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Par

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Co-développement d'un modèle d'aide à la décision pour la gestion intégrée de la flore adventice. Méta-modélisation et analyse de sensibilité d'un modèle mécaniste complexe (FLORSYS) des effets des systèmes de culture sur les services et disservices écosystémiques de la flore adventice.

Thèse présentée et soutenue à l'INRA, le 26/03/2018

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Avant-propos

Je me suis toujours intéressée aux plantes et particulièrement à comprendre pourquoi une plante pousse. Mon cursus s’est concentré sur la biologie des plantes et leur écologie, avec un entr’aperçu de l’agronomie dans mon master (Forêt, Agronomie et Gestion de l’Environnement dans l’université Henri Poincaré à Nancy, maintenant université de Lorraine). Après un stage très technique sur la mesure de l'humidité du sol, comprendre la dynamique de populations de plantes m'a poussé vers un stage effectué à l’université de Stockholm. Ce stage avait une vision spatio-temporelle longue (quelques centaines d’années) pour des plantes prairiales et l’effet de la fragmentation du paysage. Après ces expériences de recherche, j'ai fait un service civique pour constituer une promenade permettant de visiter la diversité des arbres du campus de l’université de Limoges, rappelant le stage volontaire fait entre la licence et le master, qui consistait en un inventaire de l’arboretum de l’INRA de Nancy.

Même en n'ayant qu'une faible formation en agronomie, j'ai eu envie de travailler pendant plus de trois ans sur les problématiques de production durable de nourriture. Ayant plutôt étudié les plantes, sur de longues périodes (forêts, prairies pâturées depuis longtemps, au moins depuis l’installation de vikings), j’ai découvert la période plus courte, du combat entre cultures et adventices dans un environnement perturbé comme un champ. En plus de m’approprier ce pas de temps court, j'ai aussi eu l’opportunité durant cette thèse de faire le lien entre l'agronomie, les statistiques et l'informatique grâce à mes trois encadrants de thèse Nathalie, Jean-Pierre et Jean.

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i Listes des productions scientifiques

i.1 Articles dans des revues internationales à comité de lecture

i.1.1 Articles dans le cadre de la thèse

Colas, F., Colbach, N., Cordeau, S., Jeuffroy, M.-H., Granger, S., Queyrel, W., Pointurier, O., Rodriguez, A., Villerd, J., (in preparation) Co-development of a decision support system for integrated weed managment: contribution from future users.

Colas, F., Colbach, N., Pointurier, O., Villerd, J., (in preparation) Which cultural techniques drive weed dynamics and impact? Sensitivity analysis of a cropping system model to support integrated weed management.

Colas, F., Gauchi, J.-P., Villerd, J., Colbach, N. Simplifying a complex computer model: sensitivity analysis and metamodelling of the complex process-based model FLORSYS. Ecological Modelling, submitted.

Colbach N., Bockstaller C., Colas F., Gibot-Leclerc S., Moreau D., Pointurier O. & Villerd J. (2017). Assessing weed-mediated broomrape risk in cropping systems with a simulation-based indicator. Ecological Indicators 82, 280–292, dx.doi.org/10.1016/j.ecolind.2017.05.070

Colbach N., Colas F., Pointurier O., Queyrel W. & Villerd J. (2017). A methodology for multi-objective cropping system design based on simulations. Application to weed management. European Journal of Agronomy 87, 59–73, https://doi.org/10.1016/j.eja.2017.04.005

Gauchi J.P., Bensadoun A., Colas F., Colbach N. (2017). Metamodelling and global sensitivity analysis for computer models with correlated inputs: a practical approach tested with a 3D light interception computer model. Environmental Modelling & Software Environmental Modelling and Software, 2017, 92, 40-56. http://dx.doi.org/10.1016/j.envsoft.2016.12.005

Colbach, N., Bertrand, M., Busset, H., Colas F., Dugué, F., Farcy, P., Fried, G., Granger, S., Meunier, D., Munier-Jolain, N., Noilhan, C., Strbik, F., Gardarin, A. (2016). Uncertainty analysis and evaluation of a complex, multi-specific weed dynamics model with diverse and incomplete data sets. Environmental Modelling & Software, 86, 184-203 (http://dx.doi.org/10.1016/j.envsoft.2016.09.020)

i.1.2 Articles hors cadre de la thèse

Plue, J., Colas, F., Auffret, A. G. and Cousins, S. A. O. (2016). Methodological bias in the seed bank flora holds significant implications for understanding seed bank community functions. Plant Biol J. (http://dx.doi.org/10.1111/plb.12516)

i.2 Revue nationale sans comité de lecture

Colbach N., Bockstaller C., Colas F., Gibot-Leclerc S., Granger S., Guyot S., Mézière D., Moreau D., Pointurier O., Queyrel W., Villerd J. & Voisin A.-S. (2017). Conception de systèmes de culture multiperformants à l'aide de modèles prédisant la nuisibilité et les services dépendant des adventices. Innovations Agronomiques 59, 191-203.

i.3 Présentations à des congrès

Colas F., Cordeau S., Jeuffroy M.-H., Granger S., Queyrel W., Pointurier O., Rodriguez A., Villerd J., Colbach N. (2017). Développement d'un outil d'aide à la décision pour la gestion intégrée des adventices: implication des futurs utilisateurs. Séminaire de restitution à mi-parcours du projet de recherche ANR CoSAC, Paris, France, 31 janvier-1er février 2017,79-80 (poster).

Colas F., Cordeau S., Jeuffroy M.-H., Granger S., Villerd J., Colbach N. (2017). Comment les conseillers et les agriculteurs raisonnent la gestion des adventices? Séminaire de restitution à mi-parcours du projet de recherche ANR CoSAC, Paris, France, 31 janvier-1er février 2017, 59-61 (communication orale).

Colas F., Gauchi J.-P., Villerd J., Colbach N. (2017). Méta-modélisation de l'interception de la lumière dans un couvert cultures: adventices. Séminaire de restitution à mi-parcours du projet de recherche ANR CoSAC, Paris, France, 31 janvier-1er février 2017,46-47 (poster).

Colas F., Villerd J., Colbach N. (2017). Prototypes d'outil d'aide à la décision à partir de FLORSYS pour la gestion intégrée des adventices. Séminaire de restitution à mi-parcours du projet de recherche ANR CoSAC, Paris, France, 31 janvier-1er février 2017, 32-33 (communication orale).

Colas F., Villerd J., Colbach N. (2017). Prototypes d'outil d'aide à la décision à partir de FLORSYS pour la gestion intégrée des adventices. Journée des doctorants l'UMR Agroécologie, 10 avril 2017, Dijon, France (communication orale).

Colbach N., Colas F., Pointurier O., Queyrel W., Villerd J. (2017). Proposition d'une méthodologie de conception multi-objective de systèmes de culture à partir de simulations. Application à la gestion des adventices. Séminaire de restitution à mi-parcours du projet de recherche ANR CoSAC, Paris, France, 31 janvier-1er février 2017, 64-66 (communication orale).

Colas F., Cordeau S., Jeuffroy M.-H., Granger S., Queyrel W., Pointurier O., Rodriguez A., Villerd J., Colbach N. (2016) Développement d'un outil d'aide à la décision pour la gestion intégrée des adventices. In: 23e Conférence du COLUMA - Journées internationales sur la lutte contre les mauvaises herbes, Dijon, France, 467-476 (poster).

Colas F., Gauchi, J.-P., Villerd J., Colbach N. (2016) Meta-modeling light interception in crop:weed canopies 14th ESA Congress, 5-9 September 2016, Edinburgh, Scotland, 43-44 (poster).

Colas F., Granger S., Villerd J., Colbach N. (2016) 1st steps of participatory design for a weed maangement decision support system. 14th ESA Congress, 5-9 September 2016, Edinburgh, Scotland, 43-44 (poster).

Colas F., Granger S., Villerd J., Darmency H., Colbach N. (2016) Which decision-support systems for sustainable weed management: why, how and when to use it? International Weed Science Congress, Prague (poster).

Colbach N, Colas F, Moreau D, Gibot-Leclerc S, Pointurier O, Queyrel W, Bockstaller C (2016). Ex ante evaluation of weed-mediated pests and environmental benefits of cropping systems with simulation-based indicators. The fourteenth congress of the European Society for Agronomy, 5-9 September 2016, Edinburgh, Scotland, 9-10 (communication orale).

Colas F., Cordeau S., Jeuffroy M.-H., Villerd J., Colbach N. (2015) Which decision-support system for sustainable weed management: needs and constraints of crop advisors 17th European Weed Research Society Symposium, “Weed management in changing environments", 23-26 June 2015, Montpellier, France, 239 (poster).

Colas, F., Colbach, N., Gauchi, J.-P., Villerd, Développement d’un outil d’aide à la décision pour la gestion intégrée de la flore adventice. J.. Journée des doctorants de l’UMR Agroécologie, 16 mars 2015, Dijon, France (poster).

i.4 Conférences de vulgarisation

Colas F., Gauchi, J.-P., Villerd J., Colbach N.. Nuit européenne des Chercheurs – speed searching, Dijon (21), vendredi 29 septembre. Développement d’un outil d’aide à la décision pour la gestion intégrée des adventices.

Colas F., Gauchi, J.-P., Villerd J., Colbach N.. Expérimentarium - de jeunes chercheurs à la rencontre d'élèves de la primaire au lycée, Collèges et lycées, Dijon (21), mars 2017. Développement d’un outil d’aide à la décision pour la gestion intégrée des adventices.

Colas F., Gauchi, J.-P., Villerd J., Colbach N.. Expérimentarium - de jeunes chercheurs à la rencontre d'élèves de la primaire au lycée, Lycée, Nevers (58), novembre 2016. Développement d’un outil d’aide à la décision pour la gestion intégrée des adventices.

Colas F., Gauchi, J.-P., Villerd J., Colbach N.. Expérimentarium - de jeunes chercheurs à la rencontre du grand public, Bibliothèque de Fontaine d'Ouche, Dijon (21), 5 novembre 2016. Développement d’un outil d’aide à la décision pour la gestion intégrée des adventices.

Colas F., Gauchi, J.-P., Villerd J., Colbach N.. Festival des Expérimentariums - de jeunes chercheurs à la rencontre du grand public, Lycée et Maison natale de Pasteur, Dole (25), 20-22 mai 2016. Développement d’un outil d’aide à la décision pour la gestion intégrée des adventices.

Colas F., Gauchi, J.-P., Villerd J., Colbach N.. Expérimentarium - de jeunes chercheurs à la rencontre du grand public, Ferme des Gêtes, Villers-sur-Port (70), 1er mai 2016. Développement d’un outil d’aide à la décision pour la gestion intégrée des adventices.

Colas F., Gauchi, J.-P., Villerd J., Colbach N.. Expérimentarium - de jeunes chercheurs à la rencontre d'élèves de la primaire au lycée, Lycée, Sémur-en-Auxois (21), mars 2016. Développement d’un outil d’aide à la décision pour la gestion intégrée des adventices.

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Lexique

b : Paramètre de forme pour la distribution des feuilles vs. la hauteur de la plante

CART : Classification and Regression Trees , Arbres de classification et de régression

DSS : Decision Support System = outil d'aide à la décision

FLORSYS-metaLight : FLORSYS méta-modélisé pour le module d'interception de la radiation lumineuse

GRCETA : Groupement Régional des Centre d'Etudes Techniques Agricoles

IFT : Indice de fréquence de traitement

IFTh : IFT concernant les herbicides

IWM: Integrated Weed Management : gestion intégrée des adventices

k : Coefficient d'extinction d'une espèce, correspond à la perte d'énergie du rayonnement solaire passant par la plante.

LA : Aire foliaire totale de la plante

LASSO : Least Absolute Shrinkage and Selection Operator : une méthode de régression pénalisée pour sélectionner des variables.

LASSO-PLS : utiliser la sélection de variables de LASSO pour sélectionner des monômes des polynômes de chaos combinés à la régression PLS.

LHS : Latin Hypercube Sampling, méthode pour tirer aléatoirement des valeurs d'entrée pour de multiples variables et répartir de façon uniforme les points d'échantillonnage.

ME : Modelling Efficiency : efficacité de modélisation

Méta-modèle: émulateur ou modèle d'un modèle permettant de prédire les sorties du modèle à partir des entrées du modèle.

Modèle : « représentation simplifiée, relativement abstraire, d'uin processus, d'un système, en vue de le décrire, de l'expliquer ou de le prévoir » (Dictionnaire de l'environnement, 2015).

Modèle mécaniste : « Modèle fondé sus des sous-modèles qui sont des proposition d'explication des processus biologiques ou physiques (Colbach, 2006).

OAD : Outil d'Aide à la Décision

PAR : Rayonnement photosynthétiquement actif

PARa : Proportion du PAR absorbé par la plante à l'échelle

PARaP : Proportion du PAR absorbé par la plante à l'échelle de la plante

PARaC : Proportion du PAR absorbé par la plante à l'échelle du 1 cm3

PCE : Polynômes du chaos (Polynômial Chaos Expansion), modèle additif de monômes combinant toutes les variables jusqu'à un degré défini/choisi

PCE-OLS : Indice de sensibilité de type régression des moindres carrés (Ordinary Least Square Regression) estimés à partir d'un polynôme du chaos.

PCE-PLS : Indice de sensibilité estimés à partir d'un polynôme du chaos et de la régression PLS

PLS : Partial Least Squares Regression : régression des moindres carrés partiels.

Q2cum : Critère de qualité d'ajustement d'un modèle propre à la régression PLS

RH50 : Hauteur relative de la plante en dessous de laquelle la moitié de l'aire foliaire est située

rPARi : Proportion relative du PAR intercepté par la plante par rapport à la radiation incidente au-dessus du couvert végétal

rPARibase : Proportion relative du PAR intercepté par la base de la plante par rapport à la radiation incidente au-dessus du couvert végétal

rPARitop : Proportion relative du PAR intercepté par le haut de la plante par rapport à la radiation incidente au-dessus du couvert végétal

RMSEP : Root square Mean Squared Error of Prediction error Erreur de prédiction quadratique moyenne.

RRMSEP : Erreur relative de prédiction quadratique moyenne.

SID : Intensité d'ombrage journalière, i.e. Proportion de la radiation incidente au-dessus du couvert végétal qui n'atteint pas la plante

Système de culture :

VIP : variable importance, importance de la variable calculée par des méthodes CART et forêt aléatoire

Voxel : pixel 3D

Xmax : Taille de la parcelle virtuelle dans le sens est-ouest

Ymax : Taille de la parcelle virtuelle dans le sens nord-sud.

Chapitre I : Etat de l'art et problématique

INTRODUCTION

L’augmentation de la population humaine et les innovations dans l’industrie chimique ont entraîné la mise en place d’un système agricole principalement basé sur l’apport d’intrants chimiques, augmentant ainsi les impacts négatifs sur les écosystèmes, comme l’eutrophisation des rivières et la diminution du nombre des bourdons (Matson et al., 1997; MAE, 2005; Tilman et al., 2002). Des solutions pour produire de la nourriture sans détruire les écosystèmes sont à trouver, soit en reconstruisant les systèmes alimentaires (du système de production jusqu’au consommateur), en modifiant l’utilisation des surfaces (en augmentant les surfaces agricoles), ou en modifiant les systèmes de culture (Lamine, 2011; Muller et al., 2017). Pour une agriculture durable, il faut forcément avoir une réflexion à l’échelle du système de culture, car il faut prendre en compte toutes les interactions biotiques et abiotiques (Hill and MacRae, 1996). Une des menaces pesant sur l’agro-écosystème, conduisant à un fort usage de produits chimiques, est la flore adventice. En effet, les adventices sont les principales menaces de la production (Oerke, 2006) et les herbicides sont le moyen de les gérer le plus simple et efficace. Cependant, les herbicides sont une menace pour la santé humaine et l’environnement (Waggoner et al., 2013; Wilson and Tisdell, 2001). Il faut par conséquent pouvoir réduire leur utilisation. Un système de culture[1] est un ensemble logique de pratiques complémentaires et en interaction ; pour réduire l’usage des herbicides il faut donc compenser par d’autres pratiques (Colbach and Cordeau, 2018a; Wezel et al., 2014). **Ce travail de thèse va contribuer à la diminution de l’utilisation des herbicides en proposant des connaissances et, surtout, un outil pour aider la réflexion sur la gestion de la flore adventice, à l’échelle systémique et en considérant à la fois les services et disservices dépendant de cette flore.** Ce premier chapitre a pour but de replacer ce travail dans le contexte scientifique et de présenter les objectifs de la thèse.

I.1 Les adventices des grandes cultures

Dans les grandes cultures, afin d’améliorer le rendement, les adventices sont à contrôler en priorité, étant les principaux bioagresseurs si rien n’est fait pour les gérer (Oerke, 2006). Les adventices sont des plantes qui croissent spontanément dans des milieux anthropisés alors que l’agriculteur ne les a pas semées dans son champ (Godinho, 1984). En France, le nombre d’espèces d’adventices est estimé à 1200 espèces (Jauzein, 1995). Cela comprend des espèces sauvages comme le vulpin (*Alopecurus myosuroides Huds.*), le coquelicot (*Papaver rhoeas L.*), ou encore des plantes issues de semences perdues et produites par d’anciennes cultures, comme les repousses de colza (*Brassica napus L.*). Il y a également une grande diversité de familles botaniques (poacées, astéracées, caryophyllacées) ou de périodes de levée (printemps, automne ou même toute l’année).

[1] Système de culture : l'ensemble des modalités techniques mises en œuvre sur des parcelles cultivées de manière identique. Chaque système se définit par : (1) la nature des cultures et leur ordre de succession, (2) les itinéraires techniques appliqués à ces différentes cultures, ce qui inclut le choix des variétés.

I.2 La dualité des adventices, bioagresseurs et composants de la biodiversité

En entrant en compétition pour les ressources (lumineuses, nutritives, hydriques…) avec les espèces cultivées, les adventices sont à l'origine de pertes de rendement importantes (Caussanel, 1989; Munier-Jolain et al., 2008; Oerke, 2006). Elles peuvent aussi diminuer la qualité d'une récolte en contaminant les produits récoltés par leurs semences ou des débris, et même poser des problèmes techniques sur les outils agricoles. De plus, ces « mauvaises herbes » ont une image négative auprès des agriculteurs, un champ sale (i.e. avec des mauvaises herbes visibles) est un problème pour nombre d'entre eux (Mézière et al., 2015d). Cependant, les adventices produisent aussi des services écosystémiques, en étant à la fois ressources trophiques et habitats pour de nombreuses composantes de la biodiversité (Petit et al., 2011). Elles servent aussi d'habitat pour des prédateurs de ravageurs des cultures (Hawes et al., 2003). Elles peuvent également être des ressources alimentaires pour les pollinisateurs, les oiseaux ou les insectes (Marshall et al., 2003). Les adventices sont aussi une composante de la biodiversité végétale avec des espèces spécialistes aux écosystèmes agricoles (Fried et al., 2010). Cette dualité des adventices fait qu'il est difficile de trouver un compromis entre nuisibilité et bénéfices de cette flore.

- ➔ Par conséquent, il faut aider les agriculteurs à gérer les adventices, en conciliant contrôle de la nuisibilité et promotion des services écosystémiques.

I.3 Gestion des adventices

I.3.1 Nécessité de réduire l'usage des herbicides

Jusqu'à récemment, la gestion des adventices était basée sur des applications fréquentes et répétées d'herbicide. Cependant, les produits phytosanitaires provoquent de nombreux problèmes de santé (Vinson et al., 2011; Waggoner et al., 2013; Wilson and Tisdell, 2001). Ils sont les principaux polluants des cours d'eau (http://www.statistiques.developpement-durable.gouv.fr/, (Croll, 1991; Lopez *et al.*, 2015)), entrainant une perte de biodiversité dans les cours d'eau (Beketov et al., 2013) et entrainant d'autres risques environnementaux. En réponse aux problèmes environnementaux et sanitaires liés aux herbicides, les gouvernements, d'abord l'Union Européenne puis le gouvernement français visent une diminution des quantités d'herbicides épandues dans les champs (Directive 2009/128/CE; Ecophyto, 2017). En outre, on observe une limitation des principes actifs autorisés dans les herbicides (Règlement (CE) N°1107/2009) en raison de leurs risques sur l'Homme, les animaux et l'environnement. Ce qui fait que les agriculteurs sont de plus en plus fréquemment dépourvus de solutions chimiques. En parallèle, apparaissent un nombre grandissant d'espèces et de populations adventices résistantes aux l'herbicides (Heap). La limitation des principes actifs autorisés dans les herbicides amplifie ce problème, puisqu'elle oblige les agriculteurs à utiliser plus souvent les mêmes principes actifs. Les plantes étant fréquemment exposées aux mêmes molécules, les cas de résistance risquent de se développer encore plus rapidement et devenir de plus en plus fréquents (Délye et al., 2013).

- ➔ Par conséquent, il est indispensable de repenser les systèmes de culture, en particulier les stratégies de gestion des adventices, afin de diminuer l'usage des herbicides.

I.3.2 Pourquoi utiliser des herbicides ?

La re-conception des stratégies de gestion de la flore adventice bute sur un obstacle majeur : les herbicides sont la solution curative la plus efficace, la plus simple et la plus rapide à mettre en œuvre. Au niveau économique, les herbicides en général permettent à court terme une diminution des adventices et une augmentation du rendement, évitant aux agriculteurs des pertes économiques, sur le court terme. Mais sur le long terme, il faut supplémenter la parcelle par d'autres produits, qui ont un impact négatif sur la balance économique des exploitations. Ainsi, plus il est nécessaire de mettre des produits chimiques, plus il est difficile économiquement de revenir à d'autres pratiques (Wilson and Tisdell, 2001). Les herbicides sont une solution curative de lutte contre les adventices en visant une espèce ou un ensemble d'espèces souvent du même type (graminées ou dicotylédones) identifiées comme problématiques dans le champ, par exemple pour un problème de Vulpin, la réponse de la flore est rapide, les plantes survivent ou disparaissent. Les autres pratiques curatives (mécanique ou thermique) agissent et se raisonnent sur le long terme, et elles sont moins efficaces (Bastiaans et al., 2008) ou plus difficiles à mettre en œuvre (Munier-Jolain *et al.*, 2008). Par exemple, l'efficacité du désherbage mécanique résulte d'une combinaison d'arrachage et d'enfouissement partiels de plantes dont certaines peuvent reprendre (Kurstjens and Kropff, 2001; Kurstjens and Perdok, 2000; Kurstjens et al., 2000). En outre, un désherbage mécanique va également perturber le sol et éventuellement déclencher de nouvelles germinations, qu'un désherbage chimique ne déclencherait pas (Bàrberi, 2002). La difficulté de mise en œuvre vient du fait que le désherbage mécanique est très dépendant des conditions pédoclimatiques de la parcelle et des stades de la culture. Ainsi, s'il pleut, les plantes arrachées peuvent reprendre, rendant le désherbage inutile, tandis que si le sol est trop sec, l'arrachage est insuffisant (Bowman, 1997; Kurstjens and Kropff, 2001; Kurstjens and Perdok, 2000; Kurstjens et al., 2000).

➔ Les techniques curatives alternatives seules ne suffisent pas pour remplacer les herbicides. Il faut combiner plusieurs techniques de désherbage et de gestion du système de culture et il faut insister sur la prévention des adventices.

I.3.3 Gestion agroécologique de la flore adventice

Pour compléter une gestion curative partiellement efficace lorsqu'on réduit l'usage des herbicides, il faut utiliser des méthodes de prévention contre les adventices et combiner tous ces leviers (Liebman and Gallandt, 1997; Colbach and Cordeau, 2018). La gestion intégrée des adventices est « un système de lutte aménagée qui, compte tenu du milieu particulier et de la dynamique des populations des espèces considérées, utilise les techniques et méthodes appropriées de façon aussi compatible que possible en vue de maintenir les populations d'organismes nuisibles à des niveaux où ils ne causent pas de dommages économiques » (Milaire, 1995). Elle repose sur la combinaison de différentes pratiques telles que : (1) la diversification de la rotation, (2) le travail du sol pour vider le stock semencier, (3) le semis tardif en automne pour éviter le pic de germination, (4) des espèces et variétés de culture compétitives pour occuper l'espace et (5) du désherbage mécanique (Deytieux et al., 2012). La gestion intégrée ne devient réellement efficace que si elle combine ces pratiques à effet partiel et raisonne à l'échelle pluriannuelle (Liebman and Gallandt, 1997).

Au-delà de la gestion intégrée, il est possible d'avoir une vision agroécologique de la gestion et d'encourager les interactions biologiques et les services écosystémiques rendus par les adventices. En effet, l'agroécologie peut se définir de nombreuses manières selon ce qui nous intéresse : la vision scientifique, le mouvement politique ou encore les pratiques culturales (Wezel et al., 2009). Un agroécosystème rend de nombreux services à l’écosystème, comme les services d’approvisionnement (de nutriments, d’eau, de matériaux et d’énergie par l’écosystème), les services de régulation (des cycles de l’eau, de l’érosion) et les services culturels (récréatifs, esthétiques et spirituels) pour la société (Tibi and Therond, 2017). Les adventices ont leur rôle à jouer dans ces services rendus notamment en tant que ressources trophiques pour la faune auxiliaire de la parcelle ou composante de la biodiversité végétale. Ce qui fait que les interactions biologiques entre les cultures et les adventices sont complexes.

Ces approches rendent souvent le travail des agriculteurs plus lourd et plus complexe. L'augmentation de fréquence des interventions mécaniques (e.g. désherbage mécanique, faux-semis…) ou une diversification des successions culturales rend l'organisation du travail plus complexe à l’échelle d’une exploitation. Les nouvelles cultures de "diversification" peuvent être moins productives ou ne pas avoir de débouchés localement, ce qui entraîne des pertes de revenus (Meynard et al., 2013). Certaines modifications de pratiques (retard de semis, variétés plus étouffantes) peuvent réduire le potentiel de rendement (Munier-Jolain et al., 2008). Le conseil agricole peut aussi être insuffisant, à la fois pour les nouvelles cultures ou les techniques alternatives (Pasquier and Angevin, 2017). En revanche, ces techniques peuvent aussi réduire le coût lié à l’usage des produits phytosanitaires et peuvent conduire à une diminution d’émission des gaz à effet de serre, même s’il y a une augmentation des passages d’engins agricoles, le gaz émis est compensé par une utilisation moindre de fertilisants azotés, très émetteurs de gaz à effet de serre (Deytieux et al., 2012).

➔ La gestion de la flore adventice économe en herbicides nécessite un raisonnement sur le long terme, en combinant les pratiques culturales préventives et curatives.

I.4 L’échelle "système de culture"

De nombreuses pratiques culturales et combinaisons de ces pratiques peuvent être mises en œuvre pour gérer les adventices. Il est important de réfléchir sur le long terme, car les semences adventices survivent pendant plusieurs années (Burnside et al., 1996; Conn et al., 2006; Gardarin et al., 2010; Murdoch and Ellis, 2000), une décision prise pendant l'année a des répercussions pendant de nombreuses années après. Ce n'est généralement pas l'adventice de l'année N qui embête les agriculteurs, mais les centaines voire milliers de semences produites qui lèveront les années suivantes, ce qui oblige à penser la gestion de la flore adventice dans le temps, sur plusieurs années. Cela entraîne une complexité de pratiques et d’interactions de pratiques dans la gestion des adventices, qu’il faut prendre en compte en concevant un système de culture durable. Afin de prendre en compte ces effets et combinaisons d’effets, il faut réfléchir à l’échelle du système de culture (Bàrberi, 2002).

I.4.1 Qu’est-ce qu’un système de culture ?

Un système de culture se définit par : « la nature des cultures et leur ordre de succession et les itinéraires techniques appliqués à ces différentes cultures, ce qui inclut le choix des variétés » (Sebillotte, 1990), où les itinéraires techniques sont des combinaisons logiques et ordonnées de techniques culturales permettant de contrôler le milieu et d’en tirer une production donnée (Sebillotte, 1974, 1978). Un système de culture se construit dans les grandes lignes en prenant des décisions stratégiques pour l'exploitation (choix des cultures, des outils…) et de manière plus fine avec les décisions tactiques liées à la conduite des cultures et adaptées à l'état de la parcelle (la météo, le type de sol…). Dans le cadre de cette thèse, c'est la vision stratégique qui est utilisée pour une gestion préventive et sur le long terme. Les techniques culturales comprises dans le système de culture ont de nombreux effets sur les adventices. Le choix des cultures actuelles et précédentes (Fried et al., 2008; Bohan et al., 2011), le travail du sol, le désherbage chimique ou le désherbage mécanique (Chicouene, 2007) ont des impacts majeurs sur la communauté des adventices. Des variations dans les dates de semis peuvent modifier la dynamique de cette flore (Liebman and Dyck, 1993). Les pratiques réalisées dans un système de culture sont très dépendantes de la situation de production, c'est-à-dire les conditions pédo-climatiques (ex : température moyenne, quantité de pluie annuelle), économiques et sociales (ex : la présence de filières dans la région) (Aouadi et al., 2015; Lechenet et al., 2016).

➔ Pour analyser un système de culture, il est donc essentiel de prendre en compte la situation de production.

I.4.2 Quelles méthodes pour concevoir de nouveaux systèmes de culture ?

La modification d'un système de culture existant, afin qu'il soit plus durable environnementalement, socialement et économiquement, s'organise autour de trois niveaux de modification (Hill and MacRae, 1996):

- l'efficience, où l'on optimise les pratiques en place, par exemple en optimisant l'usage d'herbicides (ex : drones et robot pour ne traiter que les zones avec adventices), les dates d'application, les doses ou les produits;
- la substitution, où l'on remplace une pratique par une autre (ex : pesticides remplacés par du biocontrôle) ;
- la reconception, où différentes techniques et pratiques vont être mises en œuvre pour modifier le système de culture (ex : réduire l'usage d'intrants *via* la gestion intégrée).

Pour concevoir un nouveau système de culture, il existe plusieurs méthodes (Loyce and Wéry, 2006) :

- Améliorer l'existant en faisant un diagnostic agronomique des systèmes existants chez les agriculteurs pour identifier les pratiques intéressantes permettant d'améliorer le système, à partir d'enquêtes (Doré et al., 1997) ou de réseaux comme le réseau DEPHY (Ecophyto, 2015)
- Le prototypage est une approche participative avec co-construction de systèmes avec différents experts au cours d'ateliers où les participants vont échanger leurs connaissances (Hossard, 2012; Lefèvre *et al.*, 2014).
- Utiliser des modèles pour tester un grand nombre de systèmes rapidement (Bergez *et al.*, 2010; Messean *et al.*, 2010), car si un modèle n'est jamais vrai, certains permettent de comparer des systèmes entre eux et de savoir si un système est meilleur qu'un autre.

Les deux premières méthodes mobilisent beaucoup de temps, d'espace et de ressources et posent un risque de confusion d'effets entre les pratiques et le contexte, car un système vient souvent avec une situation de production particulière. En outre, la modélisation permet de sortir des sentiers battus pour la conception de systèmes de culture et permet de tester des combinaisons de pratiques (Andrew and Storkey, 2017). Elle permet également de calculer des indicateurs afin d'évaluer les systèmes de culture (Bockstaller *et al.*, 2008).

➔ Lorsque l’on souhaite concevoir et évaluer le plus de systèmes possible, le virtuel avec un modèle est donc tout adapté (Jouy and Tournier, 2011).

I.4.3 Quels outils pour évaluer l’impact de la flore sur les systèmes de culture ?

Afin d’évaluer des systèmes de culture pour déterminer leur aptitude à gérer la flore adventice, il est possible de faire des observations agronomiques comme des relevés de flore *in situ*, des mesures de rendement ou de stock semencier. Ces observations ont les mêmes contraintes que les tests en réel, d’où l’intérêt de passer par des modèles. Pour évaluer les systèmes de culture sur plusieurs critères, notamment sur les trois piliers du développement durable (économie, environnement et social), des outils, comme MASC (Sadok et al., 2009a) ou DEXiPM (Pelzer *et al.*, 2012), vont calculer des indicateurs de durabilité du système à partir de plusieurs sous-variables de type rendement, charge de travail ou fréquence de traitement herbicide dans le système. Pour les impacts de la flore adventice, il y a des indicateurs (Colbach et al., 2017b; Mézière et al., 2015d; Queyrel and Colbach, 2015) pour prendre en compte les impacts négatifs de la flore, directs (pollution de la récolte, difficulté de récolte) ou indirects (risque augmenté de maladie) et indicateurs d’impacts positifs directs (limitation de la lixiviation en interculture) et indirects (ajout de ressources pour les pollinisateurs). Les indicateurs de nuisibilité développés par Mézière et al (2015c) sont issus d’enquêtes auprès d’agriculteurs et répondent donc à leurs besoins. Les indicateurs de services rendus par la flore ont été développés en interaction avec des écologues et agronomes et sont essentiels pour quantifier les effets de la dualité des adventices.

➔ Il faut utiliser des outils proches des problèmes des agriculteurs ainsi que des indicateurs concernant la durabilité environnementale pour trouver un compromis de gestion durable des systèmes de culture.

I.4.4 Qui serait intéressé par des outils pour aider la gestion des adventices ?

Différents acteurs sont concernés par la gestion des adventices : les agriculteurs sur la première ligne ; les conseillers agricoles qui appuient les agriculteurs ; les agronomes qui produisent de nouvelles connaissances ; les décideurs pour l’établissement des normes et des lois. Il a été remarqué que les connaissances produites ne transitaient pas assez vers la profession (Dubrulle *et al.*, 2014). C’est donc vers les conseillers agricoles et les agriculteurs, des acteurs de premier plan pour la gestion des adventices, qu’il faut nous tourner pour leur transmettre les connaissances produites sur la gestion des adventices. D’autant plus que Il faut engager un dialogue avec ces acteurs afin de bien définir leurs besoins pour identifier comment leur fournir le mieux les connaissances existantes pour que ce soit utile et utilisé (Cerf et al., 2012a).

➔ Il faut impliquer les conseillers et agriculteurs dans le développement d’outils pour les aider à gérer les adventices.

I.5 Les outils existants pour aider à la gestion des adventices

En reprenant les conclusions des paragraphes précédents, identifiés comme les éléments importants pour la gestion des adventices, nous pouvons déjà établir une ébauche de cahier des charges pour un outil aidant à la gestion intégrée des adventices, tout en réduisant l'utilisation des herbicides :

- Un outil pour concilier contrôle de la nuisibilité et pour promouvoir de la biodiversité dépendant des adventices.
- Un outil qui prenne en compte les techniques curatives alternatives et la prévention des adventices.
- Un outil qui raisonne et évalue la gestion sur le long terme, et combinant les pratiques culturales pour gérer la flore adventice.
- Un outil avec en sortie des indicateurs proches des problèmes liés aux adventices des agriculteurs, ainsi que des indicateurs pour le compromis de gestion durable des systèmes de culture.

Nous avons étudié des modèles et outils sur la flore adventice afin de voir s'ils répondaient à ces critères.

I.5.1 Les modèles biophysiques et de dynamique de la flore adventice

Concernant la gestion des adventices, de nombreux modèles existent. Certains se focalisent sur la compétition à la lumière entre adventices et cultures, sous forme empirique (Cousens, 1985) ou mécaniste (Kropff and Spitters, 1992). Des modèles plus globaux synthétisent les connaissances sur le cycle de vie de la flore dans un système biologique (Swinton and King, 1994; Colbach et al., 2006; Renton and Chauhan, 2017). Ce sont souvent des modèles analysant les effets des techniques culturales sur une seule espèce d'adventice au fil des années, réduisant souvent le système de culture aux seules cultures et herbicides (Colbach and Debaeke, 1998; Holst et al., 2007; Freckleton and Stephens, 2009). Certains de ces modèles sont plus complets, considérant un ensemble plus large de techniques culturales, mais généralement sans intégrer les interactions avec les états du milieu, interactions indispensables pour pouvoir prédire un effet moyen d'une technique, mais également sa variabilité en fonction des autres techniques culturales et des conditions pédoclimatiques (Colbach and Debaeke, 1998; Colbach et al., 2005; Colbach, 2010). Or, la prédiction de cette variabilité est importante pour les agriculteurs, afin qu'ils puissent juger du rapport coût/bénéfice de leurs décisions et des risques d'effets opposés à ceux recherchés.

Le modèle FLORSYS (Gardarin et al., 2012; Munier-Jolain et al., 2013; Colbach et al., 2014b) tente de dépasser ces limites, en simulant la dynamique pluriannuelle de plusieurs adventices en fonction du système de culture, en interaction avec le pédoclimat. C'est un modèle de recherche qui permet de réaliser des expérimentations de systèmes de culture sur des parcelles virtuelles. Il est très utile pour la recherche, pour tester et évaluer des systèmes de culture, mais il est complexe d'utilisation pour des personnes non initiées. C'est souvent le cas des modèles de recherche, ce qui les rend peu adaptés à l'aide à la décision par les différents acteurs du monde agricole (Becu et al., 2008; Antle et al., 2017).

I.5.2 Les outils d'aide à la décision pour la gestion de la flore adventice

Il existe de nombreux outils d'aide à la décision basés sur différentes fonctions, entre de l'aide à la reconnaissance d'espèces (e.g. InfloWeb (Terres Inovia et al.)), un guide de traitements herbicides (e.g. HADSS (Lassiter et al.)) et un logiciel permettant de totalement piloter sa culture (e.g. WECOF-DSS (Neuhoff et al., 2002)) (Table I. 1). Cependant, un manque d'outil d'aide à la décision au niveau de la gestion stratégique de la flore adventice est ressorti chez différents groupes d'experts (Dubrulle et al., 2014; GIS GC HP2E, 2011). En effet, un tel outil est nécessaire, mais complexe car il doit pouvoir :

- évaluer des combinaisons de différentes pratiques culturales, à l'échelle du système de culture ;
- évaluer des rotations diversifiées avec de nombreuses cultures ;
- prédire les effets des pratiques sur la dynamique pluriannuelle des espèces adventices.

Dans le Table I. 2, les différents outils présentés dans le Table I. 1 sont analysés afin de voir s'ils répondent aux objectifs fixés pour un OAD stratégique de gestion des adventices. Par exemple, ODERA (Agro-Transfert Ressources et Territoires) évalue le risque moyen de salissement par adventices dans un système, pour ensuite orienter l'utilisateur vers de nouvelles pratiques. ODERA est basé sur des additions de scores et ne permet pas d'avoir les effets combinés des pratiques sur la dynamique adventice. Il ne convient donc pas à nos objectifs. Un autre exemple est Décid'herb (Munier-Jolain et al., 2005) qui propose des programmes de traitements herbicides en fonction de risques adventices, avec des notes d'efficacité de contrôle et d'impact écotoxicologique. Il s'agit d'un outil d'aide à la décision de choix d'herbicide, et non pas d'un outil de stratégie de conception de systèmes de culture. Ces outils d'aide à la décision ne permettent pas de retirer des informations sur la perte de récolte due aux adventices ou sur le salissement du champ qui sont pourtant des critères d'évaluation très importants pour les agriculteurs (Mézière et al., 2015d). Ces outils n'évaluent pas non plus les bénéfices apportés par les adventices, éléments importants pour la biodiversité et la gestion durable de l'environnement. Comme les effets des adventices sont multiples, aussi bien nuisibles qu'intéressantes pour les services écosystémiques, il faut pouvoir évaluer de façon multicritère les systèmes de culture. Il y a donc besoin d'un outil permettant de faire de la conception multiobjective de systèmes de culture.

Table I. 1: Description d'outils d'aide à la décision existant pour gérer les adventices en grandes cultures, revue bibliographique.

Nom	**Référence**	**Description**
Agrovisioflore	(Syngenta)	Clé de détermination pour reconnaitre les adventices
Bay+ CIBlé®	(Bayer Cropscience)	Proposition de traitements herbicides en fonction des conditions climatiques des dates de semis et des variétés
Betsy	(Itb)	Proposition de traitements herbicides post-émergence dans la betterave, en fonction des adventices, de leurs stades et de la région
Cambio'net	(De Sangosse)	Aide à la reconnaissance des adventices, identification du risque et propositions de traitements herbicides (de la marque Cambio)
DECID'herb	(Munier-Jolain et al., 2005)	Estimation du risque adventice et proposition d'un programme de lutte de désherbage (mécanique et chimique)
ECOHERBI	(Rodriguez et al., 2014)	Guide qui à partir d'un système de référence qui propose des alternatives économes en herbicides pour 3-4 pédo-climats différents
GESTINF	(Berti and Zanin, 1997)	Estimation de la nuisibilité des adventices via des densités observées et prédiction les pertes de rendement, donne différents scénarios de gestion leur rendement net et leur impact sur l'eau
HADSS™	(Lassiter et al.)	Evaluation économique de différentes stratégies de gestion des adventices en fonction de la flore initiale et impacts sur la flore des traitements
Infloweb	*(Terres Inovia et al.)*	Clé de détermination pour reconnaitre les adventices, information sur la biologie des espèces et conseils de lutte
Le guide Optimaïs	(Réseau Gab-Frab)	Guide pour déterminer quand faire le désherbage mécanique et quels sont les meilleurs outils
MaïsExpert	(Syngenta)	Conseil de traitement du maïs en fonction de la météo
OdERA-Systèmes	(Agro-Transfert Ressources et Territoires)	Aide à la conception de nouveaux systèmes de culture en évaluant le risque d'adventices
OFSAT	(Colomb et al., 2013)	Evaluation de différents systèmes de culture bio, pour trouver le système de culture le plus adapté par essai erreur
Phytnès	(In vivo)	Optimisation du choix des semences et des traitements en fonction des risques d'adventices, évaluation agronomique, économique et environnementale
RIM	(Pannell et al., 2004)	Outil bioéconomique pour conduire des expériences virtuelles en testant différentes combinaison de traitement et voir leurs effets sur le ray-grass, le rendement et l'économie
RIMPhil	(Beltran et al., 2011)	Outil bioéconomique pour conduire des expériences virtuelles de gestion herbicide du Panic pied-de-coq dans le riz et voir leurs effets sur le ray-grass, le rendement et l'économie
R-sim	(Lievin et al., 2013)	Estimation d'un risque de résistance pour chaque culture et à l'échelle de la rotation
SELOMA	(Stigliani and Cosimo, 1993)	Estimation de la compétition avec les adventices en donnant des conseils de gestion ou non par désherbage chimique et mécanique
WECOF-DSS	(Neuhoff et al., 2002)	Guide pour déterminer des stratégies efficaces pour la gestion du blé en bio à l'échelle européenne
Weed Manager	(Tatnell et al., 2006)	Suite de modèle pour établir des stratégies de gestion d'adventices
WeedSOFT®	(Neeser et al., 2004)	Outil pour tester différents scénarios de gestion d'adventices, en essayant différentes densités et stades cultures ou adventices
Voir la page suivante pour la suite du tableau		

Table I. 2 : Détails/particularités des outils d'aide à la décision précédemment décrits (Tableau 1).

Nom	**Quelle échelle ?**	**Quelles pratiques culturales ?**	**Quelles cultures ?**	**Quelles adventices ?**	**Modélisation de la dynamique adventice ?**	**Quels utilisateurs ?**
Agrovisioflore	Non pertinent	Non pertinent	Non pertinent	Nombreuses	Non pertinent	Agriculteurs
Bay+ CIBlé®	Culture/parcelle	Désherbage chimique et dates de semis	Blé et Orge	Aucunes ou pas d'info	Non	Agriculteurs
Betsy	Culture	Désherbage chimique	Betterave	Nombreuses	Non	Agriculteurs
Cambio'net	Culture	Désherbage chimique	Maïs	Plusieurs	Non	Agriculteurs
DECID'herb	Culture	Désherbage chimique et mécanique	Espèces de grande culture	Plusieurs	Oui mais peu robuste	Conseillers et agriculteurs
ECOHERBI	Système de culture	Nombreuses pratiques culturales (faux-semis, décalage de la date de semis, couvert d'interculture et labour)	Espèces de grande culture	Non pertinent	Non	Agriculteurs
GESTINF	Culture	Désherbage chimique et mécanique	2 : Soja et Blé d'hiver	Plusieurs	Non	Non spécifié
HADSS™	Culture	Désherbage chimique	4 : Maïs, coton, soja, cacahuète	Nombreuses	Non	Agriculteurs et conseillers
Infloweb	Non pertinent	Non pertinent	Non pertinent	Nombreuses	Non pertinent	Agriculteurs et conseillers
Le guide Optimaïs	Culture	Désherbage mécanique	Maïs	Plusieurs	Non	Agriculteurs
MaïsExpert	Culture	Nombreuses pratiques culturales	Maïs	Plusieurs	Non	Agriculteurs
OdERA-Systèmes	Système de culture	Nombreuses pratiques culturales (succession, date semis, labour, interculture…)	Espèces de grande culture	Plusieurs	Non (mais système additif)	Agriculteurs et conseillers
OFSAT	Système de culture	Nombreuses pratiques culturales (succession, date semis, labour, interculture…)	Espèces de grande culture	Nombreuses	Non	Agriculteurs et conseillers
Phytnès	Culture	Nombreuses pratiques culturales (succession, date semis, labour, interculture…)	Espèces de grande culture	Plusieurs	Non	Conseillers et agriculteurs
RIM	Système de culture	Nombreuses pratiques culturales (succession, date semis, labour, interculture…)	Espèces de grande culture	1 : Lolium rigidum	Oui	Agronomes, agriculteurs et étudiants
RIMPhil	Système de culture	Nombreuses pratiques culturales (succession, date semis, labour, interculture…)	Riz	1 : Echinochloa crus-galli	Oui	Agronomes, agriculteurs et étudiants
R-sim	Système de culture	Désherbage chimique	Espèces de grande culture	Nombreuses	Non	Agriculteurs

Nom	Quelle échelle ?	Quelles pratiques culturales ?	Quelles cultures ?	Quelles adventices ?	Modélisation de la dynamique adventice ?	Quels utilisateurs ?
SELOMA	Culture	Désherbage chimique et mécanique	7 : Blé, Maïs, Betterave, Orge…	Plusieurs	Non	Conseillers et agriculteurs
WECOF-DSS	Système de culture	Nombreuses pratiques culturales (écartement du rang, orientation du semis, potentiel allélopatique…)	Blé d'hiver	Plusieurs	Non	Agriculteurs et conseillers
Weed Manager	Système de culture	Nombreuses pratiques culturales (succession, date semis, labour, interculture…)	Blé	Plusieurs	Oui	Agriculteurs, agronomes et Distributeurs de semences
WeedSOFT®	Culture	Désherbage chimique	4 : Coton, Soja, Maïs et Blé	Nombreuses	Non	Agriculteurs et conseillers

I.5.3 Le recyclage c'est important

Nous l'avons vu dans les deux parties précédentes, des outils et des modèles existent, et il faut en profiter. Deux possibilités s'offrent à nous pour obtenir un outil permettant de gérer de façon intégrée les adventices en faisant de la conception multiobjective de systèmes de culture : soit combiner des OAD existants entre eux, soit utiliser un modèle complexe permettant déjà de faire cela et le simplifier. Les OAD existants n'ont en général pas le même fonctionnement ni le même objectif, leurs entrées et sorties sont donc différents. Les faire communiquer demanderait un gros travail de correspondances entre les référentiels des outils et de trouver des valeurs par défaut, quand l'information n'est pas présente d'un outil à l'autre, à dire d'expert ou via la littérature. En outre, les OAD sont souvent à un niveau plus simplifié des connaissances scientifiques, et ainsi, augmenter la simplification et utiliser des valeurs par défaut pourrait faire perdre la cohérence des résultats. En partant d'un modèle complexe, il n'y a pas le travail de mise en forme et d'approximation, et moins de risques de perte d'information. C'est pourquoi nous avons pris le parti de partir d'un modèle complexe, FLORSYS, et de le simplifier.

I.5.4 FLORSYS : un modèle de recherche qui pourrait s'adapter à plus d'utilisateurs

Les outils existants ne permettent pas d'évaluer des systèmes de culture contrastés, sur plusieurs années, en prédisant la variabilité d'une technique en fonction des autres techniques culturales et des conditions pédoclimatiques. En outre, les outils existants ne concernent pas plusieurs espèces d'adventices, avec des sorties autorisant le calcul de nombreux indicateurs de nuisibilité et de bénéfices liés aux adventices. En revanche, le modèle FLORSYS (Colbach et al., 2016b; Colbach et al., 2014b; Colbach et al., 2014c; Gardarin et al., 2012; Mézière et al., 2015d; Munier-Jolain et al., 2014; Munier-Jolain et al., 2013), issu de la recherche et destiné à la recherche, est très complet et complexe avec de nombreuses entrées et sorties permettant de tester différents systèmes de culture.

I.5.4.1 Les entrées de FLORSYS

FLORSYS est un modèle mécaniste qui simule les impacts du système de culture sur la dynamique adventice à l'échelle de la parcelle, en fonction du pédoclimat dans une « parcelle virtuelle ». En entrée, de nombreuses variables sont nécessaires pour décrire le système de culture, le pédoclimat et le stock semencier adventice initial. Le système de culture est décrit de façon très détaillée, par une liste d'opérations avec dates et options, incluant : la rotation (ex : espèces, variétés, mélanges d'espèces), le semis (ex : densité et profondeur de semis, orientation des rangs), la récolte et la fauche (ex : date de coupe, hauteur de coupe), le travail du sol et le désherbage mécanique (ex : outil, profondeur, vitesse), les herbicides (ex : produit, dose), la fertilisation minérale et organique, l'irrigation et les autres pesticides. Le sol est décrit en terme de ses caractéristiques physiques et chimiques (ex : texture, profondeur, taux de cailloux). La météo provient de relevés de stations météorologiques (ex : la quantité de radiation journalière, les précipitations, les températures). Le stock semencier des adventices initial est décrit par les espèces et les densités de graines à différentes profondeurs. Comme connaitre le stock semencier est très compliqué (Dessaint *et al.*, 1986), les stocks semenciers initiaux sont généralement estimés à partir de connaissances sur la flore régionale issues d’enquêtes floristiques (Colbach et al., 2016b), comme par exemple le réseau Biovigilance-Flore (Fried *et al.*, 2008).

I.5.4.2 Le contenu biophyisque de FLORSYS

FLORSYS fonctionne au pas de temps journalier, où les options de gestion et les variables environnementales vont influencer le cycle de vie des cultures et adventices, prédisant pour chaque jour : la densité des semences viables, dormantes et germées, la densité, la position, la biomasse, et le stade des plantes émergées, ainsi que la production de graines. Le modèle est une combinaison de différents modules modélisant plus spécifiquement par exemple : la germination et la croissance pré-levée des plantules, interception du rayonnement lumineux et la photosynthèse, la croissance des plantes, le calcul des indicateurs… Par exemple, la germination et la croissance pré-levée des semences dépendent de leur état (âge, niveau de dormance, position dans le sol) et de leur environnement (structure du sol, température, potentiel hydrique). Le couvert culture:adventice est décrit en 3D par une représentation individuelle simplifiée de chaque plante. Les processus post-levée (ex : photosynthèse, respiration, croissance, étiolement) sont déterminés au niveau de chaque plante et dépendent de son état (stade, ombrage passé, position dans la parcelle) et de leur environnement (disponibilité de la lumière, température de l’air).

Le modèle combine à la fois des approches déterministes et stochastiques. Par exemple, la probabilité de survie d’une plante adventice est calculée de façon déterministe en fonction des opérations de gestion (travail du sol, application d’herbicides, désherbage mécanique, fauche, récolte), et en fonction de l’environnement biophysique et du stade et de la morphologie de la plante. La survie est déterminée stochastiquement pour chaque plante, en comparant la probabilité de survie à une probabilité aléatoire.

I.5.4.3 Le domaine de validité

L’évaluation de FLORSYS avec des données indépendantes provenant d’observations sur le terrain dans différences régions de France (Colbach et al., 2016b) a montré que le rendement des cultures, la densité journalière d’adventices et les densités moyennées sur les années de simulations sont classées correctement par le modèle, ce qui permet de comparer des systèmes de culture entre eux, l'erreur de prédiction est acceptable. La prédiction est moins bonne pour les variables sommées sur toutes les espèces vs. par espèce, ainsi que pour les variables au pas-de-temps journalier vs. moyennées sur la rotation. La flore adventice est souvent surestimée et la production agricole sous-estimée. Cependant, la flore est souvent trop variable sur le terrain pour vraiment conclure (Colbach et al., 2014d).

I.5.4.4 Les indicateurs d’impacts de la flore adventice

En sortie, FLORSYS prédit les densités et biomasses de tous les stades des adventices et cultures pour chaque jour de simulation, ce qui permet d'analyser finement les effets des techniques culturales. Afin de simplifier la comparaison de systèmes de culture, ces nombreuses sorties ont été traduites en indicateurs d’impact de la flore adventice (Mézière et al., 2015a; Colbach et al., 2017). Ce sont des indicateurs de services et disservices des adventices. La plupart des indicateurs de disservice des adventices ont été développés avec des agriculteurs (Mézière et al., 2015b). Ils estiment la nuisibilité directe des adventices sur la production agricole (perte de rendement due aux adventices et pollution de la récolte par des débris d'adventices), les soucis techniques (problèmes lors de la récolte en cas de biomasse verte qui bloque la moissonneuse-batteuse). Les indicateurs vont aussi estimer le salissement de la parcelle pendant la croissance des cultures qui est considéré comme problématique, même en l'absence de perte de rendement. Ce salissement est un problème plus sociologique d'image auprès des autres agriculteurs. D'autres indicateurs de nuisibilité indirecte des adventices sont aussi calculés, en fonction de la capacité des adventices à augmenter la survie et la dispersion de certains bioagresseurs : augmentation des pertes de rendement dues au piétin échaudage des céréales (Gaeumannomyces graminis var. tritici) qui est transmis par les adventices graminées (Mézière et al., 2013) et le risque de parasitage par l'orobanche rameuse Phelipanche ramosa dû à la transmission par les adventices (Colbach et al., 2017).

Les indicateurs de services écosystémiques ont été développés avec des experts en écologie et par de la recherche bibliographique (Mézière et al., 2013). La biodiversité fonctionnelle a été estimée par la contribution des adventices aux ressources trophiques des oiseaux, descarabes granivores et des abeilles domestiques. Deux autres indicateurs permettent d'estimer la contribution des adventices à la biodiversité sauvage, avec la richesse spécifique et l'équitabilité de répartition des espèces. Un dernier jeu d'indicateurs est encore en développement et concerne la contribution des adventices à réduire les impacts environnementaux du système de culture en calculant par la réduction de l'érosion du sol, la réduction du ruissellement des herbicides ou de la lixiviation des nitrates (Queyrel and Colbach, 2015).

I.5.4.5 FLORSYS : un modèle complexe

FLORSYS, par sa capacité à tester en virtuel des systèmes de culture très détaillés et à les évaluer par de nombreux indicateurs, en fait un outil intéressant pour aider les conseillers agricoles et les agriculteurs à concevoir des systèmes de culture multiperformants. FLORSYS est un modèle de recherche, très détaillé et relativement lent à utiliser. Par exemple, une simulation « standard » sur 30 ans avec 10 répétitions climatiques, en demandant l'ensemble des fichiers de sortie avec un pas-de-temps journalier, va prendre en moyenne 11 heures (6-20 heures suivant les systèmes), avec un ordinateur à 16 G0 de RAM et un biprocesseur à 2 x 2.2 GHz et 2 x 4 cœurs (sachant que FLORSYS ne peut utiliser qu'un seul cœur). En l'état, FLORSYS est difficilement utilisable comme outil d'aide à la décision. Pour le transformer en outil d'aide à la décision, il faudrait le simplifier de manière à bénéficier de l'efficacité de FLORSYS pour comparer des systèmes de cultures entre eux. Il est tout à fait possible de simplifier un modèle pour faire des prédictions plus rapides, même si le contrecoup est que le modèle simple perd en fonctionnalité et en détails (Brooks et al., 2001). Donc, un outil basé sur la simplification de FLORSYS, mais ne faisant varier que certaines entrées et ne donnant en sortie que certains résultats serait plus adapté pour les utilisateurs potentiels : les conseillers agricoles et les agriculteurs.

➔ Il faut construire un nouvel outil d'aide à la décision, s'appuyant sur une simplification de FLORSYS

I.6 Développement d'un nouvel outil d'aide à la décision

En reprenant les différents points identifiés à la fin de chaque paragraphe, nous avons abouti à la constatation qu'il faut un outil d'aide à la décision pour conseillers agricoles et agriculteurs qui :

- apporte du conseil pour la gestion intégrée des adventices,
- permette l'évaluation et la conception de systèmes de culture
- donne des indicateurs d'impact de la flore adventice sur la production agricole et proche des problèmes des agriculteurs,
- concerne des indicateurs d'impact sur la biodiversité et
- soit simple d'utilisation pour l'utilisateur.

L'analyse des modèles et des outils existants, ainsi que des méthodes et connaissances disponibles pour la construction d'outils d'aide à la décision nous amène à choisir la voie de la transformation du modèle de recherche existant FLORSYS en outil d'aide à la décision. Dans la suite de ce chapitre, nous allons présenter les différentes méthodes employées au cours de la thèse pour développer un nouvel outil d'aide à la décision à partir du modèle FLORSYS. C'est-à-dire que nous présenterons comment il nous a été particulièrement nécessaire d'accélérer les simulations de FLORSYS et d'impliquer les futurs utilisateurs.

I.6.1 Simplifier un modèle par méta-modélisation et analyse de sensibilité

L'analyse de sensibilité permettra d'identifier les variables d'entrées les plus influentes sur les sorties (Casadebaig et al., 2016; Ganji et al., 2016; Ruget et al., 2002) et la méta-modélisation d'un modèle permettra de simplifier ce modèle (souvent complexe) et de l'accélérer (Kleijnen and Sargent, 2000; Ryan et al., 2017; Villa-Vialaneix et al., 2012). Un méta-modèle est un modèle de modèle, qui va imiter le modèle complexe en s'appuyant sur des entrées qui peuvent être plus synthétiques ou ne concerner qu'une fonctionnalité du modèle. Pour méta-modéliser, un grand nombre de simulations est nécessaire, toutefois, ce n'est pas toujours faisable, surtout dans le cas de modèles lents, comme FLORSYS. Une solution est de réaliser le travail en deux étapes, en méta-modélisant d'abord une partie seulement du modèle complexe pour l'accélérer comme l'ont fait (Marie and Simioni, 2014). Cette accélération permettra alors de nombreuses simulations pour construire une grande base de données de simulations couvrant la diversité de situations que l'analyse du modèle complet doit couvrir. La deuxième étape consistera ensuite à méta-modéliser le modèle complet, en travaillant avec la version accélérée.

Il existe différentes méthodes d'analyse de sensibilité et de méta-modélisation (Ellouze et al., 2010; Luo et al., 2013; Rothenberg and Wang, 2016). Il faudra par la suite évaluer par de la revue bibliographique et des tests lesquelles de ces méthodes sont les plus adéquates pour chacune des deux étapes de simplification de FLORSYS, cela grâce à de la revue bibliographique et des tests. Cette réflexion devra non seulement prendre en compte des considérations purement statistiques et techniques, mais aussi la destination finale du méta-modèle, en tant que composante d'un outil d'aide à la décision. Certaines méthodes de méta-modélisation s'y prêtent mieux que d'autres. Par exemple, des méthodes empruntées à la fouille de données ont déjà fait leurs preuves, à la fois pour méta-modéliser des modèles et pour fournir des conseils (Hill et al., 2014). Ainsi, les forêts aléatoires (Breiman, 2001) sont souvent utilisées en méta-modélisation pour leur qualité prédictive. Elles fournissent de plus un classement des entrées les plus influentes via les VIP. En revanche, elles ne possèdent pas de représentation graphique interprétable. Les arbres de classification et régression (CART) (Breiman *et al.*, 1984), offrent précisément cette représentation interprétable et peuvent servir de support au conseil.

I.6.2 Implication des futurs utilisateurs dans le développement de l'outil

L'évaluation des impacts des systèmes de culture sur la flore adventice, et les conséquences de celle-ci sur la production agricole et la biodiversité, est d'intérêt pour de nombreux acteurs de l'agronomie : les conseillers est les agriculteurs. Identifier les systèmes de culture optimaux, adaptés au contexte actuel de changement, que ce soit changement de règlementation ou changement climatique, est réalisé par ces différents acteurs. De plus, ceux qui prennent les décisions dans les champs sont les agriculteurs, alors, pour éviter de perdre des informations dans les intermédiaires, il est logique d'orienter le développement d'un outil d'aide à la décision à destination de conseillers et d'agriculteurs. Les agricultures et conseillers agricoles n'ont pas forcément un langage commun ou une utilisation similaire de l'outil. C'est pourquoi il est important d'impliquer ces deux acteurs dans le développement de cet outil. En outre, comme les utilisateurs ont généralement des usages variés d'outil d'aide à la décision, comme par exemple comparer ce qu'ils ont obtenu avec ce que l'outil a prédit, utiliser l'outil pour voir l'effet seul de l'application des herbicides, il est nécessaire de tous les impliquer dans le développement (Cerf and Meynard, 2006). Pour aider à la simplification et à la transformation de FLORSYS, il est essentiel de bien cerner les différents problèmes de ces acteurs de la gestion des adventices. Il faut donc établir un dialogue avec les futurs utilisateurs afin de les impliquer dans la conception de manière à obtenir un outil utile et utilisé. Ces interactions, peuvent avoir la forme d'enquêtes auprès des futurs utilisateurs (Merot *et al.*, 2008) ou des rencontres et des ateliers (Hossard *et al.*, 2013) pour les mettre dans une situation d'utilisation de l'outil. Mais souvent, ces méthodes utilisent un modèle existant avec des utilisateurs (Figureau et al., 2015; Patel et al., 2007) ou bien construisent un modèle avec les utilisateurs (Christen *et al.*, 2015).

➔ Il est essentiel d'impliquer les futurs utilisateurs de l'outil d'aide à la décision dès les premières étapes de développement à partir du modèle de recherche pour que le l'outil soit à la fois utile et utilisé.

I.7 Les méthodes pour développer ce nouvel outil dans ce projet de thèse

Dans cette thèse, pour co-développer un outil d'aide à la décision pour la gestion intégrée des adventices à l'échelle du système de culture qui soit adapté aux besoins des conseillers agricoles et des agriculteurs. Un outil informatique pour la prise de décision lors de la conception de systèmes de culture ainsi que l'évaluation de systèmes de culture. Nous proposons un développement en différentes étapes, combinant des approches statistiques et d'agronomiques, présenté dans la Figure I. 1 afin de bien transformer le modèle de recherche en outil utile. La première étape (Figure I. 1 étape 1) est d'identifier les besoins et attentes des futurs utilisateurs. Nous avons choisi de les impliquer dans la réflexion via des enquêtes pour définir leurs besoins, leurs objectifs et leurs contraintes. La méthodologie employée sondera les futurs utilisateurs sur les questions auxquelles doit répondre l'outil et la présentation des entrées et résultats. Puis, différentes étapes de simplification et d'accélération du modèle seront nécessaires (Figure I. 1 étapes 2, 3 et 4), notamment par méta-modélisation et analyse de sensibilité. Mais pour l'accélération du modèle en méta-modélisant un module de FLORSYS et pour l'analyse de sensibilité globale de FLORSYS, différentes méthodes vont devoir être développées et employées. En utilisant de nombreux systèmes de culture variés, nous pourrons trouver les variables du système de culture influençant le plus la dynamique adventice et les services et disservices qui en découlent. Cette analyse de sensibilité permettra de hiérarchiser les entrées et d'identifier les techniques culturales les plus influentes sur l'impact des adventices. Ceci nous permettra de proposer un prototype d'outil qui sera testé avec des acteurs (Figure I. 1 étape 5), pour continuer le dialogue commencé plus tôt. À l'issue de ces tests, nous aurons des retours qui permettront d'améliorer le prototype, qui devra être testé et amélioré jusqu'à arriver à un outil fonctionnel. Les étapes suivantes nécessaires, comme l'"emballage" par une interface humain-machine, et l'optimisation informatique, ne feront pas partie de ce travail de thèse.

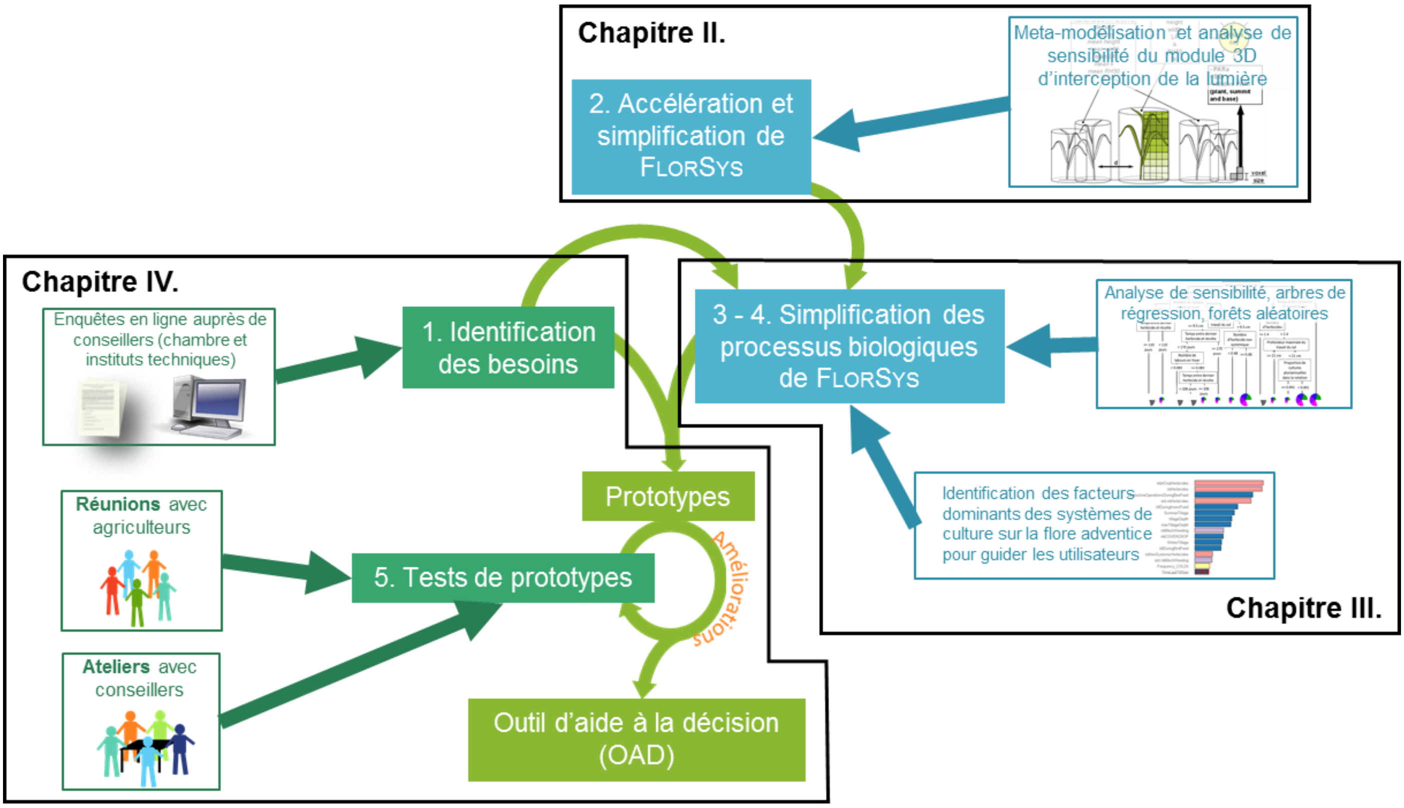


Figure I. 1 : Articulation des différentes parties de la thèse pour le développement d'un outil d'aide à la décision.

I.8 Objectifs du travail de thèse

Objectif global : Quelles méthodes et comment les appliquer pour développer un outil d'aide à la décision pour des conseillers agricoles et des agriculteurs, à partir d'un modèle de recherche « parcelle virtuelle » ?

Ci-dessous, les différentes questions pour les grandes parties (1 à 5) de cette thèse, avec les propositions qui seront explorées dans ce travail pour y répondre.

(1) Identification des besoins des futurs utilisateurs : quels sont les besoins en outil d'aide à la décision pour la gestion intégrée de la flore adventice ?

Les conseillers ont une certaine image des problèmes crées par les adventices et une certaine manière de les gérer.

Il y a différents profils de conseillers et donc différents niveaux d'utilisation et besoins d'un OAD.

Tous les indicateurs d'impact de la flore adventice n'ont pas la même utilité pour les différents conseillers.

(2) Accélération de FLORSYS : comment accélérer les simulations de FLORSYS ?

Il faut développer une méthode de méta-modélisation adaptée à des modèles complexes et gourmands en temps.

À cause de cette complexité, il faut séparer la méta-modélisation en plusieurs étapes, méta-modélisant plus particulièrement un module modèle.

(3) Identification et classement des composantes des systèmes de culture en fonction de leurs effets sur la flore adventice ainsi que son impact sur la production agricole et la biodiversité : quelles sont les pratiques culturales les plus influentes sur les adventices ?

En évaluant de nombreux systèmes de culture, il est possible d'identifier les pratiques et combinaisons de pratiques ayant le plus d'effet sur la dynamique adventice.

Pour identifier des systèmes de culture qui concilient diminution de nuisibilité des adventices et augmentation de biodiversité, il faut évaluer les systèmes de culture en fonction de leur situation de production.

(4) Simplification des processus biologiques de FLORSYS : comment transformer le contenu de FLORSYS pour permettre l'aide à la décision ?

Il est possible de synthétiser les systèmes de cultures en utilisant des méta-règles de décision.

Pour guider sur les pratiques les plus influentes et celles au contraires qui ne le sont pas, il faut hiérarchiser les entrées les plus influentes sur les indicateurs d'impact des adventices. Dans ce but, il est possible d'utiliser les indices d'importance des variables calculés par des forêts aléatoires qu'il faut construire à partir d'une grande base de données de systèmes de culture.

Utiliser des arbres de décision pour montrer aux personnes non initiées à FLORSYS comment les entrées se combinent pour aboutir aux sorties et ainsi comparer des systèmes de culture et leurs pratiques culturales.

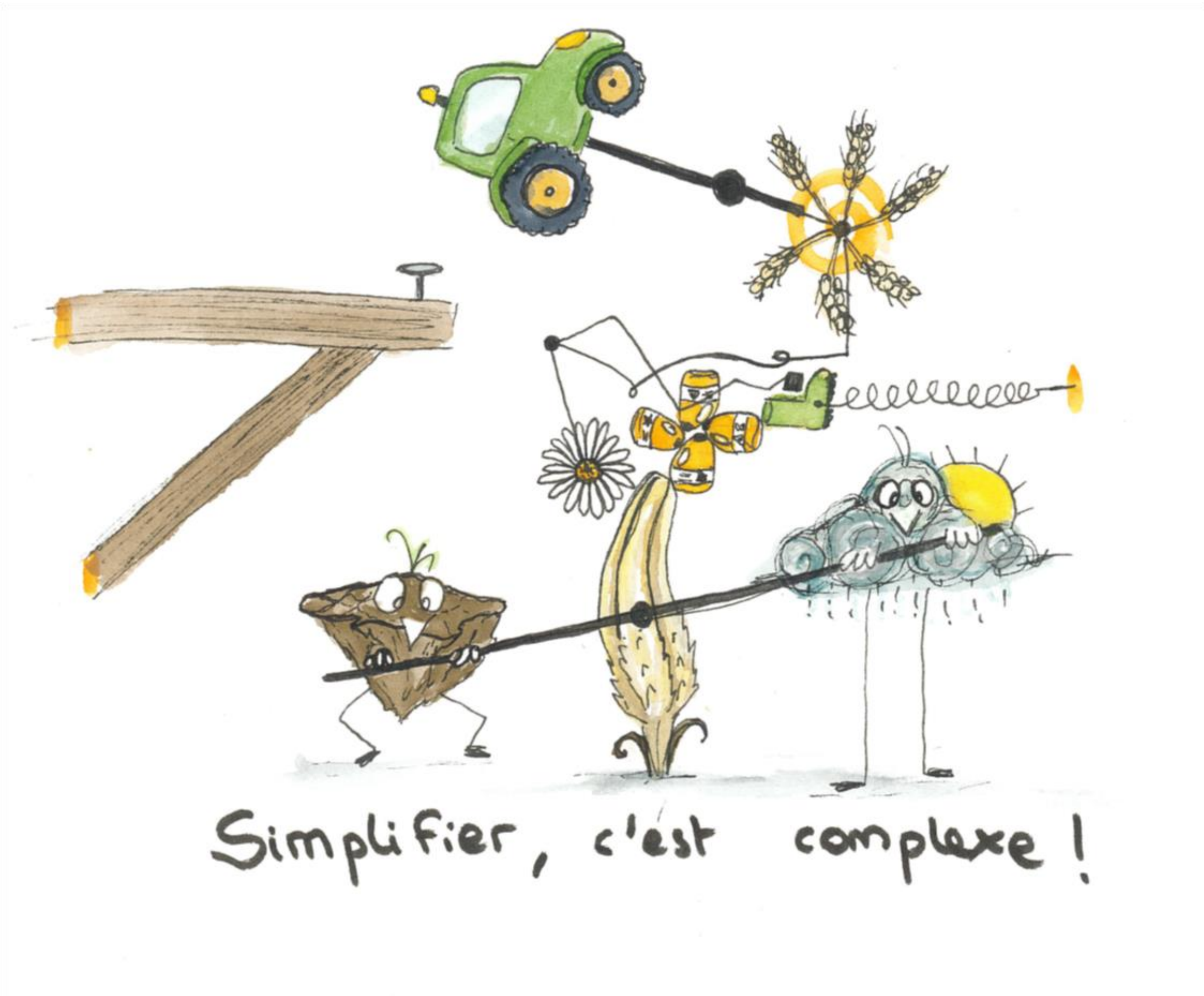
Utiliser les forêts aléatoires pour permettre de tester des systèmes plus rapidement qu'avec le modèle mécaniste et sans perdre trop de qualité de prédiction.

(5) Tests de prototypes avec les futurs utilisateurs : comment améliorer l'outil d'aide à décision en le confrontant à des utilisateurs ?

Pour définir la structure la plus efficace de l'outil, il faut le confronter à de futurs utilisateurs et tester différentes formes de sorties. L'amélioration de l'outil vient des discussions entre les différents acteurs sur leur expérience avec l'OAD.

Chapitre II : Analyse de sensibilité et méta-modélisation d’un module du modèle mécaniste complexe FLORSYS

SIMPLIFIER C’EST COMPLEXE



II.1 Objectif et démarche

Le développement d'un outil d'aide à la décision basé sur le modèle FLORSYS nécessite de simuler de nombreux systèmes de cultures variés. Seulement, comme nous avons vu dans le chapitre I, les simulations de FLORSYS sont assez lentes. Pour pouvoir simuler suffisamment de systèmes, il faut donc accélérer FLORSYS. FLORSYS est complexe et constitué de nombreux modules, dont le module d'interception de la radiation lumineuse qui est responsable de 70% du temps de calcul. Nous avons choisi de simplifier ce module d'interception de la radiation pour accélérer les simulations de FLORSYS. Ce module représente la parcelle en voxels, des pixels 3D, où l'interception de la radiation lumineuse est estimée pour chaque voxel. Une plante est alors constituée de plusieurs voxels. Ramener cette estimation à l'échelle de la plante entière et non plus du voxel est notre proposition pour accélérer le modèle. Pour cela, il est nécessaire d'identifier les variables d'entrée les plus importantes dans l'interception de la radiation et de créer un méta-modèle, c'est à dire un modèle du modèle, qui va simplifier le calcul à l'échelle de la plante. Pour finir, il faudra intégrer le module méta-modélisé à FLORSYS et évaluer le modèle méta-modélisé. **L'objectif de ce chapitre est de faire l'analyse de sensibilité et la méta-modélisation du module d'interception de la radiation lumineuse.**

Pour cela le travail a été divisé en différentes étapes, après avoir défini les limites du module, les entrées à faire varier et les sorties essentielles pour FLORSYS, nous avons étudié un cas simple d'une plante isolée dans le champ. Comme il a fallu développer une méthode permettant de faire de l'analyse de sensibilité sur des entrées corrélées, cette partie a fait l'objet d'un article décrivant la méthode et dont le cas simple d'une plante isolée dans le champ est présenté comme application de la méthode. Cette partie n'est pas inclue dans le corps du manuscrit, seul un résumé est présent section 2.4.1.3 et l'article (Gauchi *et al.*, 2017) se trouve en annexe A1 du manuscrit. En revanche la suite du travail est présentée en détail dans ce chapitre. Cela concerne l'application de cette méthode dans le cas plus complexe d'une plante entourée d'autres plantes, la combinaison des différents méta-modèles créés et l'addition de modèles supplémentaires pour intégrer dans FLORSYS et conserver la qualité de prédiction en évaluant les simulations avec FLORSYS. Le travail présenté dans ce chapitre a fait l'objet d'un article soumis à Ecological Modelling. Des résultats préliminaires de ce travail ont aussi présentés au congrès européen de l'ESA.

Gauchi J.P., Bensadoun A., Colas F., Colbach N. (2017). Metamodelling and global sensitivity analysis for computer models with correlated inputs: a practical approach tested with a 3D light interception computer model. Environmental Modelling & Software Environmental Modelling and Software, 2017, 92, 40-56. http://dx.doi.org/10.1016/j.envsoft.2016.12.005

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Colas F., Gauchi, J.-P., Villerd J., Colbach N. (2016) Meta-modeling light interception in crop:weed canopies 14th ESA Congress, 5-9 September 2016, Edinburgh, Scotland, 43-44 (poster).

II.2 Simplifying a complex computer model: sensitivity analysis and metamodelling of the complex process-based model FLORSYS

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Abstract

Complex biological models such as mechanistic research models often need to extend their current use to a broader audience. Simplification and faster simulations are solution to increase their use. A step-by-step methodology was developed and applied to partially metamodel, hence accelerate, a mechanistic model FLORSYS. FLORSYS is a process-based, multiannual and multispecies model ("virtual field") where cropping systems can be tested and evaluated for crop production and biodiversity, but it is too time-consuming for practical use. Especially when we need to design cropping systems reconciling crop production and biodiversity, we need tools to test numerous and diverse cropping systems.

(1) First, the 3D voxelized light interception submodel was identified as the slowest submodel. (2) We developed a metamodel predicting light interception and absorption directly at the scale of the plant instead of the voxel, first in the simplest situation, *i.e.* a single plant in a field and (3) then extrapolated the method to more complex situations, *i.e.* a plant in diverse crop:weed canopies. We used the global sensitivity method based on a truncated Legendre polynomial chaos expansion (PCE) whose coefficients were estimated by PLS regression (PCE-PLS) to simultaneously (i) rank inputs with respect to their polynomial and total effects on outputs via the so-called PCE-PLS sensitivity indices, and (ii) provide metamodels predicting light interception and absorption at the plant level. These metamodels were then shortened into parsimonious metamodels via a LASSO-PLS method. (4) Additional equations and decision rules were needed to replace the original process-based submodel by the metamodels. (5) The evaluation of the metamodelled FLORSYS, called FLORSYS-metaLight, with independent field observations, showed adequate prediction quality combined with an increased speed at fine-grained scale since the metamodelled version was 28 times faster than the process-based version.

Highlights

- A step-by-step guide was proposed to metamodel a complex process-based model.
- Additional equations and decision rules were needed to obtain a simulation model.
- Metamodels were better than the mechanistic model to reconcile precision and simulation speed.

• The metamodel was 28 times faster than the process-based model.
• Plant height and width were the key factors for radiation interception by plants

Keywords

Metamodel; light interception; photosynthetically active radiation PAR; crop:weed canopy; sensitivity analysis; simulation time

II.2.1 Introduction

The study of biological problems usually requires complex mechanistic models, especially when dealing with weed dynamics (Holst et al., 2007). Weeds are both harmful for crop production (Oerke, 2006) and important for biodiversity (Marshall et al., 2003; Petit et al., 2011). However, health issues, environmental concerns and new policies oblige farmers to reduce their herbicide use (Liebman, 2001). To date, no alternative weed control technique is, alone, as efficient as herbicides, and thus, several cultural techniques must be combined to control weeds (Liebman and Gallandt, 1997). Techniques influence above-ground vegetation or below-ground seed bank, they interact with other agricultural practices (*e.g.* tillage effects depend on crop rotation) and their effects can be either in the short or the long term and depend on the weed species present (Bàrberi and Lo Cascio, 2001; Cardina et al., 2002; Fried et al., 2008; Menalled et al., 2001). Thus, modelling weed dynamics is complex. Many weed dynamics models exist to understand and predict weed dynamics (Colbach, 2010; Holst et al., 2007). Only a few take into account the long-term effects of the weed impacts on crops, the multiplicity of weed species, the complexity of cropping systems, or the impact on crop production and biodiversity. Weed Manager (Tatnell *et al.*, 2006), RIM (Pannell *et al.*, 2004) or GESTINF (Berti and Zanin, 1997) respectively take into account the long term, the detailed cropping systems or the multi species community, but not all three aspects. The one exception is FLORSYS (Colbach et al., 2014c; Gardarin et al., 2012; Munier-Jolain et al., 2013). This is a process-based "virtual field" model which simulates the effects of cropping systems on weed dynamics as well as on crop production and weed-related biodiversity, thus making possible a multiobjective design of cropping (Colbach et al., 2017e). Unfortunately, models like FLORSYS that are accurate enough to reproduce the effects of agricultural practices on weed dynamics are time-consuming and complex (Colbach, 2010). In order to use FLORSYS to evaluate numerous cropping systems to designing herbicide-sparse cropping systems, the model must be accelerated and simplified. Since many research models are not used enough, the underlying problematic of simplifying and increasing the simulation time of FLORSYS is common to other mechanistic models.

To simplify a complex mechanistic model, it is possible to decrease the precision level as some problems dos not require the same high precision level (Kleijnen and Sargent, 2000; Renton, 2011). However, for a simpler model with the same precision different methods must be considered, global sensitivity analysis can explore the model and understand its behaviour to identify which inputs change the outputs the most. This allows to assign constant values to minor inputs and to simplify equations (Cox et al., 2006). Global sensitivity analysis then helps to find the correct level of complexity for the metamodel by identifying the non-influential inputs (Mahévas and Iooss, 2013). Then, metamodelling itself aims at emulating the original model, linking inputs and outputs by less detailed but faster equations. Some example are metamodelling of the noTG forest model (Marie and Simioni, 2014) and the bio-geo-chemical DNDC-EUROPE model (Villa-Vialaneix *et al.*, 2012).

Sometimes, metamodelling a whole model can be impractical, particularly if there are too many inputs and outputs. A more practical solution, as our mechanistic model being composed of numerous submodels, is to perform a local metamodelling on the submodel using most of the computing time (Marie and Simioni, 2014). Metamodelling requires several steps (Kleijnen and Sargent, 2000) that summarize as (1) what is the purpose of the metamodel (*i.e.* what goal, what is the accuracy needed), (2) what do we know about the model to be metamodelled (*i.e.* which inputs, which domain of applicability, which outputs), (3) what method to use (which type of metamodel to use, which experimental design) and (4) how to evaluate the metamodel (*i.e.* what fitting, which validity).

Many sensitivity analysis and metamodelling methods exist like the widespread Sobol indices or FAST. Mahévas and Iooss (2013) identified three criteria to select the best sensitivity analysis for a complex model: (1) the number of possible simulation runs, (2) the number and (3) type of inputs. The feasible number of runs, depending on the simulation time and the number of inputs are crucial to select the relevant methods (Table II. 1). When little is known about the model behaviour, which is often the case for complex models, performing early tests to increase the knowledge on the model is needed.

The objective of the present paper was to accelerate and simplify a mechanistic model, by implementing efficient metamodels through: (1) identify the sensitivity analysis and metamodelling methods adapted to a slow, complex model such as FLORSYS, (2) identify the important inputs, (3) simplify equations and shorten the computing time. We focused here on the reasoning for choosing the sensitivity and metamodelling methods and how they were combined with the other steps needed to transform a metamodel into a simulation model. The chosen method is fully developed in Gauchi *et al.* (2017) for a preliminary study. This global sensitivity analysis method is able to deal with both dependent and independent inputs. It is based on a truncated Legendre polynomial chaos expansion (PCE) whose coefficients are estimated by PLS regression (Gauchi et al., 2017) aiming to simultaneously rank inputs as a function of their polynomial and total effects on outputs via the so-called PCE-PLS sensitivity indices, and to provide precise and fast metamodels. Finally, the metamodels were reduced into parsimonious metamodels via a LASSO-PLS regression method. Here we present the methodology in section 2 and the model and its submodels in section 3. In section 4, we present the metamodelization per se with the tests that led to the choice of the most suitable method and how we applied this method to cover all situations in the model. Finally, in section 5 we show how the metamodels were integrated into FLORSYS and in section 6 which model (process-based vs metamodel) was the best in terms of simulation speed and precision, depending on the model use.

Table II. 1: Compilation of different sensitivity analysis methods for independent variables depending on complex model's proprieties. From (Tenenhaus, 1998; Harrington *et al.*, 2000; Bizouard *et al.*, 2012; Faivre *et al.*, 2013; Gauchi *et al.*, 2017)(Bizouard *et al.*, 2012; Faivre *et al.*, 2013; Gauchi *et al.*, 2017; Harrington *et al.*, 2000; Tenenhaus, 1998)

		ANOVA	Sobol-Saltelli	FAST	PCE-OLS	PCE-PLS	CART; random forest	Neural network
Model characteristics	Inputs number > 10	difficult to test all interactions	Yes	difficult, too heavy	Yes	Yes	Yes	Yes
	Possible run number > 1000	Yes	Yes	Yes	Yes	Yes	Yes	Yes
	Accept correlated inputs	No	No	No	No	Yes	Yes	Yes
Sensitivity methods properties	Estimates sensitivity indices	Yes	Yes	Yes	Yes	Yes	No	No
	Evaluates inputs for their importance	Yes	Yes	Yes	Yes	Yes	Yes	Yes
	Provide a metamodel	Yes	No	No	Yes	Yes	Yes	Yes
	Simulation design available from: LHS, Sobol sequence, Monte-Carlo, Hadamard, Full factorial design, Morris, OAT, numerous data from different sources	all	LHS, Sobol sequence, Monte-Carlo	Monte-Carlo	LHS, Sobol sequence, Monte-Carlo	LHS, Sobol sequence, Monte-Carlo	all	all

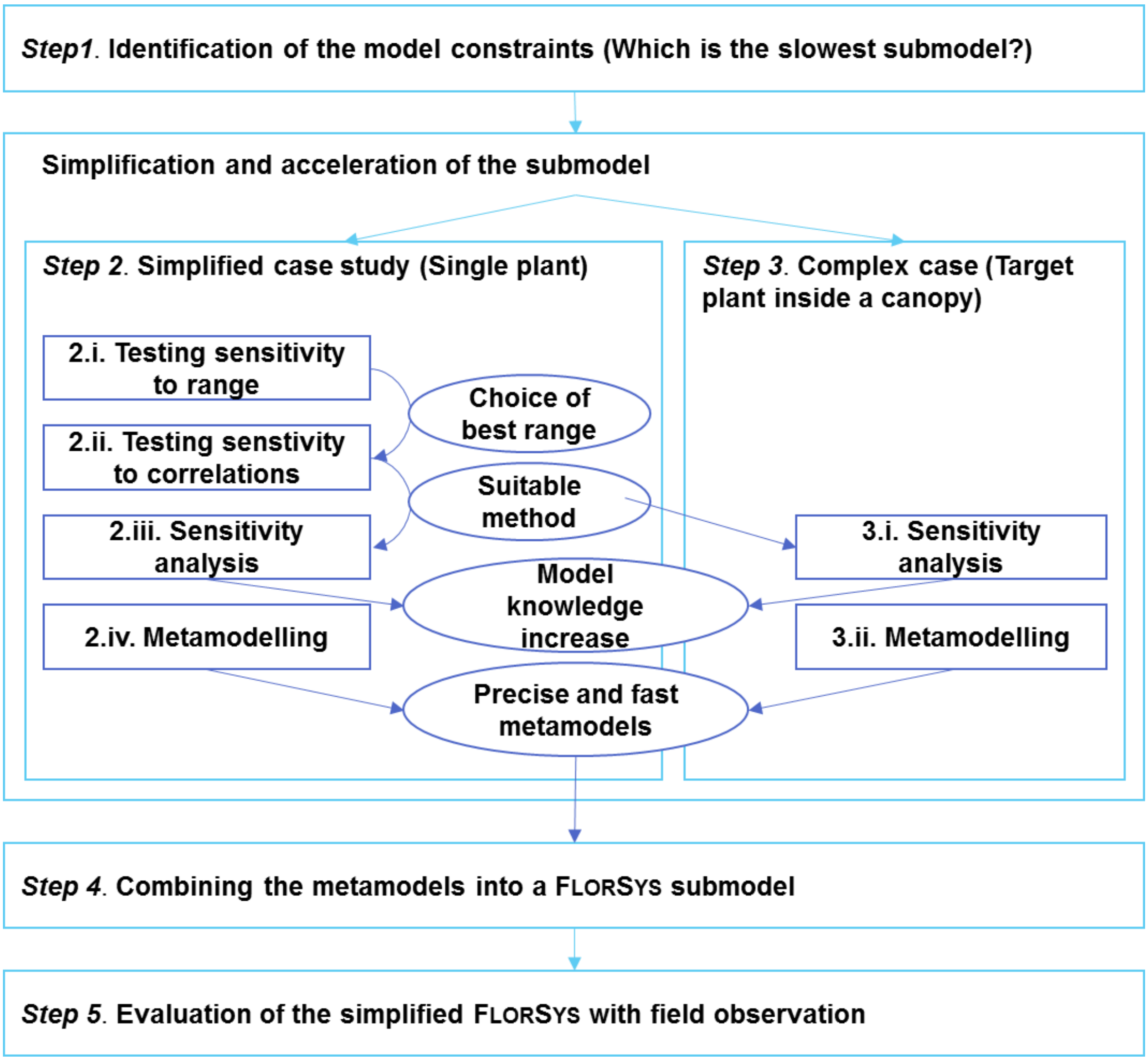

Figure II. 1: Schematic representation of the steps of the simplification and acceleration of the model FLORSYS. The numbers and roman numbers correspond respectively to the sections and sub-sections of the paper (Floriane Colas © 2017).

II.2.2 Step-by-step methodology to simplify a complex model

The methodology to accelerate and simplify FLORSYS involves several steps (Figure II. 1). The first step was to identify the most time-consuming submodel of FLORSYS and to determine the nature and ranges of its inputs and outputs appropriate for metamodelling. The second step was to find the most suitable method for analysing and simplifying this submodel. To facilitate this task, we worked with the simplest possible case for the submodel (*i.e.* a single plant in the field). Different methods of sensitivity analysis and metamodelling were tested to choose the method most suitable for a slow and complex model such as the process-based submodels of FLORSYS. In the third step, this method was applied to more realistic but more complex occurrences relevant for the submodel, *e.g.* target plants surrounded by neighbour plants. Step 5 shows how the metamodels were implemented into FLORSYS to replace the existing process-based submodel, with decision rules to determine which metamodel to use in which situation. The last step evaluated the whole new FLORSYS including the metamodels (hence FLORSYS–metaLight) with independent field observations to determine the loss of precision due to the metamodels and which model version (metamodelled or process-based) was best, depending on the model use.

II.2.3 Identification of the model constraints (step 1)

II.2.3.1 Presentation of FLORSYS

FLORSYS (Colbach et al., 2016; Colbach et al., 2014; Gardarin et al., 2012; Munier-Jolain et al., 2014; Munier-Jolain et al., 2013) is a mechanistic (*i.e.* process-based) model which simulates multispecies weed dynamics depending on cropping system and pedoclimate in a "virtual field". Its purpose is to experiment numerous cropping systems to design sustainable weed management strategies that reconcile crop production and biodiversity. FLORSYS models the annual life-cycle of crop and weed plants at a daily time-step and is a combination of submodels such as plant emergence, plant growth or radiation interception. FLORSYS inputs are daily weather, soil characteristics, initial weed seed bank, and cropping system practices (crop succession and detailed list of cultural operations). Outputs include crop yield, daily weed seed bank, plant densities and biomass. As FLORSYS consists of a collection of submodels, the simplification should not concern the whole model, but one individual submodel should be simplified at a time to keep modularity and access to specific submodels outputs.

II.2.3.2 Identification of the most time-consuming submodel in FLORSYS (step 1)

The computing time for each FLORSYS submodel was registered for a simulation with diverse crops and cultural practices over 13 years corresponding to a cropping system trial (Colbach et al., 2016a). Code profiling of the C++ source code of FLORSYS showed that the 3D radiation interception submodel was by far the most time-consuming submodel. This submodel predicts the photosynthetically active radiation (PAR) intercepted by each plant of the crop:weed canopy volume discretised into voxels (3D pixels). It used 57%, 64% and 99% of total simulation time with a voxel edge size of 7, 4 and 1 cm, respectively. The second most time-consuming submodel was the germination/emergence submodel which used 20%, 7% and 0.04% of the computation time for the three voxel edge sizes. Consequently, we will focus here on simplifying and accelerating the radiation interception submodel.

II.2.3.3 A short presentation of the 3D radiation interception submodel

The 3D radiation interception submodel (Munier-Jolain *et al.*, 2013) simulates a 3D sample of the virtual field where the space is discretised into voxels. Crop and weed plants are placed onto this field, with plant position and morphology resulting from other FLORSYS submodels. Crop plants can be sown in rows or broadcast (*i.e.* random position in the field); weeds can be positioned randomly or in species-specific patches. The radiation interception submodel calculates the amount of photosynthetically active radiation (PAR) that arrives on top of the crop:weed canopy and that trickles down to the voxels in the underlying layers, depending on plant leaf areas, species radiation extinction coefficients and solar angle (which depends on latitude and season). In total 14 input variables can be modified in the submodel for 5 different outputs.

II.2.3.3.1 3D radiation interception inputs

Plants are represented as cylinders delimited by their height and width (Figure II. 2, Table II. 2.A). The leaf area (LA) of the plant is distributed in the successive voxel layers of the cylinder, with 50% of the cumulated leaf area below relative median leaf height (RH50) of the plant and its distribution governed by the shape parameter, b. The species radiation extinction coefficient (k) and the plant leaf area inside each voxel determine how much incident radiation of the voxel is absorbed by the plant's leaves. The radiation absorbed by each plant (PARa) is the sum of the radiation absorbed by its leaves in the different voxels. Other inputs describe the location: (1) the field sample, *i.e.* dimensions in the north-south and in the east-west directions, as well as the grain of the discretization, *i.e.*, the voxel edge size, and (2) the position of the solar angle, *i.e.* latitude of the simulated field and the Julian day.

II.2.3.3.2 3D radiation interception outputs

Outputs of this submodel (Table II. 2.B) are used for different purposes in FLORSYS: the photosynthetically active radiation absorbed by a plant (PARaP) drives biomass accumulation in the growth submodel, the daily shading intensity perceived by the plant (SID) drives etiolation in the morphology submodel, and the relative photosynthetically active radiation intercepted by a plant (rPARi) and arriving below it on the soil surface ($rPARi_{base}$) are used as proxies for herbicide penetration and interception in the canopy in the herbicide treatment submodel. As single plants are not shaded by neighbouring plants, their relative PAR intercepted on the plant's top ($rPARi_{top}$) is always 1. Thus, for the single plant case, only four outputs were studied, *i.e.* PARaP, SID, rPARi, $rPARi_{base}$. For the "plant in a canopy" step, the five outputs are studied (Table II. 2.B). Plant growth is driven by the PARa value per plant (PARaP), but the metamodels also predict PARa per cm² (PARaC), *i.e.* relative absorption efficiency for a given plant volume.

Table II. 2: Definition, range variation and unit for of the inputs and outputs of the 3D radiation interception submodel.

A. Inputs

Types	Name	Short explanation	Step§	Range of variation	Unit
Physical environment	Latitude	Latitude of the simulated field	both	[-66; +66] single plan [0; +66] plant in a canopy	angle degree
	Day	Julian day	both	[1; 365]	no unit
Model precision	Xmax	Field sample size in the East-West direction	SP	[1; 4]	m
	Ymax	Field sample size in the North- South direction	SP	[1; 4]	m
	Voxel	Voxel edge size	SP	[1; 20]	cm
Target-plant variables	Height	Plant height	both	[1; 250]	cm
	Width	Plant width	both	[1; 200]	cm
	LA	Total plant leaf area	both	[1; 10^5]	cm2
	k	Species radiation extinction coefficient	both	[0.01; 1.1]	no unit
	RH50	Relative median leaf height below which is located half of the leaf area	both	[0.01; 1]	$cm \cdot cm^{-1}$
	b	Shape parameter for leaf distribution vs. plant height	both	[0.01; 6]	no unit
Neighbour mean plant variables	Density	Total plant density of the disc of plants (crops + weeds), including the target plant	PIC	[0.1; 3000]	$plant.m^{-2}$
	Distance to neighbour	Distance of the target plant to the furthest neighbour	PIC	[0.1; 3]	m
	Height	Plant height averaged over all neighbours and weighted by the inverse of distance to target plant	PIC	[0; 240]	cm
	Cover	Plant base area (superposed plants are added to the value) averaged over all neighbours and weighted by the inverse of distance to target plant	PIC	[0; 20000]	cm^2
	LA	Plant leaf area averaged over all neighbours and weighted by the inverse of distance to target plant	PIC	[0; 100000]	cm^2
	k	Species extinction coefficient averaged over all neighbours and weighted by the inverse of distance to target plant	PIC	[0; 0.7]	no unit
	RH50	Plants relative height averaged over all neighbours and weighted by the inverse of distance to target plant	PIC	[0; 115]	cm

§ Input used in the "Single Plant" step (SP), the "Plant Inside a Canopy" step (PIC) or both

B. Outputs (for target plant)

Use for FLORSYS	Name	Short explanation	Step§	Range of variation	Unit
Growth submodel	PARaP	Proportion of PAR* absorbed by the plant at the plant scale compared to the PAR above canopy.	both	[0; 1]	MJ cm^{-2} MJ^{-1} cm^2 $plant^{-1}$
	PARaC	Proportion of PAR absorbed by the plant for 1 cm^3 compared to the PAR above canopy	both	[0; 1]	MJ cm^{-2} MJ^{-1} cm^2 cm^{-3}
Morphology submodel	SID	Daily Shading Intensity , *i.e.* proportion of incident radiation above canopy that does not reach the plant	both	[0; 1]	MJ MJ^{-1}
Herbicide treatment submodel	rPARi	Proportion of radiation intercepted by the plant relative to incident radiation above canopy	both	[0; 1]	$MJ.cm^{-2}$ MJ^{-1} cm^2
	$rPARi_{top}$	Proportion of radiation intercepted by the top of the plant relative to incident radiation above canopy	PIC	[0; 1]	$MJ.cm^{-2}$ MJ^{-1} cm^2
	$rPARi_{base}$	Proportion of radiation intercepted by the base of the plant relative incident radiation above canopy	both	[0; 1]	$MJ.cm^{-2}$ MJ^{-1} cm^2

* PAR: Photosynthetically Active Radiation; § Output computed for the "Single Plant" step (SP), the "Plant Inside a Canopy" step (PIC) or both

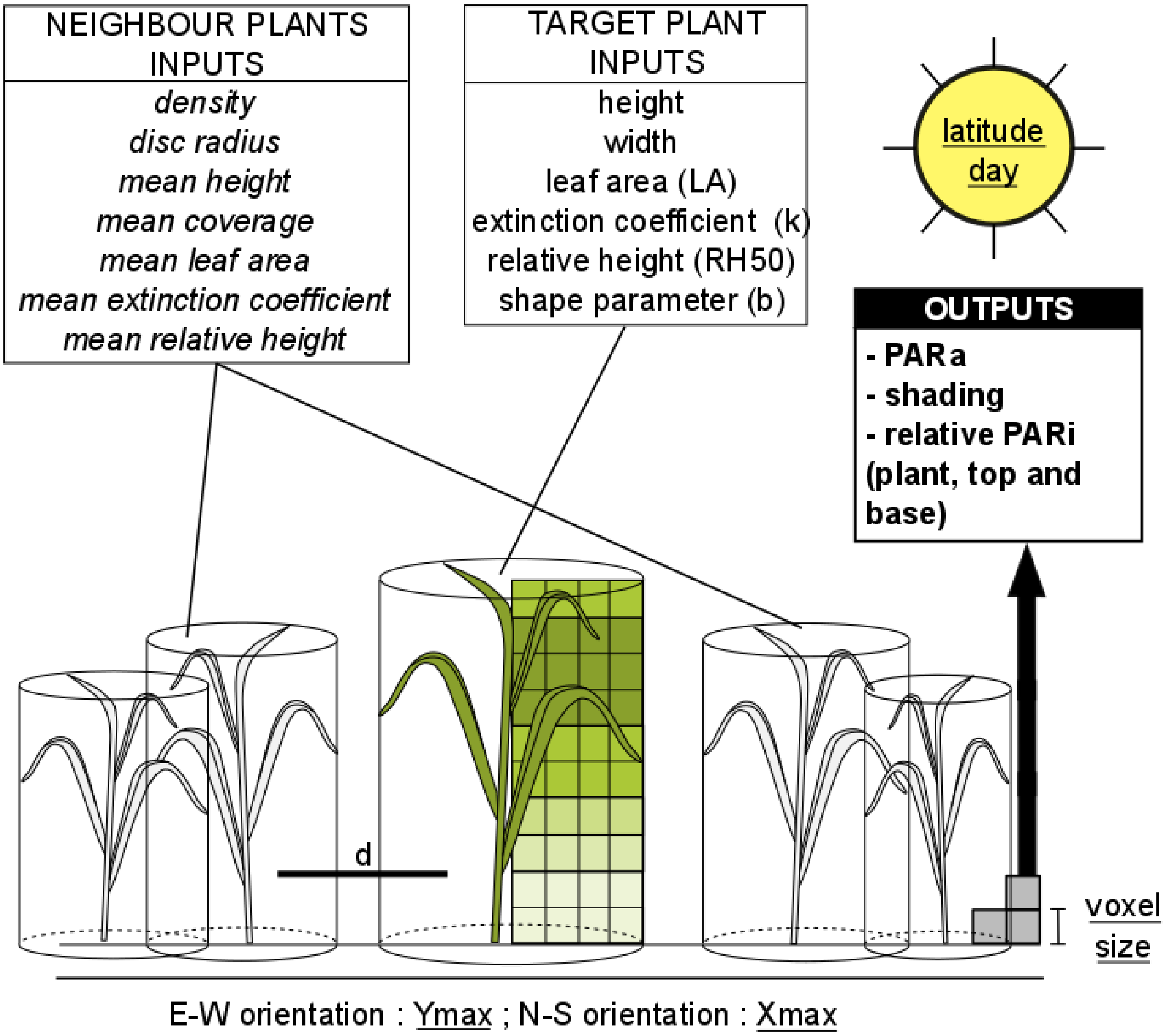

Figure II. 2: Schematic representation of the inputs and outputs of the 3D radiation interception submodel, with environmental and precision inputs (underlined), *plant in a canopy inputs (italics)*, single plant common inputs (standard font) and outputs (bold). For abbreviations, see Table II. 2. (Floriane Colas © 2017 based on (Gauchi et al., 2017))

II.2.4 Simplification and acceleration of the 3D radiation interception submodel

To find the best metamodelling and sensitivity analysis method for the radiation-interception submodel, we started with the simplest possible situation for this submodel which consists in a single plant in a field, without shade due to surrounding plants (step 2 in Figure II. 1). Once identified, this method was then applied to more realistic but more complex occurrences relevant for the submodel, *e.g.* target plants surrounded by neighbour plants (step 3 in Figure II. 1). To improve readability for all the steps, the sub steps (from i to iv) are included in the titles of the following sub-sections.

II.2.4.1 Simplified case study with single target plants (step 2)

This section aims (1) to test the effect of the range of variation in inputs, (2) to test the effect of correlations between inputs, (3) to analyse the sensitivity indices for unshaded (single) plants, and (4) to evaluate the metamodels predicting the radiation interception variables for unshaded plants.

II.2.4.1.1 Testing the sensitivity to the range of the inputs (step 2.i)

Input ranges were shown to influence the results of sensitivity analyses. Two inputs range sizes were tested following a Plackett & Burman experimental design (Plackett and Burman, 1946) with an experimental design of 12 combinations of the two extreme ranges for the 11 inputs (annex A3 section 1): (1) a small range corresponding to France, focusing on spring and summer, and the plant morphologies most common in fields and (2) a large range for all possible plant morphologies growing, all year and all around the world. For each of the 12 combination of ranges, a Latin Hypercube Sampling (McKay et al., 2000), LHS, was created for the 11 inputs and 29200 rows (this number was dependent of the number of day number and the number of different voxel values). For each configuration of ranges, Sobol sensitivity indices (Saltelli, 2002) were estimated, being the most used sensitivity indices, that can be robust enough to complex models (Gauchi et al., 2017). This estimation gave a set of 12 sensitivity indices for each of the 11 inputs. A linear regression of theses sensitivity indices was fitted, the coefficients were indications of the importance of the effect of the range. Absolute values and ranking of sensitivity indices of the various inputs changed for all outputs when a small input range was used instead of large one (annex A3 section 1). Not all inputs were, though, concerned and the concerned ones depended on the analysed output, *e.g.* the range of the voxel was important for the relative intercepted PAR (PARi) but not for the shading index (SID). Consequently, for the subsequent steps, the large input ranges were used to cover all the possible input situations and notably for novel combinations of species traits, *e.g.* resulting from new crop varieties or invasive weed species.

II.2.4.1.2 Sensitivity indices estimation via Sobol-Salteli method and via Polynomial Chaos Expansion

The objective of this part was to compare the Sobol sensitivity indices that we estimated in section 2.4.1.1 with a method that both estimates sensitivity indices and fits a metamodel. The Polynomial Chaos Expansion (PCE) method uses the same principle as Sobol sensitivity indices *via* Ordinary Least Square Regression (Sudret, 2008), here shortened to PCE-OLS. For each input, the sensitivity indices estimated by the polynomial chaos expansion are (1) the polynomial effect that accounts for the effect of the input only (*i.e.* the main effect of the input) and (2) the total effect (*i.e.* quantifying all the interactions of this input with other inputs). These indices are respectively comparable to the first order indices and the total effect indices of Sobol indices. The large range experimental design *via* Latin Hypercube Sampling, LHS (McKay et al., 2000), created in the previous section was used to estimate both indices. PCE-OLS indices were similar to Sobol indices computed on the same dataset (annex A3 section 2). The largest difference was of 0.13 for the total effect of the voxel on the radiation intercepted by the target plant (rPARi). The ranking of the inputs was the same with both methods. We thus preferred PCE in the following steps since it both estimates sensitivity indices and fits a metamodel, which is needed to simplify the radiation interception submodel.

II.2.4.1.3 Sensitivity indices with correlated inputs (step 2.ii)

The method for estimating PCE-OLS indices assumes that inputs are independent and uncorrelated. However, some inputs of the radiation interception submodel are correlated, *e.g.* plant height and the total leaf area are strongly linked (*e.g. Galium aparine L.* (Klem et al., 2014)). We thus tested the effect of including correlations among inputs on the estimation of the sensitivity indices and see whether the method needed to be adapted. This part was fully presented in Gauchi *et al.* (2017) and further details can be found in annex A3. In summary, the space filling LHS design of section 2.4.1.1 was modified to include correlations among inputs following the Iman and Conover method (Iman and Conover, 1982). These correlations (annex A3 section 3) were fully described in the previous paper (Gauchi *et al.*, 2017) and were estimated on simulated plants occurring in 12 diverse cropping systems (Colbach et al., 2016b). A number of 10000 runs were selected out of a total of 29200 runs to remove outputs too close to the limit of the ranges. Adding correlations to the space filling design of the inputs changed absolute values of sensitivity indices PCE-OLS for all outputs and gave deviant values (negatives or > 1).

Consequently, it was essential to find a method better adapted to correlation inputs. Gauchi *et al.* (2017) proposed to calculate the sensitivity indicies (*i.e.* polynomial effect and total effect) by estimating the coefficients of Polynomial Chaos Expansion using a Partial Least Squares method, namely a Partial Least Squares Regression (PCE-PLS, see (Wold *et al.*, 2001)). Here, the resulting PCE metamodels were though too huge to speed up FLORSYS computations. We thus built more parsimonious and faster metamodels, using a LASSO regression (Tibshirani, 1996) to select monomials via GLMSELECT (SAS). With the selected monomials we performed a new PLS regression for the final parsimonious metamodel (hence, "fast" metamodel). This combination of methods was hence referred to as LASSO-PLS. The resulting single plant PCE-PLS metamodels (full and fast) were evaluated via a PLS specific criterion, the Q^2_{cum} (Lazraq et al., 2003; Tenenhaus, 1998) for fitting and prediction qualities. We used the same principle and stopping rule as in Gauchi *et al.* (2017) giving a $Q^2_{cum}(h^*)$ referred to as Q2cum in this paper. This cross-validated fitting prediction criterion is bounded between 0 and 1; the closer to 1 it is, the better the metamodel is in terms of prediction and fitting. This method was used for the sensitivity analysis and metamodelling of the single-plant case (sections 2.4.1.5) and then for the more complex case with target plants surrounded by neighbouring plants (section 2.4.2).

II.2.4.1.4 Identify the key inputs that drive radiation interception of single plants (step 2.iii)

The sensitivity analysis based on PCE-PLS showed that that the most important inputs for the photosynthetically active radiation absorbed by the plant (PARaP, which drives plant growth) were voxel size and plant width (Figure II. 3). The second most important inputs were the target-plant characteristics driving potential leaf area absorption ability, *i.e.* total plant leaf area and species extinction coefficient. Total leaf area and plant volume (determined by its width and height) affected PARaP more than leaf distribution (RH50 and b) counts more than plant shape. The environmental variables (latitude and day) as well as the field size had little small but non-negligible impacts. All inputs strongly interacted, with interactions making up between 46 % (voxel edge size) and almost 100% of the total effect (all others except plant width). Consequently, the sign of the main regression coefficient of an input was useless to assess how an output varied with an input. Graphs of outputs vs. inputs confirmed that interactions made it usually impossible to identify general tendencies, except that PARaP tended to decrease with increasing plant height and width, indicating a self-shading effect (annex A3 section 5).

The same general tendencies as for PARaP were observed for the other outputs, *i.e.* all inputs matter, voxel edge size and target plant variables mattered more than physical variables and field size (though voxel size could be less important for some outputs such as the shading index, SID); plant volume (though the most relevant variable could be height rather than volume) and leaf area mattered more than plant shape and leaf distribution (annex A3 section 4).

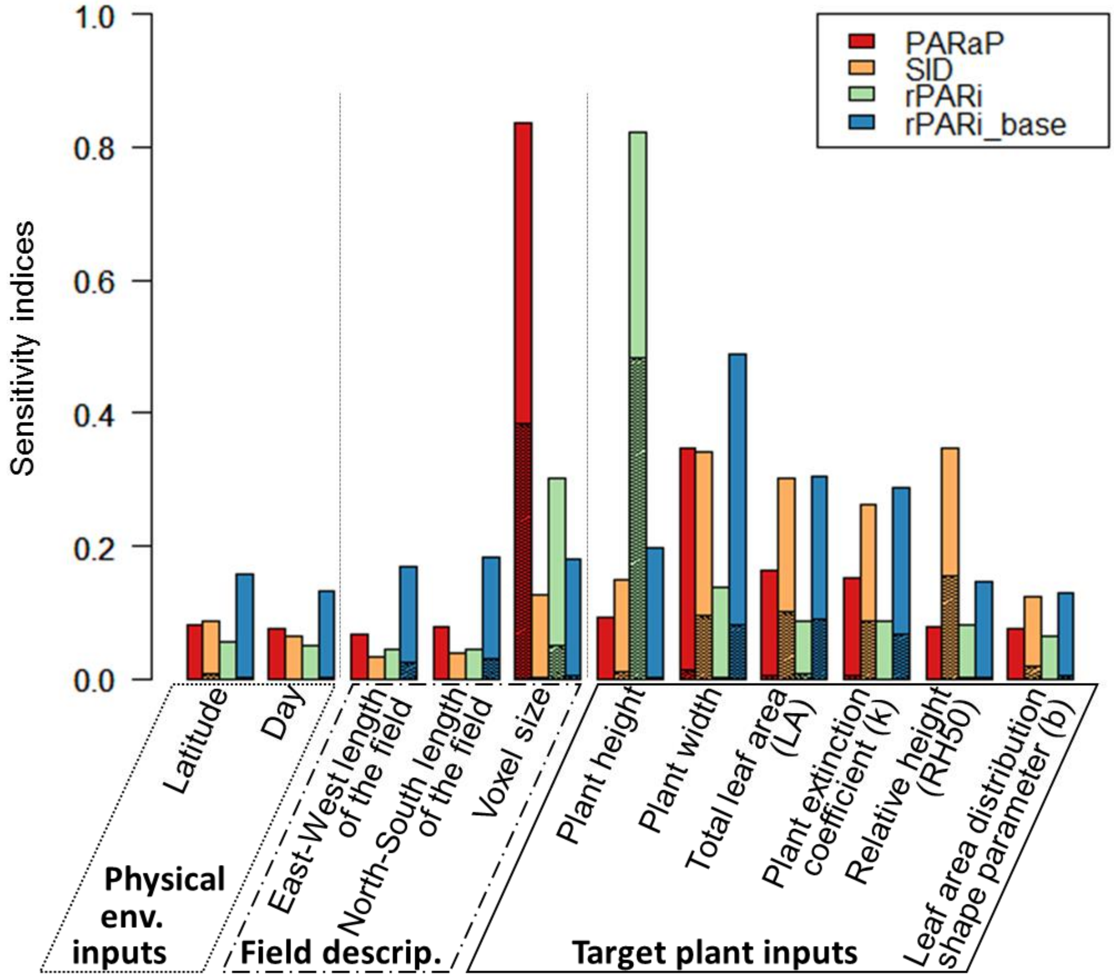

Figure II. 3 : Overall view of sensitivity indices for radiation interception outputs of a target plant alone in a field. Inputs were ranked by decreasing sensitivity. In hatched colours polynomial effects (*i.e.* disregarding interactions), in plain colours total effect (including interactions) of the inputs, environmental and precision inputs (underlined) and single plant input (normal font). The outputs are the Photosynthetic Active Radiation (PAR) absorbed by the target plant (PARaP), shading index (SID), relative PAR intercepted by the whole plant (rPARi) or at the base of the target plant ($rPARi_{base}$). (Floriane Colas © 2017)

II.2.4.1.5 Metamodels for a single plant (step 2.iv)

The metamodels for a single target plant in the field included all inputs as the sensitivity analysis indicated that all were influential, albeit to varying degrees. The full metamodels included 4367 monomials resulting in a good (*i.e.* close to 1) Q2cum (0.93 - 0.98) (Table II. 3 A lines 1, 3, 5, 7) and a low prediction error (RRMSEP = 0.15 – 0.25 $MJ \cdot MJ^{-1}$) (annex A6 section 3). LASSO-PLS selection produced simpler and faster metamodels, with only 25 to 27 monomials, resulting in a quite good Q2cum (0.70 - 0.90) but a slightly worse prediction error (RRMSEP = 0.35 – 0.55 MJ·MJ^{-1}, lines 2, 4, 6, 8). Regardless of the metamodelling approach (fast or full), radiation interception at the base of the target plant (rPARi$_{base}$, a proxy for the total herbicide penetration in the canopy) is the least well predicted output. This was also the only output that was not calculated at the scale of the plant but at the field scale.

Table II. 3: Synthesis of the different 3D radiation interception metamodels (fast and full) computed *via* polynomial chaos expansion and PLS regression for the single plant in the field (A) and the plant in a canopy of neighbour plants (B). Fast metamodels result from full metamodels via a LASSO-PLS monomials selection.

A.

	Radiation-interception model Output	Metamodel type	Polynomial degree	Monomial number	Fitting prediction Q2cum
[1]	PARaC	full	5	4367	0.96
[2]	PARaC	fast	5	26	0.85
[3]	SID	full	5	4367	0.98
[4]	SID	fast	5	26	0.82
[5]	rPARi	full	5	4367	0.95
[6]	rPARi	fast	5	27	0.90
[7]	rPARi$_{base}$	full	5	4367	0.93
[8]	rPARi$_{base}$	fast	5	25	0.70

B.

	Radiation-interception model Output	Metamodel type	Polynomial degree	Monomial number	Fitting prediction Q2cum
[9]	PARaC	full	4	3875	0.83
[10]	PARaC	fast	5	30	0.56
[11]	SID	full	4	3875	0.75
[12]	SID	fast	5	29	0.30
[13]	rPARi$_{top}$	full	4	3875	0.71
[14]	rPARi$_{top}$	fast	5	28	0.27
[15]	rPARi	full	7	4000	0.82
[16]	rPARi	fast	5	35	0.52
[17]	rPARi$_{base}$	full	4	3875	0.76
[18]	rPARi$_{base}$	fast	5	35	0.37

II.2.4.1.6 Summary for single target plants

We tested different sensitivity analysis methods that increased our knowledge on the 3D radiation interception submodel. This resulted in a more appropriated method that accounted for the correlated inputs. We then proposed a handy solution for more parsimonious and faster metamodels. Part of the methods were developed in a previous study on a single output (Gauchi et al., 2017) and were completed here before being applied to a larger set of outputs.

II.2.4.2 Case for a target plant inside a canopy (step 3)

Fields (or even field portions) rarely only comprise a single plant. Step 4 thus focused on radiation interception of target plants surrounded by neighbouring plants. The method developed in the previous step to analyse and metamodel radiation interception from target-plant, environmental and precision inputs was adapted to (1) include contrasting canopies representing the diversity in crop:weed canopies in arable fields in the simulation plan while (2) limiting the amount of additional inputs needed to describe the canopy surrounding the target plant.

II.2.4.2.1 Simulation plan

A canopy is a complex set of plants of different species, sizes, widths, positions… To have diverse plant canopies it was necessary to vary numerous variables: plant density (crop density, weed density, amount of bare field area), the position of weeds (random or in patches, number of patches in the field), the position of crop plants (row vs broadcast sown, inter-row width), canopy structure (presence and diameter of canopy gaps surrounding target plants…), the heterogeneity of plant morphology (mean and variation coefficient of target plant characteristics), weed populations being more heterogeneous than crop population (*i.e.* presenting a larger range of variation) (see annex A4). These preliminary inputs were used in a LHS design of 20440 rows. Correlations were added in the same way as for the single-plant study, with the Iman and Conover method. The diverse canopies were built by placing the plants on a virtual field and attributing morphologies, and then radiation interception and absorption was simulated with the FLORSYS radiation interception submodel. Cases with outlying values were removed as well as output values too close to the range limit (*i.e.* 0, 1 or 100 depending on the output) to avoid side effects due to computation errors; 2536 canopies remained after the sorting. The PCE-PLS method was used to metamodel and perform the sensitivity analysis.

II.2.4.2.2 Describing the canopy

Many detailed variables are needed to create contrasting canopies in FLORSYS, but only a limited number of inputs was allowed to keep the metamodel simple. The detailed canopy variables were thus aggregated into five mean canopy inputs (Table II. 2), to account for the canopy effect in the metamodel. The nearer the neighbours are to the target, the more their characteristics contribute to the variables describing the average canopy characteristics, here the example of the canopy height (cm):

Eq. 1

$$mean\ height = \frac{\sum_{i=1}^{n}\left(\frac{1}{d_i + 1} * height_i\right)}{\sum_{i=1}^{n}\left(\frac{1}{d_i + 1}\right)}$$

where d the distance (m) of the target plant to the closest neighbour plant i (+1 to account for a zero distance when the neighbour is located in the same voxel as the target), $height_i$ is the height (cm) of neighbour i and n the number of neighbour plants in the field sample. For the equations of the other canopy variables, see annex A4 section 4.

In addition to these aggregated canopy inputs, we added: (1) the plant density and the maximum distance between the target plant and neighbour plants, (2) target plant variables (as in the single plant case) and (3) two environmental variables (latitude and day), resulting in 15 metamodel inputs (Table II. 2). To reduce the number of inputs, field dimensions (Xmax and Ymax) whose effect was shown to be slight in the single-plant sensitivity analysis of the single plant (section 2.4.1.4) were both fixed at 8 m which allowed to have large plants in the virtual field sample. The voxel size was shown to be important for most outputs (section 2.4.1.4), but to simplify and accelerate the simulation plan, we kept it constant. Additional simulations (annex A3 section 6) showed that a voxel edge size of 4 cm was the best compromise between the precision of the radiation interception submodel output and the computation time.

II.2.4.2.3 Sensitivity indices (step 3.i)

The sensitivity analysis of radiation interception outputs to inputs depicting target plant, physical environment and neighbour plants showed that input effects were almost entirely due to interactions among inputs (Figure II. 4). Globally, target-plant inputs had the most and neighbour-plant inputs the least impact. Inputs of a given type had similar effects, except for the relative PAR intercepted by the target plant (rPARi) whose height effect was several times the effect of any other inputs. As for the single-plant scenario (section 2.4.1.4), the interactions among inputs were generally too complex to identify general tendencies, whether from the signs of the polynomial effects or from graphs (annex A3 section 5). And again, outputs were sensitive to all inputs *via* interactions with other inputs and none of latter could be set at a default value in the following metamodels.

II.2.4.2.4 Metamodels (step 3.ii)

The metamodels for target plants surrounded by neighbour plants included all inputs, *i.e.* for describing the target plant, the physical environment and the biological environment due to the neighbour plants. The polynomial degree of these metamodels was smaller than for the single-plant ones, except for the relative intercepted PAR rPARi, (Table II. 3. B lines 14-15); the Q2cum was always lower and the prediction error higher (Table II. 3. B vs A). Further increasing the polynomial degree did not improve the Q2cum or reduce the prediction error (results not shown). The need for a higher polynomial degree for the rPARi points to more and more complex interactions among inputs. The fast metamodels usually needed a higher polynomial degree and more complex monomials (Table II. 3. B) than full metamodels to optimize the Q2cum. The latter though remained low (0.27-0.56) and prediction error was much larger than for single plants (0.85 and 0.65). Radiation interception and absorption by a plant surrounded by neighbour plants is thus much harder to simplify *via* a small metamodel than for single plants.

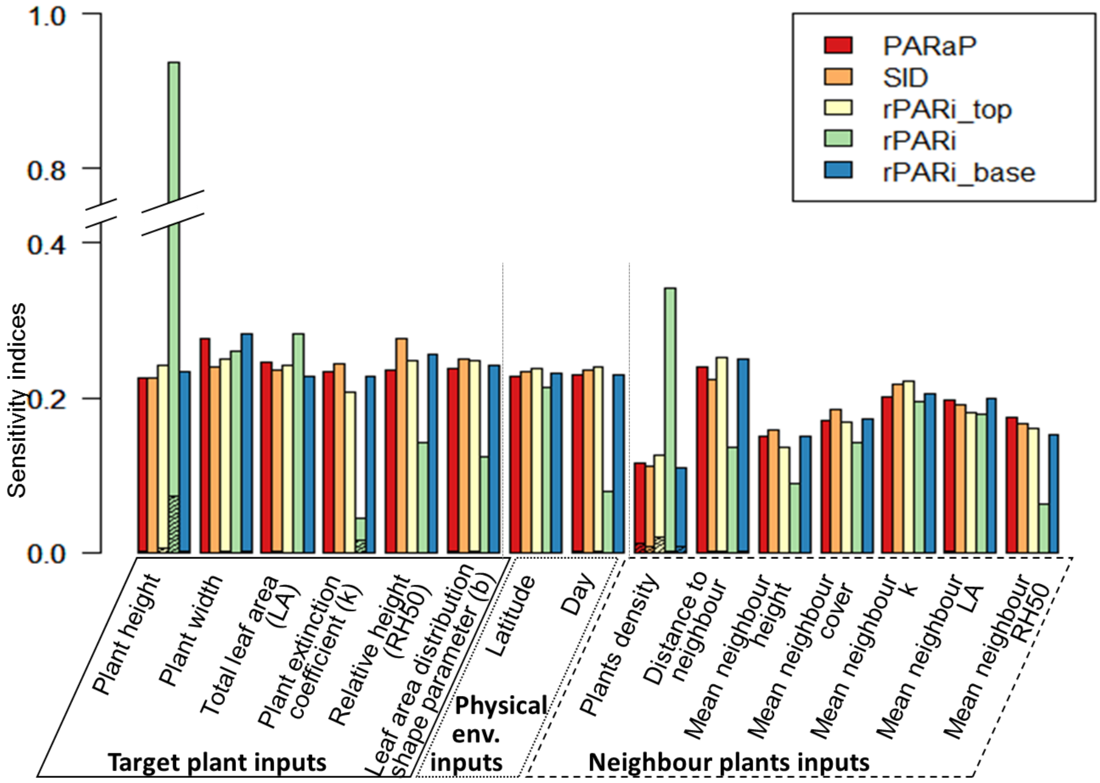

Figure II. 4: Overall view of sensitivity indices for radiation interception outputs of a target plant surrounded by neighbour plants. Total effects (plain colours) and polynomial effects (*i.e.* disregarding interactions, hatched colours) of inputs of the FLORSYS radiation interception submodel. The outputs are the Photosynthetic Active Radiation (PAR) absorbed by the target plant (PARaP), shading index (SID), relative PAR intercepted at the summit of the target plant ($rPARi_{top}$), by the whole plant (rPARi) or at the base of the target plant ($rPARi_{base}$). (Floriane Colas © 2017)

II.2.4.2.5 Summary for plants in the canopy

The metamodels for radiation interception and absorption by a plant surrounded by neighbour plants were simple enough to be implemented into FLORSYS but with a poorer prediction quality than for a single plant. The canopy creates a complex interaction with the radiation that cannot be easily simplified at a scale as large as the plant. Strong interactions between all inputs prevented us from setting the least important inputs to constants.

II.2.5 Combining the metamodels into a FLORSYS submodel (step 4)

As we had developed metamodels for two situations, *i.e.* single plant and plant in a canopy, it was necessary to establish rules to determine when to use which metamodel in a simulation using the whole FLORSYS including the metamodels (hereafter called FLORSYS-metaLight). This section present how the metamodels were combined and what else was needed to cover all likely canopy scenarios with FLORSYS-metaLight.

Table II. 4 : Synthesis of the variation in prediction error (RRMSEP) in simulations with the metamodelled *vs.* process-based model.

Output	Species scale	Time step	Type of neighbours used for calculating canopy variables		
			Local	Mixed	Average
Weed density (plants.m^{-2})	By species	Day	+9%	++%$^{\$}$	+10%
		Multiannual	-81%	-7%	-52%
	Sum of all species	Day	+9%	++%$^{\$}$	-85%
		Multiannual	-50%	-8%	+152%
Weed biomass (g.m^{-2})	By species	Day	+294%	+417%	+580%
		Multiannual	++%$^{\$}$ for process-based model		
	Sum of all species	Day	++%$^{\$}$.	+327%	+723%
		Multiannual	+1351%	+10353%	+12391%
Seedbank (seeds.m^{-2})	By species	Day	+164%	+163%	+84%
	Sum of all species	Day	++%$^{\$}$ for process-based model		
Crop yield (T.ha^{-1})	By species	Day	+61%	+6%	79%

$ RRMSEP of metamodelled simulation was >> 0 and RRMSEP of process-based simulation was < variability in observations, *i.e.* ~0, and no relative variation in RRMSEP could be calculated

II.2.5.1 Principle

Even when there is more than one plant in a field, some of these plants can be considered as single if they do not interfere with each other's radiation interception, which depends on plant sizes, solar angle and distance between plants. Consequently, each day, for each target plant (crop or weed), rules are needed to determine whether a target plant can be considered as single or as surrounded by neighbour plants (annex A5 section 2).

When building the metamodels, a large number of runs were eliminated because outputs were too close to the limits of the range or because their combination was biologically impossible and resulted in deviant values (section 2.4.2.1). This also reduced the ranges accepted by the metamodels for several key inputs such as target leaf area, making it impossible to predict radiation interception for newly emerged seedlings (*i.e.* with almost nil height, width and leaf area), voluminous single plants (having reached the maximum height and width possible for the species) or mature plants with dried leaves (with a near zero leaf area). To remedy this, further metamodels were built for the particular case of small seedlings, and for the remaining outlying situations, equations were added to predict radiation interception and absorption from ecophysiological knowledge, or from likely constants (section 2.5.3). Figure II. 5 summarizes how the different rules, equations and metamodels ware aggregated. Finally, the calculation loops over neighbour plants needed to calculate the aggregated canopy variables can be time-consuming. As a consequence, alternative methods to compute aggregated neighbour were tested (section 2.5.4).

II.2.5.2 Rules for deciding whether to use the single plant or plant in a canopy metamodel

II.2.5.2.1 Method

The PAR intercepted at the top of a target plant ($rPARi_{top}$) is relevant to identify whether radiation interception of the target plant is impacted by neighbour plants, because this output is always 1 for single targets and decreases in the presence of shading neighbours. To establish decision rules to discriminate these two situations, a regression tree was built from the data sets of sections 2.4 and 2.4.2, using the inputs listed in Table II. 2. As the metamodels in the previous sections showed that it was difficult to take account of all effects and interactions with these inputs, some were transformed and others added in the present analysis. The environmental variables were transformed to emphasize the effect related to solar angle: latitude was transformed into degrees to the equator (*i.e.* absolute latitude) and Julian days into days from the summer solstice to the winter solstice (*i.e.* between solstice days). The distance from target plant to its closest neighbour was also used as input (with distances calculated between plant centres), and all other inputs were weighted by the inverse of this distance to take into account that closer neighbours shade more than farther neighbours. Finally, the target height relative to the canopy height (overtaking percentage) was integrated *via* the ratio of the difference between the two heights (eq. 6 annex A4 section 5).

The CART method (Breiman *et al.*, 1984) was used to build a classification tree to determine the decision rules. This method successively splits the data set into two subsets along a threshold value of an input (*e.g.* distance to the closest neighbour) in order to maximize the difference between subsets in terms of output. Branches are combinations of input values that lead to output predictions contained in leaf nodes. CART also ranks the input according to their importance to explain the output.

The output analysed in the trees was not directly the $rPARi_{top}$ but a binary variable indicating whether the target plant was considered single or inside canopy, depending on whether its $rPARi_{top}$ was respectively ≥ or < a threshold value. In addition to the theoretical value of 1, ten other thresholds were tested, ranging from 0.90 to 0.99 (incremented by 0.01), in order to increase the number of single plant cases compared to canopy cases and thus the robustness of the tree. Among the 11 trees, the one corresponding to the 0.98 threshold was chosen as it was the closest to one and with the most rules to use the single plant metamodel. The latter allows to accelerate calculations because the single-plant metamodels were simpler and did not need to calculate the aggregated canopy variables.

II.2.5.2.2 Decision tree to determine where a target is shaded by neighbours

The rules determining whether a target plant can be considered as single are shown in Figure II. 6. For example, if the nearest neighbour is further than 1.6 m, and the target plant is taller than the neighbouring canopy, the target can be considered as single. Surrogates of the tree (*i.e.* variables correlated to the variable in the tree that could also explain the segmentation, but to a lesser degree) and ranking of variables in their order of importance (annex A4 section 6) showed that nearest neighbour distance and interactions are predominant to determine whether the target plant is single or within a canopy.

The decision rules provided by the tree did not cover all likely situations in the field and did not sufficiently accelerate computer time. Consequently, we added a further logical rule: if there are no neighbours whose height exceeds the distance separating the outer limits of the neighbour and target plants, the target is considered as single. In that case, even if the sun is low on the horizon, the closest neighbour is too far to shade the target (annex A5). The combination of the decision tree and this additional rule constitute step A in Figure II. 5.

II.2.5.3 Adding equations at the limits of the input ranges

The input ranges of the metamodels missed small seedlings for which good prediction is essential as their initial growth determines which plants outgrow the others. Consequently, we ran a further simulation plan to build a third metamodel focusing on small seedlings (Step C, Figure II. 5), using the method developed in section 2.4.1.3(annex A5 section 4). This additional metamodel was still inadequate for fresh seedlings whose leaf area is lower than the metamodel's accepted input range. In that case, as there is neither shading nor self-shading, the PARa absorbed by the plant is the product of the incident PARa, the plant leaf area times its extinction coefficient, based on Beer's law (Monsi and Saeki, 1953, 2005) (step B in Figure II. 5). This works fine for single plants that are unshaded by neighbours. To include either small plants surrounded by neighbours or any plants by small neighbours outside the canopy metamodel range, a linear combination of predictions for single plants (either small or large) and plants in canopy was used, step G in Figure II. 5. This was particularly true for canopy leaf area whose lower range limit was extremely high (Table II. 2). Single-plant predictions and target-in-canopy predictions were weighted by respectively 1 and the canopy leaf area, and divided by the same of these weights (annex A5 section 4).

The metamodels do not include voluminous or mature leaf-less plants either. As these have finished their growth, outputs were simply fixed either to a minimum or maximum value, or linked with a simple regression if one input was out-of-range (step Figure II. 5). The values were based on graphs of outputs *vs.* inputs from the complete data set including the outliers that were ousted during metamodel construction (annex A5 section 4). If several inputs were out of range, the output was estimated based on the analysis of the most influential input, with the strongest polynomial effect in the sensitivity analysis (annex A5 section 4). For example, if a target plant surrounded by neighbours is taller than 254.8 cm, then its relative intercepted PAR is 0.00649 $MJ \cdot MJ^{-1}$.

II.2.5.4 Different methods to aggregate neighbour plants into canopy variables

We proposed three different methods to calculate the aggregated neighbour variables of each target plants: (1) all neighbours close to the target are used for the computation ("local" neighbours), (2) all plants in the field are averaged and the same aggregated variables were used for all target plants ("average" neighbours), (3) a mix between the previous two methods, using average canopy variables when the plant density exceeds 500 plants.m^{-2}, and local neighbours otherwise. The effect of the aggregation method on prediction error and simulation speed of the whole FLORSYS-metaLight was evaluated in section 2.6.

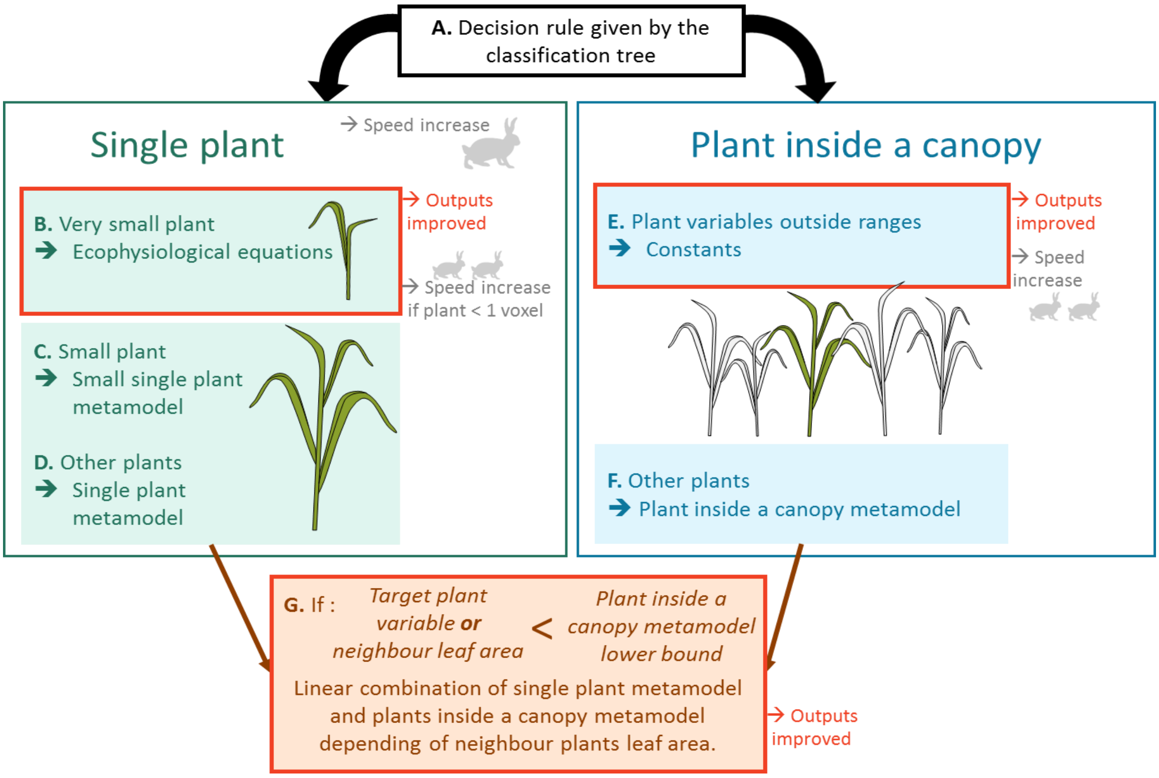

Figure II. 5: The different metamodels and when they are used in FLORSYS-metaLight depending on target plant variables, neighbour plant variables and environmental variables. (Floriane Colas © 2017)

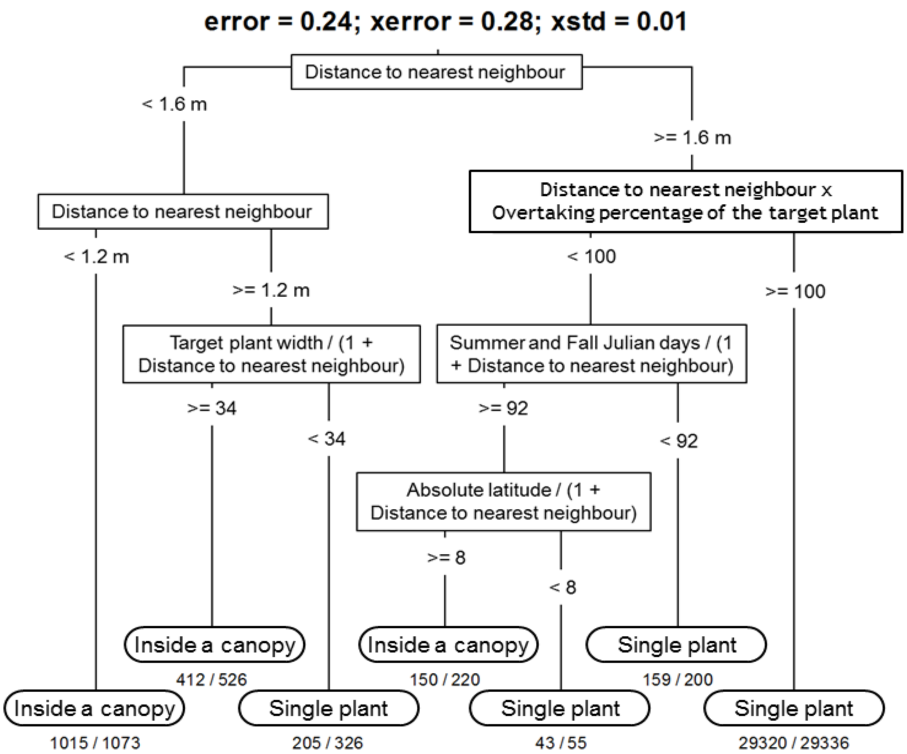

Figure II. 6: Classification tree (CART) to decide whether a target plant is single or inside a canopy. The segmentation is based on relative photosynthetically active radiation on target-plant top $rPARi_{top}$> 0.98. Error is the adjustment error or training error, xerror is the cross validation error and xstd is standard deviation of cross validation. (Floriane Colas © 2017)

II.2.6 Evaluation of the simplified FLORSYS-metaLight with field observations (step 5)

II.2.6.1 Objective

Sections 2.4.1.5 and 2.4.2.4 evaluated the prediction quality of the individual metamodels. Here, the objective was to evaluate how good and fast the predictions produced by FLORSYS-metaLight compared to the process-based FLORSYS, by comparing simulations to field observations following the methods developed in a previous paper (Colbach et al., 2016b). Different voxel edge sizes and the three methods for aggregating neighbour plants were tested.

II.2.6.2 Materiel and methods

II.2.6.2.1 Field observations and features common to all simulations

Observations were taken from the INRA long-term field experiment at Dijon-Epoisses (Burgundy) (Chikowo *et al.*, 2009) where weed and crop variables (plant and seed densities, plant biomass, yield) were monitored from 1999 to 2012. Details can be found in (Colbach et al., 2016b).. This trial included ten fields with diverse crop rotations, ranging from intensive herbicide-based to herbicide-free systems and varying degrees of tillage and mechanical weeding. Weed flora was assessed, with species identification, plant density, above-ground biomass and seed bank measurements. Crop yield was also estimated.

II.2.6.2.2 Simulation plan

The simulation combined (1) the FLORSYS version (metamodelled or process-based), with (2) the voxel edge size (1, 4 or 7 cm) which determined the precision of plant location (all FLORSYS versions) and plant morphology (processed-based version). The FLORSYS-metaLight version moreover tested (3) different methods for aggregating neighbour plants (local, average, or mixed), and the process-based version tested (4) field sample areas (1m × 1 m, 3 m × 3 m, and 6 m × 3 m) with a 7-cm voxel. Unless otherwise indicated, field area was 6 m × 3 m. In total, nine scenarios were run with FLORSYS-metaLight version and six with the process-based one. Each of the ten field histories was simulated over 13 years, using the weather measured at the local weather station (INRA Climatik) and starting with the weed seed bank observed at the onset of the simulation. Each scenario was repeated ten times, to account for stochastic effects. Outputs were produced for all the days where observations were carried out in the fields. Simulations were run with a computer with two 2GHz processors and 16 Go RAM and their simulation time was recorded and averaged over repetitions for the different methods.

II.2.6.2.3 Evaluation criteria

Simulations with the metamodelled FLORSYS-metaLight and process-based FLORSYS were compared to field observations. Prediction error was assessed with the relative root square mean squared error of prediction (RRMSEP) corrected for variability in observations (due to measurement errors and intra-field variability) and simulations (due to stochasticity). The prediction error RRMSEP is described by Colbach *et al.* (2016b) and details can be found in annex A6 section 1. Outputs were analysed at two temporal scales, either corresponding to the individual observation dates (daily scale), or values averaged over the simulation (multiannual scale).

II.2.6.3 Results

II.2.6.3.1 Mean simulation time results

The simulation time of the process based FLORSYS for all cropping system tested, decreased with voxel edge size. When voxel edge size increased from 1 to 4 cm, simulation time was divided by approximately 20 (Figure II. 7.a). Increasing voxel size further from 4 to 7 cm decreased simulation time by an additional 43%. Increasing voxel size from 7 to 10 cm did not decrease simulation time any further. The slowest scenario took 259 times more time than the fastest. The fastest scenario with the 7 cm voxel edge size and 1 m² field sample took 4 minutes for a repetition of the 13 year long cropping system, compared to more than 18 hours for the slowest, with the 1 cm voxel and the 18 m² area. Conversely, simulation time increased with field sample area (annex A6 section 2). Increasing area from 1 to 9 m² multiplied the simulation time by approximately 8; doubling the field sample area to 18 m² only increased the simulation time by a further 10%. The field size multiplies the simulation time by 1.15 for every m² of a 13 year simulation

The simulation time of the metamodels remained stable for all voxel sizes, but it depended on the method for calculating neighbouring canopy variables (Figure II. 7.a). The metamodel with average neighbours was fastest and the one combining local and average neighbours was nearly as fast. Always using local neighbours made simulations considerably slower than with the process-based model, and simulation time even increased with voxel edge size. Indeed, in metamodels, the voxel determines plant location, and the larger the voxel is, the more plants are in each voxel. So when the metamodel searches through the voxels surrounding the target plant to compute the canopy inputs, it must compute more plants, which takes longer. Metamodels are considerably faster than the voxel-based model with small voxel edge sizes, *i.e.* 28 times faster for the metamodel with average neighbours.

II.2.6.3.2 Prediction error

In process-based simulations, the prediction error tended to slightly increase with increasing voxel size (Figure II. 7.b). The same trend was observed for prediction error in metamodelled simulations for larger voxels, suggesting a sensitivity to plant position which is less precise if the voxel is large. Simulations with a 1-m² field sample produced slightly better results than 18-m² and larger areas (*e.g.* for the multiannual weed density for all species summed, the RRMSEP for 1 × 1, 3 × 3 and 6 × 3 m² field samples was respectively 63, 113 and 116 $MJ \cdot MJ^{-1}$, details in annex A6 section 3), probably because it increased interspecific competition between weed species by increasing the probability of overlapping species patches. However, small fields potentially miss rare species, and overestimate interspecific competition in case of high weed densities.

Generally, the error was larger for metamodel-based vs. process-based simulations, particularly for weed plant biomass (Table II. 4), and it varied more among repetitions (annex A6 section 3). Error was often smaller than the variability in observations, pointing to a negligible prediction error, and making it impossible to calculate the relative variation in error for metamodelled vs process-based simulations (Table II. 4). Conversely, the metamodelled FLORSYS was better than the process-based one to predict multiannual weed plant densities.

Usually, metamodels using either local or average neighbours respectively had the smallest and largest errors, whereas the ones using both average and local neighbours were intermediate (Figure II. 7.b, Table II. 4). Regardless of the evaluation criteria, there was no model version (process or metamodel-based, approach for calculating canopy variables in metamodels) or precision level (voxel size, field sample area) that optimized the precision of all model outputs.

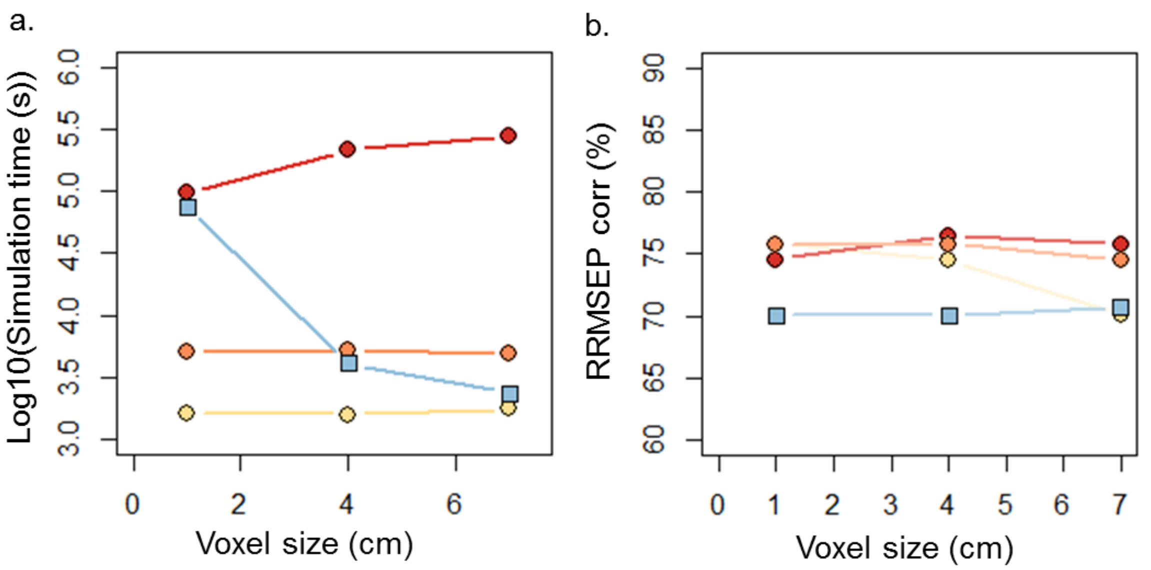

Figure II. 7: Simulation time (a) and prediction error (RRMSEP, b) of the daily weed seedbank by species for the different FLORSYS versions (squares: process-based, circles: metamodelled), neighbour aggregrating methods (dark red: local neighbours, light yellow: average, orange:mixed) and voxel edge sizes. (Floriane Colas © 2017)

II.2.7 Discussion

II.2.7.1 Simplify a complex process-based model

In this article, we presented a method to accelerate and simplify a complex process-based model. The paper is of interest for non-statisticians that want to metamodel complex models and are often baffled by statistical methods and how to apply them in their real-life complicated situation. Another particularity of our work was that we did not use the metamodel as such but integrated it into a larger model and evaluated the latter with independent field data, two steps that have been, to the best of our knowledge, rarely carried out in the past. The originality of the approach lies in (1) the choice of metamodelling only the most time-consuming part of the model (*i.e.* the 3D radiation interception submodel), (2) the choice of an innovative metamodelling method that handles correlated inputs and selects monomials, (3) the integration of the metamodelled submodel into the complex model and (4) the description of the nearby canopy with a limited number of inputs. This work did not compare different metamodelling methods (Villa-Vialaneix *et al.*, 2012) but provided practical guidelines for choosing and tuning metamodelling methods with respect to the complex model constraints (*e.g.* correlated inputs). It extended what was done in the previous paper (Gauchi et al., 2017) by showing the whole approach to simplify a complex model. Usually, metamodelling via polynomial chaos expansion allows to reduce the number of inputs in the model by setting the inputs to average values (Luo *et al.*, 2013; Rothenberg and Wang, 2016). Here, however, no input could be omitted because all either influenced radiation interception outputs directly or in interaction with other inputs. Usually, the whole model is metamodelled, avoiding the need to integrate the metamodel into a larger model (Cohen and Prinn, 2011; Luo *et al.*, 2013). Here, we metamodelled a single time-consuming submodel in order to accelerate the simulations of the whole FLORSYS model, and we thus had to integrate the metamodels, together with complementary equations, into FLORSYS. In SIRIUS (Brooks *et al.*, 2001), only a few equations were metamodelled. No implementation of the metamodel was necessary, as the metamodel was as good as the whole SIRIUS to predict the yield, which was the study's goal. The constraints of this approach were manageable for the 3D radiation interception of FLORSYS even though the number of inputs already needed to be decreased with the help of aggregated canopy variables. But these constraints probably make it impossible to apply this metamodelling method to bigger models like the whole FLORSYS with its many more inputs and correlations.

II.2.7.2 Experimental design for analysing a complex model

The numerical space filling design, LHS, is usually appropriate to explore the whole space of possible input combinations. It worked less well for the dynamic FLORSYS model, especially at the outer bounds of input ranges that were not sampled enough. This was particularly problematic at the onset of the plants' life-cycle (*i.e.* for small plants) as imprecise early predictions would amplify the next days' prediction errors, thus setting off the plants' growth and development in entirely the wrong direction. We improved the metamodelling by adding a metamodel for small plants only, but it was still insufficient for tiny plants, hence the simplified ecophysiological equations added to the model. The latter approach was acceptable here as these plants do not self-shade and are rarely shaded by neighbours. The inability of the metamodels to correctly predict small plants is explained by three combined reasons: (1) we chose a broad input range to cover all possible plant morphologies in the field, which reduced the probability of drawing many low input variables, (2) as the simulated plants were the combination of several inputs, the probability of drawing a small plant combining low values of all inputs (*e.g.* low height, width and leaf area) was even lower, particularly as the space filling design was balanced, (3) the equilibrated design also drew plants combining high values for some inputs with low values for others, resulting in biological impossible morphologies (*e.g.* tiny plants with an enormous leaf area) and non-logical output values. These plants had to be removed from the data set, decreasing even more the occurrence of extreme input values used in the metamodels. For models with a high number of inputs it is thus better to sample stepwise rather than have a unique sampling design. Surprisingly, adding correlation to inputs did not help to ensure many small and plausible plants.

II.2.7.3 Which method for which application?

To metamodel and perform a sensitivity analysis, many methods exists and many comparative studies exists, we decided to propose here the entire path when choosing and applying a method to transform a complex slow model into a faster meta-model. Polynomial chaos metamodelling accepts only a small number of inputs, hence the aggregation of neighbour plant variables into a small number of synthetic canopy variables. Unfortunately, the aggregation step, particularly the loop computing the plants close to the target plant, cancelled part of the simulation time saved thanks to the metamodels. Another way to speed up simulations would be to use the initial process-based interception submodel and to decrease the precision of the canopy structure by increasing the voxel edge size which governs the precision of plant locations and volumes as well as leaf distribution along plant height. We thus identified two ways to save simulation time, either by decreasing the precision of the plant and canopy description (process-based light interception submodel with a large voxel edge size) or that of the light interception (metamodelled submodel with a small voxel edge size).

With the decrease of precision comes a loss of quality, depending on the use of the model, choosing rapidity over precision can be appropriate, for example when needing quick simulations for workshops with farmers to co-design cropping systems (Bergez et al., 2010). The choice of the approach then depends on the target output (Table II. 5). When plant location is essential (*i.e.* when testing site-specific weed management, small sowing interrows, row-only nitrogen fertilization…) (Berge *et al.*, 2013), then a voxel size of 1 cm is needed, and the metamodelled FLORSYS-metaLight would allow faster and thus more simulations than the process-based FLORSYS. When both moderate simulation time and prediction quality are needed, the process based FLORSYS with a voxel size of 4 cm would be best. For cropping system tests, a quantitative precision is less essential as long as the management recommendations are correct (Renton, 2011).

II.2.7.4 Towards a larger simplification of FLORSYS

The simplification of the radiation interception was simpler for a single plant in a bare field, than for a plant located inside a canopy. Indeed, (1) the interaction with the canopy is harder to metamodel, and (2) the aggregated inputs simplify the canopy too much. Simplifying a complex model with many inputs is a principal issue when metamodelling. The complexity of the relationship between inputs is also an issue; for the 3D radiation interception, even small variations in outputs need to be accurately predicted, because small errors amplify over time as a result of the daily retro-acting interactions of light interception and growth. Metamodels based on polynomials are efficient to model all the single variations of the function (Hussain *et al.*, 2002), hence were adapted for the submodel. However, for a general trend, metamodelling based on polynomials cannot provide such a smooth answer. The present study suggests that the polynomial chaos expansion metamodelling, even when performed step by step and improved with expert knowledge, would be inadequate to metamodel the whole FLORSYS model, with its many and diverse inputs. To build a metamodel and estimate sensitivity indices, this method was the most suitable as there is no method that can handle many inputs, metamodelling and estimation of sensitivity indices at the same time. For a global emulation of FLORSYS, in order to synthesize and make available to farmers the knowledge comprised in FLORSYS to help with decision making (Wilkerson et al., 2002), other methods need to be considered. In that case, non-parametric methods can be helpful. Villa-Vialaneix *et al.* (2012) showed that metamodelling methods based on machine learning have good results for medium and large data sets. This is particularly true for Random Forests (Breiman, 2001) which provide the best trade-off between speed and accuracy. Moreover, non-parametric methods can tolerate heterogeneous data sets. This is crucial as FLORSYS with its numerous inputs precludes building a suitable experimental design as the one needed for the present approach.

II.2.8 Conclusion

To simplify a complex process-based weed dynamics model such as FLORSYS, we had to try different methods of sensitivity analysis to increase our knowledge on the 3D radiation interception submodel. Taking into account the correlations among inputs was essential and the tested range of inputs variation could not be reduced to make the simulation plan more efficient. The PLS regression combined with a polynomial expansion chaos model produced simple metamodels, especially with the method to select the most influential monomials. A combination of several experimental plans, metamodels and expert knowledge was needed to replace the initial process-based submodel. The complexity of radiation transmission and interception inside crop-weed canopies, particularly due to shading by neighbour plants, makes it difficult to directly predict radiation absorption at the plant scale. Simulation speed could be increased by decreasing either the accuracy of the plant and canopy description by reducing 3D definition in the process-based model, or the accuracy of the radiation interception by using metamodels. By evaluating the various approaches with independent field observations, we assessed the trade-off between prediction accuracy and simulation speed to identify which modelling approach was best, depending on the objective of the model use.

Acknowledgements

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Table II. 5 : Synthesis table to guide the choice of the best simulation method with the smaller RRMSEP depending on the goal and the target output.

Output	Species scale	Time step	Simulation goal	
			Farmer's workshops (fast simulations: 7 cm voxel, 6x3 m² field)	Site-specific weed management (precise simulations : 1 cm voxel, 6x3 m² field)
Weed density (plants.m^{-2})	By species	Day	Process-based	Process-based #
		Multiannual	Metamodelled with average neighbours	Metamodelled with average neighbours *
	Sum	Day	Process-based	Process-based #
		Multiannual	Process-based	Process-based
Weed biomass (g.m^{-2})	By species	Day	Process-based	Metamodelled with local + average &
		Multiannual	Metamodelled with local neighbours	Metamodelled with local + average neighbours
	Sum	Day	Process-based	Metamodelled with local + average &
		Multiannual	Metamodelled with local neighbours	Metamodelled with local + average neighbours
Seedbank (seeds.m^{-2})	By species	Day	Process-based *	Process-based
	Sum	Day	Metamodelled with local + average &	Metamodelled with local neighbours
Crop yield (T.ha^{-1})	By species	Day	Process-based	Process-based

Other methods that are also close in the RRMSEP value: * all of the other methods; & metamodel with average neighbour; # metamodel with local neighbours

II.3 Conclusion du chapitre

Dans cette partie est présentée une démarche pour accélérer et simplifier des modèles mécanistes complexes. Cette démarche tient compte d'entrées corrélées et permet, avec le même jeu de simulation, de faire de l'analyse de sensibilité et de la méta-modélisation. Les premières étapes de construction des méta-modèles sont assez génériques, mais les étapes d'implémentation dans le modèle global sont moins courantes car souvent les méthodes statistiques sont développées et testées sur des cas simplistes ce qui fait que les adaptations qui ont été nécessaires ici peuvent servir de guide pour aider à la méta-modélisation de modèles complexe. Au final, pour une précision moyenne en termes de placement et/ou description de plante, FLORSYS méta-modélisé n'est pas plus rapide que FLORSYS d'origine (FLORSYS voxélisé). C'est seulement pour une précision élevée que les méta-modèle à l'échelle de la plante plutôt qu'à l'échelle du voxel sont intéressants et permettent ainsi d'évaluer plus précisément des pratiques spatialisées telles que le désherbage de précision. Pour l'identification des pratiques culturales les plus influentes sur la dynamique adventice.

Nous avons ici réalisé la méta-modélisation avec un plan d'expérience régulier (c'est-à-dire le LHS). Ce plan est idéal pour des cas simples avec peu d'entrées mais est moins adapté aux situations avec plus d'entrées, comme le cas plus complexe des plantes cibles entourées d'autres plantes. Lorsque le nombre d'entrées augmente encore, il n'existe pas de méthode simple et complète pour échantillonner tout l'espace des combinaisons d'entrées possibles, tellement celui-ci est grand. Nous ne pouvons donc utiliser une analyse de sensibilité classique avec un plan d'expérience régulier pour développer l'outil d'aide à la décision souhaité car celui-ci nécessite une analyse de sensibilité de FLORSYS tout entier pour identifier les techniques culturales les plus influentes sur la flore adventice suivi d'une méta-modélisation de FLORSYS. C'est pourquoi dans le chapitre suivant, nous allons développer une autre approche pour s'affranchir des limites de l'analyse de sensibilité classique.

Chapitre III : Analyse de sensibilité globale de FLORSYS pour identifier les techniques les plus influentes sur les impacts des adventices

TORTURER FLORSYS AUTANT QU'IL NOUS TORTURE

III.1 Objectifs de ce chapitre

Pour développer un outil d'aide à la décision pour la gestion intégrée des adventices, nous avons voulu, à l'étape précédente, accélérer le modèle pour faire de nombreuses simulations. **La deuxième étape et l'objectif de ce chapitre consistent en l'identification des techniques culturales les plus adaptées à la gestion intégrée des adventices.** Pour cela, un grand nombre de systèmes de cultures doit être simulé afin de pouvoir faire une analyse de sensibilité. Seulement, les méta-modèles créés à l'étape précédente ne permettent pas d'augmenter fortement le nombre de simulations réalisables. Par conséquent, il est impossible d'utiliser des plans expérimentaux classiques comme ceux utilisés au chapitre précédent pour cette analyse de sensibilité. Nous avons donc proposé un nouveau type de plan adapté à nos contraintes, tirant parti des simulations déjà existantes de systèmes de culture réalistes et de les compléter à la fois par des systèmes contraints dans lesquels nous avons modifié une technique clé et par des systèmes de cultures aléatoires. Ces systèmes complémentaires ont comme objectif de décorréler des techniques souvent rencontrées ensemble dans la pratique agricole. Du fait de ce plan expérimental, nous devons également adapter les méthodes d'analyses des données car nous avons vu au chapitre précédent que les méthodes plus classiques, comme les indices de sensibilités par la méthode Sobol-Saltelli, ne sont pas adaptés aux cas trop complexes. Heureusement, le domaine de la fouille de données possède des méthodes permettant la hiérarchisation des variables pour des données d'origines variées sur des entrées non paramétriques. Ce type de méthode nous permet d'analyser un modèle sans en connaître la structure, avec des entrées corrélées entre elles, comme le sont les variables de description du système de culture, mais requiert un nombre important de données.

L'identification des techniques culturales les plus importantes pour la gestion des adventices permettra de conseiller aux agriculteurs et conseillers agricoles les techniques à modifier en priorité dans un système de culture. Afin de s'assurer de la robustesse des conseils qui seront issus de simulations, nous avons voulu évaluer les prédictions des modèles crées, les forêts aléatoires, en les comparant avec un jeu de données de systèmes de culture provenant du réseau DEPHY. Ces systèmes de culture présentent en plus l'avantage de s'inscrire dans une démarche de réduction d'usage d'herbicides, ce qui coïncide avec les objectifs de gestion intégrée de l'outil d'aide à la décision. Pour le conseil, l'identification statistique des techniques culturales les plus influentes n'est suffisante, car il faut aussi que l'outil parle aux utilisateurs et qu'ils puissent manipuler les variables avec lesquelles ils sont familiers. C'est pourquoi la dernière étape de notre démarche implique les futurs utilisateurs, pour trier et sélectionner des variables d'entrée décrivant les systèmes de culture de façon explicite et pertinente.

Dans cette partie, nous utilisons une combinaison d'arbres de régression et de classification, ainsi que de forêts aléatoires pour identifier les techniques culturales les plus influentes et l'effet de la combinaison de ces techniques sur la gestion des adventices en analysant des indicateurs d'impacts des adventices sur la production agricole, du niveau d'usage d'herbicides ainsi que des services écosystémiques rendus par la flore adventice. Le travail se structure en quatre étapes :

- Application de forêts aléatoires à toutes les simulations de systèmes de culture pour hiérarchiser les techniques les plus influentes en termes d'impact de la flore adventice ;
- Classification de systèmes de culture selon leur situation de production (contexte pédoclimatique) pour, par la suite, pouvoir intégrer les effets des adaptations locales des techniques culturales et leurs interactions ;
- Construction d'un arbre de décision dans chaque situation de production pour identifier les combinaisons de techniques permettant d'atteindre une combinaison d'objectifs :

- Double évaluation des forêts aléatoires, par validation croisée sur le jeu de données de systèmes de culture d'apprentissage, puis par comparaison à un jeu de données indépendant. Ce dernier est composé de systèmes de culture innovants à faible niveau d'usage d'herbicides afin de tester la qualité de prédiction des forêts aléatoires dans son futur domaine d'application.

Dans les différentes étapes, les simulations réalisées avec FLORSYS jouent de rôle de réalité ou expérimentations virtuelles, d'abord pour analyser et modéliser les effets des techniques culturales sur les impacts de la flore adventice, puis pour tester la performance des forêts aléatoires en tant que prédicteur des effets de ces techniques culturales.

Cette partie a fait l'objet d'un article qui sera soumis à European Journal of Agronomy :

Colas, F., Villerd, J., Pointurier, O., Colbach, N. (in preparation) Which cultural techniques drive weed dynamics and impact? Sensitivity analysis of a cropping system model to support integrated weed management.

III.2 Which cultural techniques drive weed dynamics and impact? Sensitivity analysis of a cropping system model to support integrated weed management

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Abstract

Redesigning more sustainable cropping systems is essential, but to be sustainable without crop production loss due to weeds is a challenge. It can be attained by judiciously combining all cropping techniques, favouring agroecological processes over herbicide use. To assess the effects of all cropping techniques combined, in the long term, computer models are essential. FLORSYS is a process-based "virtual field" simulating the effects of cropping systems on weed dynamics as well as on crop production and weed-related biodiversity, thus making possible a multiobjective design of cropping systems. FLORSYS is, however, slow and difficult to use, which makes it unsuitable for advisors and crop managers. In order to provide biophysical knowledge to feed into a decision-support system for advisors and crop managers, we identified the key cropping techniques to predict their interacting effects on weed dynamics and the resulting impact on crop production and biodiversity. For this purpose, data mining methods were used on simulations of (1) realistic cropping systems, (2) the same realistic cropping systems but without herbicides or without tillage, to decorrelate techniques that often occur together, and (3) random cropping systems to continue the decorrelation of techniques and explore ranges and combinations that do currently not occur in fields. Random forests were applied to the simulated output, showing that tillage and herbicide strategies were the main drivers of the tradeoff between crop production and ecosystem services. Decision trees were built, first to discriminate contrasting production situations, and then to identify combinations of cropping techniques for reaching a given combination of weed impact goals. Finally, the prediction ability of the random forests was evaluated twice, via cross-validation on the learning data set and by comparison to the weed impact simulated with FLORSYS for the innovative herbicide-sparse cropping systems of the French DEPHY farm network. The forests were shown to satisfactorily rank cropping systems in terms of most weed impacts but need to be completed with missing innovative cropping techniques. Decision trees and random forests are inseparable as a basis for a future decision support tool for advisors and crop managers, with (1) random forests pinpointing the techniques to change first, (2) the decision trees showing how to combine techniques in different production situations, (3) random forests allowing a quick and easy evaluation of the major changes proposed by users.

Highlights

- Tillage and herbicide use are the main drivers of the tradeoff between crop production and ecosystem services.
- Random cropping systems combined with realistic cropping systems gave realistic results.
- To withdraw advices to manage cropping systems, the combined use of decision trees and random forests are necessary.
- User opinions are now essential to fully develop a decision-support system

Keywords

Weeds, random forest, classification and regression trees, random cropping system, DEPHY, agroecology

III.2.1 Introduction

Crop management intensification of the last 50-60 years increased negative impacts on ecosystems such as water eutrophication or bumblebee decrease (Matson et al., 1997; MAE, 2005). Solutions to produce food without destroying ecosystems are needed, either by redesigning the food systems, the land use or the cropping systems (Lamine, 2011; Muller et al., 2017). Weeds are the main threat for crop production (Oerke, 2006) and herbicides are currently the simplest and most efficient way to manage weeds. However, herbicides are a threat to human health and environment (Wilson and Tisdell, 2001) needing a reduction in their herbicide use (Directive 2009/128/CE; Ecophyto, 2017) without crop production loss is possible if all other cropping techniques are judiciously combined (Colbach and Cordeau, 2018b). Many agroecological techniques can be implemented to design sustainable cropping systems less dependent on pesticide use among which novel non-chemical curative solutions such as. antagonists of crop pests or natural pesticides, or preventive measures resulting from a combination of many partially efficient techniques such as crop choice and rotation, tillage sowing dates etc. (Bonin, 2009; Liebman and Gallandt, 1997; Wezel et al., 2014). As biological or natural measures are not yet available for weeds, agroecological and integrated weed management must focus on recombining existing cropping techniques. This is a challenge because the necessary cropping system modifications have interacting and long-term effects on both weed dynamics and their subsequent impact on crop production, by modifying environmental conditions as well as above and below-ground vegetation in the short and long term (Bàrberi and Lo Cascio, 2001; Cardina et al., 2002; Fried et al., 2008; Menalled et al., 2001). Moreover, weeds provide essential ecosystem services as wild plant biodiversity and trophic resources for pollinators (Marshall et al., 2003; Petit et al., 2011).

Cropping systems can be designed by different methods: (1) agronomical diagnosis based on surveys and in farm experiment to identify the main effects of cropping techniques (Doré et al., 2008), (2) expert design and prototyping of cropping systems that will be tested in farms and adjusted if necessary (Lançon et al., 2007), and (3) computer simulations which are much faster and test a wider range candidate systems (Bergez et al., 2010; Ould-Sidi and Lescourret, 2011). The latter is particularly adapted in the present case where we must combine many interacting and highly variable factors while aiming to reconcile multiple goals. Among current weed dynamics models, FLORSYS (Colbach et al., 2014; Gardarin et al., 2012; Munier-Jolain et al., 2013) (Mézière et al., 2015d) answers best to our requirements in terms of interactions, scales and impacts (Colbach, 2010; Colbach et al., 2014a). This process-based "virtual field" simulates the effects of cropping systems on weed dynamics as well as on crop production and weed-related biodiversity, thus making possible a multiobjective design of cropping systems (Colbach *et al.*, 2017). FLORSYS is, however, a research model, slow and difficult to use, which makes it unsuitable for advisors and crop managers (Rose et al., 2016).

To widen the range of its users, FLORSYS must be simplified. A classical way is to run a sensitivity analysis to identify which inputs the most influence the outputs (Saltelli et al., 2008), followed by metamodelling to produce a faster and simpler emulator of the original model (Brooks et al., 2001; Marie and Simioni, 2014). However, the more complex the model is, the harder it is to perform the sensitivity analysis and to metamodel (Colas et al., Sumitted). An alternative is data mining which provides non-parametric methods, allowing numerous and interacting inputs as long as the learning data set is large enough (Villa-Vialaneix et al., 2012). Classification and regression methods such as CART (Breiman et al., 1984) produce a decision tree highlighting the combinations of cropping techniques leading to different performance levels. However trees are sensitive to changes in the learning dataset and may be subject to overfitting, decreasing predictive performance. Their improvement, random forests (Breiman, 2001), combine many trees, resulting in a more stable model that can be used as a predictor, hence an emulator of FLORSYS. Being most robust, random forests provide more accurate importance of values for inputs to rank the cropping techniques depending on the resulting weed dynamics and impacts. The combination of both trees and random forests would synthesize and emulate the biophysical knowledge comprised in FLORSYS in the shape of a simpler and faster tool that could be used by cropping managers.

In this work, our objective was to (1) identify the key cropping system techniques and to (2) predict their interacting effects on weed dynamics and the resulting impact on crop production and biodiversity in order to (3) provide biophysical knowledge to feed into a decision-support system for designing sustainable cropping systems. For this purpose, we used data mining methods, first a random forest was fitted to pinpoint the most influential cropping techniques and to predict their impact on weed impact indicators. Decision trees were used as a visual guide to determine which cropping techniques should be combined to reach a given weed impact target. To account for local constraints and integrate interactions of cropping systems with pedoclimatic conditions, the trees were built for contrasting production situation (Aubertot and Robin, 2013a; Lechenet et al., 2016). Finally, the previously fitted random forest was evaluated to check whether its predictions led to the right decisions, i.e. whether the cropping systems were correctly ranked according to weed impacts on crop production and biodiversity. As our ultimate goal was to design innovative cropping systems relying on no or few herbicides, the testing data set consisted of contrasted real-life cropping systems of the French DEPHY farm network (Cellule d'animation nationale DEPHY Ecophyto, 2016; Lechenet et al., 2016) monitoring farms aiming to reduce pesticide use.

III.2.2 Materials and methods

III.2.2.1 Principle

To determine which cropping techniques drive weed impacts on crop production and biodiversity we needed to rank the cropping techniques via a sensitivity analysis of the FLORSYS model. Because of the numerous variables needed to describe cropping systems, the need to run simulations over many years, and the time these simulations take, it was impossible to use a large scale-filling method. Instead, we started with an existing database of real-life cropping systems that had already been simulated with FLORSYS and completed these with contrasting cropping systems. Part of the latter were created deterministically, by running the real-life systems with one major change (i.e. without herbicides or without tillage), to decorrelate techniques that often occur together (e.g. glyphosate is often sprayed during fallow in fields with little or no tillage). Other additional systems were based on randomly chosen techniques to continue the decorrelation of techniques and explore ranges and combinations that do currently not occur in fields. The results of the simulations were used as a learning set to build a random forest that identified the key techniques that drive weed impacts. The prediction quality of the random forest model was then evaluated using real-life integrated cropping systems of the DEPHY-FERME network (Cellule d'animation nationale DEPHY Ecophyto, 2016) simulated with FLORSYS as a test set. To provide advice for crop managers and guide them during cropping-system design, we also built decision trees to highlight combination of cropping techniques to achieve various goals in terms of crop production and biodiversity. These were built for different production situations to include interactions between pedoclimatic conditions and management techniques and provide advice adapted to the local conditions of crop managers.

III.2.2.2 The virtual field model FLORSYS

III.2.2.2.1 The model

FLORSYS (Colbach et al., 2016b; Colbach et al., 2014b; Colbach et al., 2014c; Gardarin et al., 2012; Mézière et al., 2015d; Munier-Jolain et al., 2014; Munier-Jolain et al., 2013) is a mechanistic model predicting weed dynamics in a virtual field where detailed cropping systems can be tested with different pedoclimates over several years or decades. Management operations and environmental variables influence the life cycle of crops and weeds which predicts, for each day, the density, biomass, stage or status of the soil seed bank, germinating seeds, emerged plant and seed production. For instance, weed plant survival probabilities are calculated deterministically depending on management operations (tillage, herbicides, mechanical weeding, mowing, harvesting), biophysical environment as well as weed morphology and stage; the actual survival of each plant is determined stochastically by comparing this probability to a random probability.

The evaluation of FLORSYS with independent field observations from several French regions showed that crop yields, daily weed species densities and, particularly, densities averaged over the years were usually predicted satisfactorily (Colbach et al., 2016b). Most importantly, situations were ranked correctly by the model, hence answering to our main request, i.e. allowing us to compare one cropping system vs others. Further details can be found in annexe A7.

III.2.2.2.2 FLORSYS inputs

FLORSYS requires many and detailed inputs to simulate cropping systems. The virtual field environment is described by the daily weather, the latitude and soil characteristics. The weed flora at the onset of the simulation is described by the initial soil seed bank. Seed banks are notoriously difficult to assess, and FLORSYS thus usually starts with regionalized seed banks estimated from regional weed flora surveys, method deemed satisfactory during model evaluation (Colbach et al., 2016b).

A cropping system is described by the detailed list of management operations applied to the field. Operations are defined in terms of dates of occurrence and options, e.g., a sowing operation is described by the number, species and varieties of sown crops need, the sowing density and depth of each, the sowing pattern (orientation, rows vs broadcast, interrow width, sowing precision).

III.2.2.2.3 Weed impact indicators as outputs

FLORSYS estimates the crop and weed density and biomass each day of the simulation depending on all cropping techniques. These variables are translated into weed impact indicators to simplify the comparison of cropping systems (Colbach et al., 2017b; Mézière et al., 2015c). Here, we chose to investigate those weed impact indicators that were shown to be most useful to farmers and crop advisors in surveys and workshops that we conducted in another study (chapitre IV, Colas *et al.*, in prep. a). These indicators, chosen with farmers and crop advisors, mostly assessed weed harmfulness for crop production, which we completed with an equivalent number of ecosystem service indicators as well as herbicide use intensity to consider the trade-offs among weed impacts. The focus on these trade-offs is essential to provide knowledge and tools for designing agroecological weed management strategies.

The ecosystems services consisted of five biodiversity indicators (wild plant species richness and evenness (Pielou), trophic resources for birds, granivore carabids and domestic bees); and four harmfulness indicators developed with farmers (grain yield loss, harvest pollution, harvest difficulties and field infestation). If grassland or biomass crops occurred in a cropping system, energy yield ($MJ.ha^{-1}$) and energy yield loss were computed instead of grain yield loss due to weeds. Herbicide use intensity was assessed in the shape of Treatment Frequency Index for herbicides (TFIh).

III.2.2.3 The cropping systems

III.2.2.3.1 Cropping systems for exploration and model development ("learning set")

Numerous and contrasted cropping systems are needed to identify the key cropping techniques that drive weed impacts. To cover large ranges of input values and explore both common and uncommon combinations of these techniques, we combined three sources of cropping systems: (1) real-life cropping systems from diverse regions, (2) the same excluding either herbicides or tillage to disentangle confusing effects of frequently associated techniques (e.g. fallow glyphosate and direct sowing), (3) systems based on randomly chosen techniques to further decorrelate techniques.

III.2.2.3.1.1 Real-life cropping systems

Data available from past simulation study was used, representing 200 diverse cropping systems originating from farm surveys, the Biovigilance-Flore network, expert opinion, cropping system trials, crop advisors and scientists (Colbach and Cordeau, 2018b). The cropping systems covered six French regions and a Spanish one, with diverse techniques from intensive to organic systems and from no-till to tillage intensive. Rotations were mainly based on cereals (wheat, barley, maize) and oilseed rape, with a smaller proportion of legumes (lucerne, faba bean etc), non-legume broadleaved crops (sunflower, flax etc) and temporary grassland, with proportions and crop species depending on regions (Table III. 1).

III.2.2.3.1.2 No-till and herbicide-free cropping systems

Two other series of cropping systems were based on this set of cropping systems, by removing either all tillage operations or all herbicides, without any other change in techniques to compensate for these removals. These systems aimed to discriminate the effects of herbicides or tillage on weeds and crop production from effects of changes in cultural techniques that usually accompany changes in herbicide use or tillage intensity.

III.2.2.3.1.3 Random cropping systems

To continue to discriminate effects of cultural techniques without the cropping system changes that usually accompany these changes and to explore ranges and combinations that do currently not occur in fields, random cropping systems were created. Variables were randomly selected in a probable range and comprised:

- region (defined by pedoclimate and initial weed seed bank), choosing among the 7 regions of section III.2.2.3.1.1;
- crop rotation, in terms of length, crop succession and mixtures, including cash and cover crops as well as temporary grassland;
- cropping techniques (tillage, herbicide application, mechanical weeding, irrigation, sowing, harvesting) in terms of number, dates and options of operations (e.g. tool, depth and speed for tillage; orientation, interrow, density, depth and precision of sowing),

A total of 5000 cropping systems were created, eventually resulting in 3043 systems that could be simulated with FLORSYS.

III.2.2.3.2 Cropping systems for model evaluation ("test set")

The random forest models and decision trees developed from the cropping systems of the previous section (section III.2.2.3.1) were tested with real-life cropping systems of arable-crop farms and crop-livestock farming from 21 regions recorded in the French DEPHY-FERME farm network. This network is part of a French ministerial plan aiming at reducing the use of pesticides (Ecophyto plan) and consists of more than 3000 farms, the practices of which are recorded in the Agrosyst database (Cellule d'animation nationale DEPHY Ecophyto, 2016). A computer routine was developed to extract cropping system data from Agrosyst and to fill input files for FLORSYS. Conversion rules were needed as both systems have totally different designs. Details can be found in (Colbach et al.). For instance, Agrosyst records annual crop proportions per cropping systems which had to be translated into chronological crop sequences with associated techniques for FLORSYS. Actual crops or tillage tools were sometimes replaced by the most similar species and tools parameterized in FLORSYS. Inputs that were unavailable (e.g. interrow) or missing (e.g. sowing density of 0 seeds/m²) in Agrosyst were imputed based on expert knowledge, literature, the existing database (see section III.2.2.3.1.1) or from consistent Agrosyst data. Regional initial weed seed banks were determined from the relative species densities recorded in the Biovigilance Flore database (Fried et al., 2007), using a method developed when FLORSYS was evaluated (Colbach et al., 2016b). Soil parameter files were provided by the STICS team (Huard and Ripoche, 2016; Queyrel, 2014; Ruget and Lebas, 2017) and completed when necessary with soil texture data from the Gis Sol database (Gis Sol, 2018). Weather data was extracted from the Climatik database

(AgroClim, 2018). A total of 659 Agrosyst cropping systems were simulated with FLORSYS (Table III. 1).

III.2.2.3.3 Simulation plan

In each series, each cropping system was simulated over 27 years, repeating the basic rotational pattern (e.g. oilseed rape/wheat/barley) over time. Each system was repeated 10 times with 10 different weather series consisting of 28 randomly chosen weather years from its region of origin (or region determined randomly for the random cropping systems), using the same 10 series for each system of a given region. These weather repetitions allowed us to assess the robustness of the cropping systems to weather. Cropping systems were simulated as a list of operations with fixed operation dates, and not decision rules that adapted operations to weather, environmental conditions and weed flora. This simulation plan allowed us to separate the effects of cultural techniques on weeds from the reciprocal as well as from weather effects on techniques.

III.2.2.4 Synthetic cropping system descriptors

The number and level of detail of the FLORSYS inputs are too high for sensitivity analysis methods. Thus, we transformed these inputs into synthetic cropping system descriptors that are proxies for meta-decision rules. These descriptors were computed either at the level of the cropping system (e.g. average tillage frequency or proportion of spring crops in the rotation) or per cropping period per crop (e.g. average wheat sowing date, average tillage frequency in oilseed rape) (106 descriptors for the cropping system and 60 × 9 crops for the descriptor per crops; full list and description in 0Appendix). A cropping period lasted from previous cash crop harvest to the harvest of the current crop. Only major crop species were kept for this second level (e.g. wheat, maize, pea) to limit the number of descriptors, no descriptors dedicated for mixed crops was kept.

The production situation of a field is the environment and the socio-economic drivers that impact the cropping practices of farmers (Aouadi et al., 2015; Aubertot and Robin, 2013a). The production situations of the cropping systems were discriminated here only based on pedoclimate. The 65 relevant variables (annex A7) took into account physico-chemical soil properties (e.g. gravel content, mass content of organic nitrogen) and weather (e.g. mean temperature, heat intensity, rainfall frequency, sum of daily precipitation, average radiation) for different seasons (e.g. spring and summer, winter only).

III.2.2.5 Statistical analyses

To find out which cropping practice are the drivers of weed impacts we started with an uncertainty analysis, investigating correlations among inputs as well as the relations between inputs and outputs in the learning data set of section III.2.2.3.1. Then, a random forest was fitted, providing variable importance results on the cropping descriptors that rank the descriptors according to their impact on outputs. The prediction error of the random forest was assessed, using DEPHY cropping systems of section III.2.2.3.2 as test data. To guide the design of novel weed management strategies, we built decision trees to highlight the combinations of cropping techniques leading to various levels of weed impact. All statistical analyses were carried out using the R software (R Core Team, 2017) and the various packages used are detailed in the following sections.

III.2.2.5.1 Correlation analysis and output selection

The distribution of the output variation against the input variation characterized via violin plots show the distribution of all indicators values. As ten indicators can be too much to handle when analysing the results, especially for cropping advice, we propose two solutions to decrease the number, looking at correlations between the indicators. Weed impact indicators were averaged over the simulation length and these multi-annual indicator values were analysed with a principal component analysis (PCA), using the FactoMineR package (Le et al., 2008), to identify the correlations and trade-offs among indicators. Spearman correlations were calculated among outputs to help understanding the links among indicators. They also identified highly correlated outputs, which allowed us to analyses fewer indicators in the next steps. Variability in inputs and outputs was characterized with minimum, mean, median, and maximum values.

Subsequently, we considered different indicator profiles corresponding to different farming visions: (1) agroecology profile, aiming at reconciling crop production and ecosystem services, (2) productivity profile, aiming at optimizing the crop productivity hence avoiding any harmfulness from weeds and (3) integrated weed management (IWM) profile aiming at optimizing productivity and low herbicide use. Indicators in each profile were selected in order to match the aim of the profile and not to be too redundant based on the principal component analysis and the correlations among indicators. It resulted in the following indicator selection: (1) agroecology profile, with the 10 previously described indicators, (2) productivity profile, with grain yield loss, field infestation and harvest pollution and (3) integrated pest management (IPM) profile with herbicide intensity use, and grain yield loss.

III.2.2.5.2 Random forests and decision trees

To identify and rank the most important cropping system descriptors driving the weed impact indicators, we used the data mining method of classification and regression trees (shortened to decision trees as we used a combination of regression and classification for our trees) (Breiman et al., 1984) and their improved version for prediction, the random forest (Breiman, 2001). The tree branches consist of combinations of cropping system descriptors leading to various performance levels ("leaves") in terms of weed impact and can thus be used as decision trees. To avoid overfitting, the trees where pruned using the 1-standard error rule of the overall best tree size. We used sequential partitioning to build separate trees adapted to contrasting production situations. A first classification was run on production situation variables to identify contrasting production situations, followed by a series of classifications on cropping system descriptors for each production situation (Ouellette et al., 2012). The two-step approach was performed for each of the three use profiles, i.e. "productivity", "IWM" and "agroecology". As tree leaves can consist of a combination of multiple indicators we used the mvpart package (Glenn De'ath, 2014) that implements multivariate classification and regression trees.

Table III. 1: Overview of the cropping systems used as a test data set, for each region of the DEPHY network. N is the number of cropping systems in the region

Region	N	TFIh	Tillage frequency	Spring crop proportion	Main crops
Alsace	16	[0.4, 2.6]	[2, 9.9]	[0.3, 1]	Maize (53%), Wheat (27%)
Aquitaine	26	[0, 3.5]	[0.5, 6]	[0, 1]	Maize (56%), Wheat (12%), Sunflower (12%)
Auvergne	26	[0.3, 2.7]	[0.2, 6.9]	[0, 1]	Wheat (29%), Maize (22%), Fescue_Ryegrass_Clover (14%), Barley (12%)
Basse-Normandie	28	[0, 3.1]	[1.8, 15.3]	[0.1, 1]	Maize (30%), Wheat (29%), Barley (11%)
Bourgogne (Burgundy)	14	[1.3, 5.2]	[1, 5.7]	[0, 0.7]	Wheat (30%), Oilseed rape (23%), Barley (18%), Maize (11%)
Bretagne	73	[0, 4.9]	[0, 18.9]	[0, 1]	Maize (37%), Wheat (31%)
Champagne-Ardenne	15	[1.3, 4.2]	[0.7, 6.3]	[0, 0.5]	Wheat (31%), Oilseed rape (31%), Barley (22%)
Centre	35	[0.7, 6.2]	[0.6, 12.3]	[0, 0.6]	Wheat (31%), Oilseed rape (26%), Barley (22%)
Franche-Comte	11	[0.9, 3.4]	[0, 4]	[0, 0.7]	Wheat (29%), Barley (26%), Maize (20%),
Haute-Normandie	14	[1.1, 2]	[1.2, 3.1]	[0, 0.6]	Wheat (25%), Oilseed rape (20%), Flax (20%), Sugar beet (11%)
Ile-de-France	69	[0, 5.5]	[0, 10.4]	[0, 1]	Wheat (26%), Maize (15%)
Limousin	14	[0.4, 2.4]	[0, 2.8]	[0, 0.5]	Wheat (20%), Fescue_Ryegrass_Clover (18%), Maize (18%), Barley (16%), Triticale (14%)
Lorraine	40	[0.3, 11.8]	[1.3, 6.8]	[0, 0.7]	Wheat (33%), Barley (28%), Oilseed rape (26%)
Languedoc-Roussillon	6	[1.4, 2.6]	[2, 3]	[0.4, 0.5]	Wheat (43%), Sunflower (43%)
Midi-Pyrenees	49	[0, 3.5]	[0.5, 8]	[0, 1]	Wheat (34%), Maize (23%), Sunflower (19%)
Nord-Pas-de-Calais	11	[0, 6.6]	[0.8, 5.2]	[0, 0.5]	Wheat (30%), Maize (16%), Sugar beet (14%), Barley (14%), Oilseed rape (11%)
PACA	6	[0.8, 2.3]	[0, 3.5]	[0.2, 0.5]	Wheat (24%), Sunflower (24%), Oilseed rape (14%), Maize (14%), SOJA (14%)
Poitou-Charentes	31	[0, 3.4]	[0, 5.2]	[0, 0.7]	Wheat (25%), Sunflower (15%), Maize (13%), Oilseed rape (12%)
Picardie	12	[1.7, 6.5]	[0.2, 7.5]	[0, 0.5]	Wheat (28%), Oilseed rape (21%), Sugar beet (16%), Barley (16%)
Pays-de-la-Loire	106	[0, 6]	[0, 23.2]	[0, 0.7]	Wheat (24%), Maize (24%), Fescue_Ryegrass_Clover (11%)
Rhone-Alpes	57	[0, 8.7]	[0, 15.2]	[0, 1]	Maize (29%), Wheat (24%), Barley (12%)

Random forests was fitted using the rfsrc package (Ishwaran and Kogalur, 2017). They provided variable importance (VIP, Breiman-Cutler permutation (Breiman, 2001)) values for each indicators, which we averaged to get a synthetic value, allowing us to rank cropping system descriptors depending on their impact on all indicators. Descriptors were first ranked for each indicator, and again using the mean of all indicators (after rescaling, see below) to get a global view of the importance of the descriptors. Forests were also used as predictive models, directly and rapidly calculating weed impact indicators from cropping system descriptors, contrary to the lengthy FLORSYS simulations. To make the results corresponding to the different indicators comparable and avoiding biases due to indicators with larger ranges of variation, all indicators were scaled to a [0, 1] range based on their minimum and maximum values. Once the tree and forest models were fitted, outputs were backtransformed to their original units.

The predictive performance of decision trees was assessed by the mvpart built-in cross validation error (from the rpart package Atkinson, 2018) on the learning set. The random forest model was evaluated twice, first, its fitting to the observed (i.e. simulated with FLORSYS) data, during its construction from the learning data set, called explained variance index in (Breiman, 2001) was computed as:

Eq.III. 1:

$$Explained\ variance = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2}$$

With y_i the observed values, $\hat{y}_i$ the values predicted by the random forest and $\bar{y}$ the mean of the observed data.

Finally, the random forests were evaluated, to check whether its predictions led to the right decisions, i.e. whether the cropping systems were correctly ranked according to weed impacts on crop production and biodiversity, using the DEPHY data as a test set. In addition to testing the models with independent data, this allowed testing the relevance of the model partially based on randomly constructed cropping systems for real-life cropping systems based on agronomic reasoning, with some located in regions other than those used for model building. Cropping system data were fed to the random forests to predict indicator values which were compared to the values simulated with FLORSYS which were considered here as "virtual observations". The modelling efficiency (ME) (Mayer and Butler, 1993) which correspond to the explained variance in (Table III. 2) was computed, with the virtual observations being the DEPHY simulations. The closer to 1 the modelling efficiency is, the closer the observed data are to the simulated data in terms of absolute values. It becomes negative when the assessed model is worse than a model that systematically returns the mean. The prediction error was estimated via the root mean squared error predictor RMSEP (Wallach and Goffinet, 1987, 1989):

Eq.III. 2:

$$RMSEP = \sqrt{\frac{\sum(y_i - \hat{y}_i)^2}{N}}$$

With N the number of observations. The previously fitted random forest was evaluated to check whether the cropping systems were correctly ranked according to weed impacts on crop production and biodiversity. The ranking ability of the random forest was assessed via Pearson correlations:

Eq.III. 3 :

$$r = \frac{\sum(y_i - \bar{y})(\hat{y}_i - \bar{\hat{y}})}{\sqrt{\sum(y_i - \bar{y})^2}\sqrt{\sum(\hat{y}_i - \bar{\hat{y}})^2}}$$

The closer the Pearson r is to 1, the closer the predicted values are to the observed values in terms of relative values. Finally, the Spearman correlation coefficient was calculated, using ranks of observed and predicted values in Eq.III. 3 instead of actual values. The closer the Spearman r is to 1, the more similarly the observed and predicted values are ranked.

III.2.3 Results

III.2.3.1 Which weed impact indicators to illustrate the trade-offs between crop protection and ecosystem services?

A Principal Component Analysis (PCA) was run on the weed impact indicators simulated with FLORSYS in the learning data set to identify trade-offs among impacts and to eliminate redundant indicators. All indicators except herbicide intensity use were located in the same half of the PCA correlation circle (Figure III. 1). Biodiversity indicators were clustered in two groups: (1) the three indicators in the top right part of the circle are based on weed plant densities (including flowering plants), i.e. wild plant species richness and evenness (Pielou) as well as bee food offer, (2) the two indicators in the bottom right part of the circle are based on seed densities, albeit depending on different seasons and qualities for carabids and birds.

The four harmfulness indicators were all clustered along the first PCA axis, which is consistent with their depending on the same weed state variable (i.e. plant above-ground biomass), in contrast to biodiversity indicators. Herbicide use intensity was badly represented in the correlation circle defined by the first two PCA axes and thus little correlated to the other indicators (correlation plot in annex A7). The bee food offer was the biodiversity indicator the most correlated to harmfulness indicators, generally increasing with increasing harmfulness, particularly field infestation, yield loss and harvesting pollution (Spearman correlation coefficients of 0.53, 0.31 and 0.29 respectively, see details in annex A7). Consequently, it would be difficult to find cropping systems that reconcile bee food offer and reduced weed harmfulness for crop production. Reconciling reduced herbicide use and other ecosystem services with crop production should be easier.

To check whether FLORSYS responded to the variation in inputs, distributions of outputs were analysed (Violin plot in annex A7). These showed that outputs greatly varied among cropping systems and regions and that these variations largely exceeded variations due to stochasticity in FLORSYS. For instance, yield loss varied from -100 to 100% here, with a standard-error of 25 %, whereas in the real-live cropping systems of section III.2.2.3.1.1, the difference between two successive series of simulations with a change in inputs were usually below 8% (Colbach and Cordeau, 2018b). There are usually around 14 species in the crop succession with most of the cropping systems having between 5 and 24 weed species. The distribution of the indicators is wide and covers the possible variation range defined for the indicators, knowing which outputs drives more the variation is the next step after this uncertainty analysis.

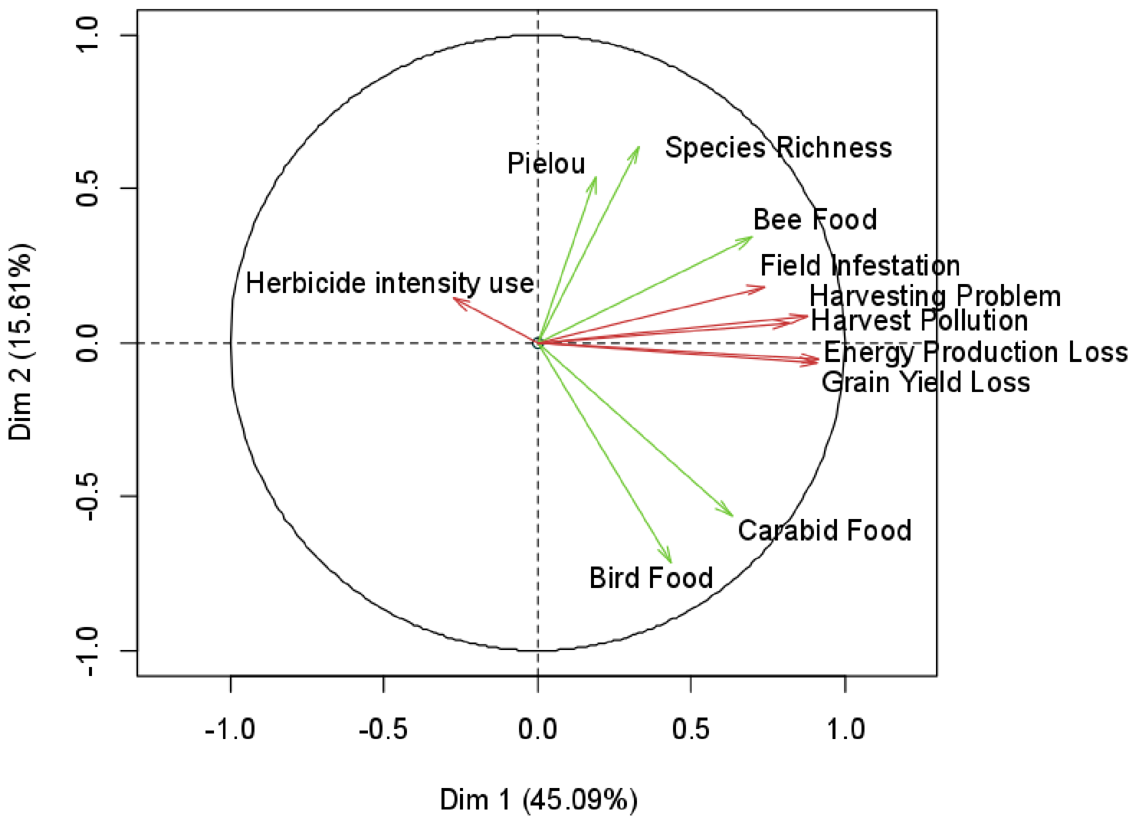


Figure III. 1: Correlations and trade-offs among weed impacts. First two axes of the principal component analysis (PCA) showing the relationships among the weed impact indicators simulated with FLORSYS on the learning data set composed of contrasted cropping systems. In red harmfulness indicators and herbicide intensity use, in green ecosystem services.

III.2.3.2 Which cropping techniques drive weed impact?

To identify key cropping techniques that drive weed harmfulness for crop production and weed-based ecosystem services indicators, we used the variable importance computed with random forests on the learning data set to rank cropping system descriptors. For instance, weed impact indicators mainly depended on techniques related to herbicide and tillage (Figure III. 2.a). Herbicide effect mostly depended on the number of operations, either during cash crops (nbInCropHerbicides) or for the whole cropping period (nbHerbicides), including interannual variation in operation frequency (std.nbHerbicides). In addition to operation frequency in different seasons (e.g. tillDuringInsectFeed, summerTillage, etc), tillage effect was most determined by depth (tillageDepth, maxTillageDepth). Direct effect of crop rotation (i.e. disregarding its effect on the choice of cropping techniques) was less important though the frequency of particular crops (here oilseed rape) was a key determinant of yield loss. When looking at a particular subset of the learning data set (Figure III. 2.b), the ranking was very similar though some descriptors could be replaced by similar ones (e.g. frequency of oilseed rape by durationCropCoverBroomrapeHosts as oilseed rape is the main broomrape host grown in Burgundy).

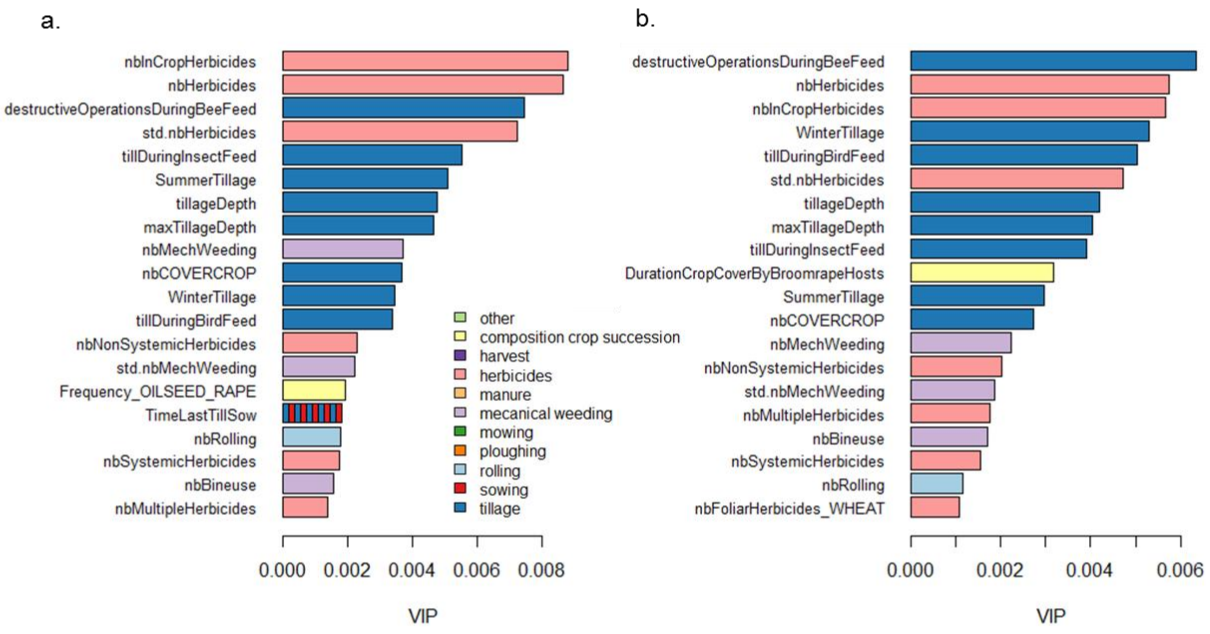


Figure III. 2: Key cropping system descriptors driving overall weed impact (mean of variable importance values of all indicators) averaged over simulation in the learning data set. Random forests VIP values for the first 20 most important cropping system descriptors for (a) the whole learning data set and (b) data from production situation PS.C (Figure III. 3). All indicators were rescaled to [0,1] before analysis. Colours represent types of cropping system descriptors, hatched bars are for descriptors concerning two different types. For the meaning of the cropping system descriptors, see Appendix. Variance explained for whole learning data set: 83.78 % and for production situation PS.C: 76.86 %.(Floriane Colas © 2018)

Generally, we found no general relationship between descriptors and weed impact indicators. Graphs plotting indicators vs descriptors usually show huge data point clouds, without any general correlation (results not shown). Among the few exceptions were bee food offer increasing with increasing oilseed rape frequency because this crop favored several weed species visited by bees, or carabid food offer as well as field infestation increasing with increasing time between last tillage and cash crop sowing because this lag time allowed weeds to emerge earlier than the crop and thus grow and reproduce better. Conversely, field infestation decreased with increasing frequency of various operations (e.g. multi-entry herbicides, summer tillage, hoeing, etc, see details in section 2 annex A7).

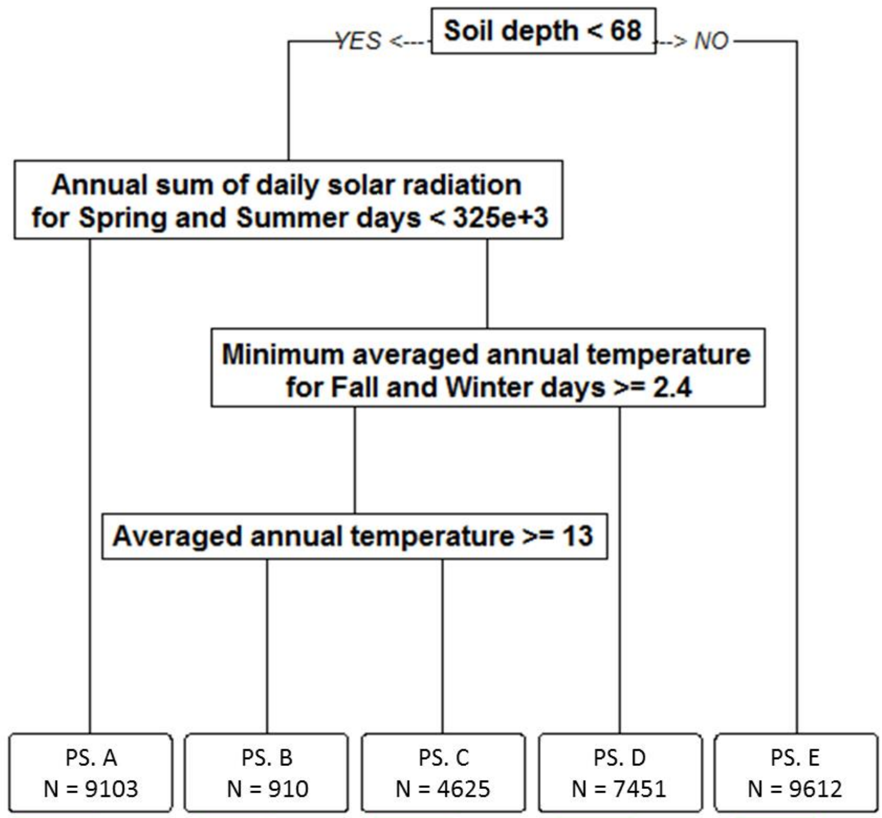
The descriptor ranking could vary, depending on the analyzed indicator. For instance, herbicide frequency was the most important to explain herbicide use intensity, wild plant species evenness, and the four harmfulness indicators (field infestation, energy production loss, harvest pollution and harvest difficulties), whereas tillage operations were crucial for wild plant species richness and the two seed-based biodiversity indicators (carabid and bird food offer). Overall, the variance importance of the different profiles did not greatly differ (see details in section 7 annex A7).

III.2.3.3 Decision trees

The previous section allowed us to identify key cropping system descriptors that drive weed impact on crop production and biodiversity. However, because most cropping techniques interact, their effect greatly depended on the other techniques implemented in the cropping system. The use of decision trees in the present section aimed to address this problem by investigating combinations of cropping techniques in contrasting production situations.

III.2.3.3.1 Determinants of production situation

Weed floras and management techniques both depend on the production situation. To guide stakeholders towards efficient weed management strategies, we thus aimed to propose decision trees for contrasting production situations. The latter were determined from a first multivariate regression carried out on the learning data set, using production situation variables only. Soil depth, radiation and average precipitation were the variables that the most discriminated weed impact indicator values in the tree (Figure III. 3). Soil depth discriminated production system E with the deepest soils from the other production situations with shallower soils. Burgundy systems were found in two production situations (PS.C and PS.D), and the soil-depth threshold segregating PS E from the rest was close to the mean soil depth observed in the learning set (mean: 70 cm, [min: 25, max: 130]). Conversely, the thresholds to discriminate production situations with high vs low radiation as well as high vs low temperatures were more extreme. The radiation threshold was below the first quantile, with annual radiation ranging from 305×10^3 to 362×10^3 MJ/year in the data set. The same was true for minimum temperature in fall and autumn (mean: 3.2°C, [min: 1.5, max: 5.1]) whereas the annual-temperature threshold exceeded the third quantile (mean: 11.5°C, [min: 9.5, max: 14.9]). The different regions clustered are Moselle, Ile-de-France and Picardie in PS.A, Aquitaine in PS.B, Burgundy in PS.C and D and Poitou in PS.E. All production situation, except PS.B, had random cropping systems in the cluster. When looking at the values of the weed impact indicators, PS.B tended to differ from the others with lower grain yield loss or species evenness. Otherwise production situations were similar, indicating that further segmentation using cropping system descriptors is needed to segregate contrasting weed impact profiles. For the following analyses, only the results on production situation PS.C are shown, corresponding to the branch with more cropping systems originating from Burgundy along with random cropping systems.



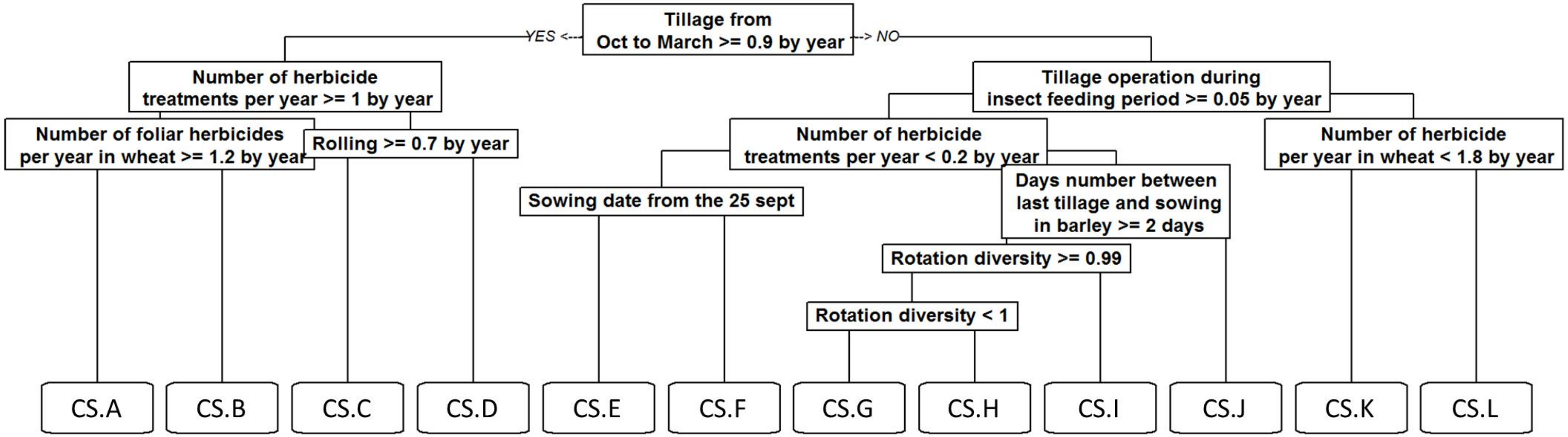
	PS. A		PS. B		PS. C		PS. D		PS. E	
Species richness	11.99	+/- 2.14	10.7	+/- 2.59	13.48	+/- 2.76	15.11	+/- 2.43	16.06	+/- 2.97
Pielou's equitability	0.33	+/- 0.08	0.19	+/- 0.14	0.26	+/- 0.07	0.32	+/- 0.08	0.31	+/- 0.08
Trophic ressources for birds	6.46	+/- 2.58	7.7	+/- 2.39	5.84	+/- 3.1	6.98	+/- 2.23	6.83	+/- 2.29
Trophic ressources for carabids	5.99	+/- 1.78	6.08	+/- 2.78	5.77	+/- 2.21	6.39	+/- 1.53	6.48	+/- 1.51
Trophic ressources for bees	2.44	+/- 0.7	1.24	+/- 0.44	1.86	+/- 0.6	2.74	+/- 0.64	2.7	+/- 0.82
Harvest pollution	3.85	+/- 1.25	1.88	+/- 0.83	3.55	+/- 1.31	3.95	+/- 1.13	4.11	+/- 1.27
Harvesting problem	4.56	+/- 1.3	2.14	+/- 0.92	4.18	+/- 1.42	4.71	+/- 1.2	4.93	+/- 1.36
Field infestation	1.76	+/- 0.99	1.32	+/- 0.7	1.75	+/- 0.99	1.81	+/- 0.8	2.64	+/- 1.11
TFI herbicide	1.12	+/- 0.89	1.24	+/- 0.57	1.09	+/- 0.74	0.97	+/- 0.83	1.01	+/- 0.82
Grain yield loss	69.55	+/- 23.2	24.95	+/- 19.26	62.6	+/- 27.17	73.05	+/- 20.28	75.93	+/- 20.81

Figure III. 3: Determinants of production situation based on pedoclimatic variables. Multivariate regression tree with the sorted on the production situation variables for all weed impact indicators and situations of the learning data set. The tree is pruned using the 1-standard error rule of the overall best tree size. All branches on the right: NO, branch on the left: YES. Indicator value show means and standard-deviations, with means coloured from white (0) to green (biodiversity) or red (harmfulness) for maximum values. Cross validation error = 0.04, for indicator range of variation rescaled to [0, 1] then back to their initial scale.

III.2.3.3.2 Multicriteria decision trees investigating trade-offs among weed impacts

The aim of the classification for a given production situation was to highlight combinations of cropping techniques that allow to reach a given goal in terms of weed harmfulness and biodiversity contribution. Because of the general trade-off between weed harmfulness and benefits, the multivariate tree for production situation PS.C of Figure III. 4 was unable to discriminate a weed impact indicator profile that combined high weed-based ecosystem services with low weed harmfulness for crop production. Profile CS.H was the best compromise, with generally low harmfulness and herbicide use intensity combined with medium biodiversity. The branch leading to this profile required less than one superficial tillage in winter, occasional summer tillage (during insect feeding season), occasional herbicide treatments, more than two days between the last tillage and barley sowing, and more than one crop in the rotation. The profile CS.G correspond to the same cropping system with the exception of monocultures *i.e.* with a rotation diversity of 1. Increase the diversity in the rotation is a simple way to improve the performance of the cropping system and pass from profile CS.G to CS.H.

Despite the inability of the tree to pinpoint agroecological solutions to reconcile crop production, low herbicide use and high weed benefits, several conclusion for weed management could be drawn. The main cropping techniques that drove weed impact indicators are tillage, herbicide strategies, rolling, sowing date and the crop rotation diversity (Figure III. 4) which is different from the variance importance of the random forests, especially for sowing date or the crop rotation diversity. While the cropping technique ranking based on the random forests (section III.2.3.2) already gave this type of information, the trees went further, indicating how techniques should be changed to improve performance. For instance, leaves CS.J, CS.K and CS.L identified solutions leading to the highest food offer for birds and carabids, e.g. less than 0.9 tillage per year in winter followed either by no summer tillage (during insect feeding periods), regardless of herbicide strategy in wheat (CS.K and CS.L), or occasional summer tillage, with herbicide treatments at least one year in five, and the last tillage in barley on sowing date (CS.J). Herbicide-free branches resulted in different performances, e.g. branch CS.C achieved low yield loss by combining frequent winter tillage and rolling operations. High tillage, during bee feeding period and shortly (less than 14 days) after the harvest is what determine a good indicator value. When aiming to reconcile a subset of weed impact goals, particular trees focusing on these indicators (e.g. productivity profile with all harmfulness indicators of IWM profile with crop yield and herbicide use) were not able to determine more efficient and precise solutions, only switching the days number between last tillage and sowing in barley and the number of superficial tillage in oilseed rape in the decision tree for the productivity profile (annex 7 section 7).



	CS.A		CS.B		CS.C		CS.D		CS.E		CS.F	
Species richness	12.13	+/- 1.57	14.49	+/- 2.28	12.64	+/- 3.6	13.78	+/- 1.85	14.7	+/- 2.68	16.55	+/- 1.12
Pielou's equitability	0.24	+/- 0.08	0.26	+/- 0.08	0.32	+/- 0.08	0.29	+/- 0.05	0.25	+/- 0.07	0.32	+/- 0.04
Trophic ressources for birds	0.53	+/- 0.51	3.62	+/- 2.19	1.44	+/- 1.42	5.12	+/- 1.01	6.44	+/- 2.1	3.29	+/- 0.82
Trophic ressources for carabids	1.49	+/- 0.34	4.42	+/- 1.61	2.8	+/- 1.16	5.15	+/- 0.8	6.11	+/- 1.11	5.87	+/- 0.56
Trophic ressources for bees	1.1	+/- 0.22	1.55	+/- 0.61	1.27	+/- 0.82	1.93	+/- 0.39	2.1	+/- 0.5	2.67	+/- 0.26
Harvest pollution	2.44	+/- 0.74	3.02	+/- 1.37	2.71	+/- 2.17	3.57	+/- 0.94	3.87	+/- 1.3	3.95	+/- 0.47
Harvesting problem	2.75	+/- 0.74	3.67	+/- 1.51	3.7	+/- 2.95	4.06	+/- 1.05	4.62	+/- 1.26	4.62	+/- 0.51
Field infestation	0.32	+/- 0.47	1.64	+/- 0.93	0.81	+/- 0.72	1.4	+/- 0.7	2.3	+/- 0.77	1.94	+/- 0.48
TFI herbicide	1.4	+/- 0.21	2.19	+/- 0.63	0	+/- 0	0.58	+/- 0.31	0	+/- 0	0.8	+/- 0.26
Grain yield loss	13.82	+/- 13.7	53.74	+/- 25.57	20.76	+/- 19.66	59.82	+/- 17.12	72.15	+/- 18.61	74.8	+/- 9.09

	CS.G		CS.H		CS.I		CS.J		CS.K		CS.L	
Species richness	13.31	+/- 2.45	11.94	+/- 3.05	14.16	+/- 2.73	14.3	+/- 1.22	9.42	+/- 2.46	13.53	+/- 1.17
Pielou's equitability	0.24	+/- 0.11	0.2	+/- 0.09	0.24	+/- 0.07	0.28	+/- 0.04	0.23	+/- 0.08	0.31	+/- 0.03
Trophic ressources for birds	6.52	+/- 3	5.54	+/- 3.13	6.25	+/- 1.97	9.5	+/- 0.3	9.24	+/- 1.55	9.81	+/- 0.09
Trophic ressources for carabids	5.13	+/- 1.3	3.85	+/- 1.66	6.11	+/- 1.17	8.26	+/- 0.27	8.35	+/- 1	8.59	+/- 0.08
Trophic ressources for bees	1.8	+/- 0.59	1.44	+/- 0.42	1.96	+/- 0.49	2.73	+/- 0.31	1.49	+/- 0.37	2.41	+/- 0.25
Harvest pollution	1.72	+/- 1.86	1.58	+/- 1.23	3.87	+/- 1.27	4.06	+/- 0.43	3.8	+/- 1.57	4.16	+/- 0.27
Harvesting problem	2.68	+/- 2.22	2.27	+/- 1.41	4.68	+/- 1.38	4.69	+/- 0.46	4.61	+/- 1.58	4.42	+/- 0.28
Field infestation	1.93	+/- 0.91	1.08	+/- 0.49	2.3	+/- 0.89	1.54	+/- 0.38	2.32	+/- 0.92	1.31	+/- 0.24
TFI herbicide	2.75	+/- 1.32	1	+/- 0	1.09	+/- 0.37	1.27	+/- 0.16	0.93	+/- 0.68	1.43	+/- 0.28
Grain yield loss	41.52	+/- 39.06	26.48	+/- 21.2	73.84	+/- 19.44	81.21	+/- 6.77	72.23	+/- 23.83	80	+/- 5.03

Figure III. 4: Multivariate regression tree identifying combinations of cropping techniques to achieve contrasting profiles of weed impact on crop production and biodiversity for the PS.C production situation (with more cropping systems from Burgundy) from Figure III. 3, sorted on the 10 weed impact indicators. The tree is pruned using the 1-standard error rule of the overall best tree size. All branch on the right: NO, branch on the left: YES. Cells were colored from white (nil) to green (maximum) for biodiversity, from white to red (maximum) for harmfulness to crop production averaged over years and weather repetitions. Uncoloured cells show standard-error including weather effects and variability among systems in a branch. Cross-validation error = 0.022, for indicator range of variation rescaled to [0,1] then back to their initial scale.

III.2.3.4 Testing the new models with DEPHY cropping systems

The random forest gave a good fitting quality with 83.78 % of explained variance. Cross-validation on the learning data set showed that the random forest produced excellent predictions for all weed impact indicators. Irrespective of the evaluation criteria, predictions were best for herbicide use intensity which directly resulted from cropping system inputs (Table III. 2). It was lower for the other indicators which all resulted from biophysical processes during FLORSYS simulations. The worst (but still well) predicted indicator was the plant species evenness, the only indicator that does not assess a weed function but only relative species densities. In conclusion, random forests are an excellent emulator of FLORSYS for cropping systems similar to those of the learning data set.

The situation was different when looking at more innovative cropping systems in the DEPHY test set. The prediction error was higher than for the learning data set, though still acceptable for the range of possible variation. The modelling efficiency was very low, showing that random forests are not very efficient for predicting absolute values of the weed impact indicators in novel cropping systems. However, the ranking ability of the random forest was much better, especially for herbicide use intensity (pearson coefficient: 0.59 and spearman coefficient: 0.72). Plant species evenness was again the worst predicted indicator.

The comparison of the range of predicted vs observed values showed that random forests were bad at predicting extreme values. The predicted range of indicator variation was only approximately 30 % of the original variability, with the worst ranked indicators (i.e. plant species evenness, field infestation, grain yield loss) having the most limited range of predicted variation.

Table III. 2: Prediction quality of the random forests assessed by comparison to independent innovative herbicide-sparse cropping systems from the DEPHY farm network. In both cases, observations were computed with FLORSYS. All indicators were rescaled to [0,1] before analysis.

Weed impact indicators	RMSEP	ME	R pearson	Spearman	Predicted vs observed range of variation: $(max_{predict} - min_{perdict}) / (max_{obs} - min_{obs})$
Plant species richness	0.22	-0.85	0.46	0.42	0.19
Plant species evenness	0.19	-0.12	0.03	0.06	0.22
Bird food offer	0.22	0.21	0.48	0.42	0.73
Carabid food offer	0.20	0.20	0.47	0.39	0.57
Bee food offer	0.15	0.15	0.42	0.38	0.27
Harvest pollution	0.17	-0.02	0.37	0.34	0.26
Harvesting difficulties	0.17	0.03	0.29	0.27	0.29
Field infestation	0.18	-0.13	0.18	0.20	0.17
Herbicide use intensity	0.31	-6.96	0.59	0.72	0.58
Grain yield loss.	0.30	-0.29	0.08	0.13	0.28

See III.2.2.5.2 for the computation of the statistical criteria.

III.2.4 Discussion

We used a combination of decision trees along with random forests to assess the cropping systems techniques that drive weed impacts on crop production and ecosystem services. The methodology based on data mining allowed us to determine that tillage and herbicide strategies are the main cropping techniques that are decisive when managing weeds. Decision trees and random forests are inseparable here as they provided complementary essential elements such as variable importance, the effects of variable combinations and the ability to rapidly predict new inputs.

III.2.4.1 Are the results consistent with field observations?

We demonstrated that herbicides and tillage are the main cropping techniques that drive weed impacts, which is consistent with previous studies (McCloskey et al., 1996; Menalled et al., 2001). We could though go much further here, specifically identifying which aspects of these techniques are essential (e.g. summer tillage) and which have little effect (e.g. winter tillage, or tillage specific to a crop). Tillage was thus described by 102 different descriptors out of 606, describing aspects such as timing in terms of season (e.g. winter or summer tillage), timing in terms of interactions with biological organisms (e.g. tillage during bird feeding period) or relatively to other operations (e.g., days from last tillage to cash crop sowing), in terms of tools (e.g. number of operations with a disk or a power harrow) or settings (e.g. maximum or average tillage depth). Similarly, herbicide strategy was described by a total of 114 descriptors. If the variable importance of these various descriptors were added, it would have increased mathematically the overall importance of tillage and herbicide use even if all descriptors are not important. The nature of the relevant descriptors selected in the trees depended not only on the production situations, but also on the presence of other techniques. This shows that many descriptors are needed to describe the complex effects of these major techniques, particularly to discriminate similar situations (e.g. number of herbicide treatments per year, followed by the number of foliar herbicide treatment in wheat, Figure III. 4, branches leading to leaves CS.A and CS.B) and to finely adjust cropping systems (Liebman and Dyck, 1993).

Crop succession composition was not very important, contrary to previous findings, both from field surveys and simulation studies (Cardina et al., 2002; Colbach and Cordeau, 2018b; Fried et al., 2008). However, the latter authors focused on one aspect of weeds (e.g. field infestation, weed-borne yield loss) whereas we investigated both harmfulness and benefits. Possibly, the various weed functions were differently impacted by crop rotation, which partially cancelled each other out when looking at the overall multicriteria ranking of cropping-system descriptors. Moreover, a large part of the crop rotation effect reported in field surveys is due to differences in cropping techniques which were captured here via a large selection of detailed cropping-system descriptors (see section III.2.4.2).

Generally, it was difficult to find previous field studies to assess the consistencies of the previous results, not only because of the level of detail we used to characterize our cropping systems but also because the decision trees and random forests focused on weed functions, i.e. harmfulness and benefits, rather than weed dynamics which are usually monitored in fields. We had the same difficulty when evaluating the FLORSYS model (Colbach et al., 2016b) which was used here as a virtual reality to build our new models. The domain of validity and the limits of the model were already discussed in several previous papers, concluding that FLORSYS's prediction quality was satisfactory, particularly for our aiming of ranking cropping systems (Bürger et al., 2015; Colbach et al., 2016b; Colbach et al., 2017d; Colbach and Cordeau, 2018b; Mézière et al., 2015d).

The lack of adequate evaluation data was one of the reasons why we ran a sensitivity analysis here. Such an analysis not only contributes to simplify a model or prioritize inputs, it can also test the robustness of a model with a wide range of input variations (Saltelli et al., 2008). Here, we especially put FLORSYS to test with the addition of random cropping systems, checking that the latter did not shift the results towards unrealistic values. For example, even with randomly chosen cropping systems where no logic compensated low herbicide use with other preventive or curative measures, we still did not observe any correlation between herbicide use intensity and weed harmfulness, just as in previous simulations with real-life systems only (Colbach and Cordeau, 2018b), cropping-system trials (Adeux et al., 2017; Chikowo et al., 2009; Colbach et al., 2016b) or farm field surveys (Lechenet et al., 2017; Petit et al., 2016). It is true that a large number of the random cropping systems could not be simulated because they resulted into situations that were so unrealistic that FLORSYS could not handle them.

The weather repetition variable was important for some indicators (e.g. field infestation, species richness, and bee food offer), reflecting the well-known effects of rainfall, temperature and radiation on biological processes such as plant growth (Andrieu et al., 2006) or seed germination (Hilhorst and Toorop, 1997). However, as in previous simulation studies (Colbach et al., 2016b; Colbach and Cordeau, 2018b) and field study (Gaudin et al., 2015), the cropping system effects largely exceeded the effect of weather. Moreover, even though indicator values varied among the weather repetitions of a given cropping systems, all repetitions were always located in the same leaf. This demonstrated that our results were robust, even though in each weather repetition FLORSYS simulated the same list of operations for a given cropping systems, without adapting dates or options to weather events or weed floras in particular repetitions. Though this might exacerbate effects, this approach was voluntarily chosen to assess effects of cropping systems on weed floras rather than the reciprocal (Colbach and Cordeau, 2018b).

III.2.4.2 New implications for weed management.

The present results indicate that the rotation or crop effects reported in field studies (Gaudin et al., 2015; Smith et al., 2008) are largely due to the associated choice in cropping techniques. Indeed, when working here with a large range of random, unreasoned cropping systems, crop species had little effect in contrast to previous simulation studies using only reasoned real-life cropping systems (Colbach et al., 2017d; Colbach and Cordeau, 2018b) and field reports(Smith et al., 2008). This is consistent with a more recent simulation study specifically focusing on species and variety effects, indicating that these effects are small compared to the rest of the cropping system even when focusing on crop yield loss only (Colbach et al.). This is good news for farmers that have little room for manoeuver in terms of crop choice, because of pedoclimatic or socio-economic constraints (e.g. no outlet to sell crop production, no advice on how to grow crops) (Meynard et al., 2013). This is where the random forests come in. allowing stakeholders to rapidly test novel combinations and ranges of cropping techniques. However, even if the present results indicate that judicious combinations of cropping techniques can achieve multiperformant weed management, the choice of combinations and techniques is severely limited by the crop choice, e.g. winter cereals do not allow winter tillage.

Moreover, despite adding more diverse cropping systems, we were unable to identify strategies that reconciled bee food offer and integrated crop protection, just as previous simulation studies working with a more limited set of real-life situations (Colbach et al., 2017d). The persisting trade-off between bee food offer and weed harmfulness control suggests that domestic-bee conservation should be achieved using habitats outside the field, which was demonstrated in a simulation-based case study comparing landsharing and landsparing scenarios in terms of reconciling crop production and biodiversity conservation (Colbach et al., 2018). Indeed, the scale needed for bee food offer appears to be larger than for other ecosystem services (Ekroos et al., 2016).

Harmfulness indicators were more correlated and thus redundant than ecosystem services. Indeed, the latter rely on broader elements in FLORSYS, such as seed densities or flowering plants, whereas weed harmfulness was mostly related to weed biomass (Mézière et al., 2015d). When solely aiming to maximise crop production, the analysis of the effects of cropping techniques on weed harmfulness for crop production and the subsequent cropping system design could thus be simplified by focusing on a single harmfulness indicator, except when farmers aim for particular production outlets such as seed production where harvest purity is a major issue.

III.2.4.3 Novel methodology

As for any model that is used for prediction and decision aid, it was essential to assess the ability of the random forests to lead to the right decision. In our case, this means that the forests must rank the cropping systems correctly whereas a correct prediction of absolute values is helpful but not (Loyce et al., 2002a). Many agronomical models are evaluated via expert knowledge. Here, in order to avoid the known confirmation bias (Palminteri et al., 2017), we chose a more objective evaluation method comparing the random-forest predictions with independent observations. However, as already mentioned above (section III.2.4.1), it was next to impossible to find adequate field observations, both in terms of situations and type of observations. Consequently, we used virtual observations, i.e. simulations with FLORSYS. The fitting of the forests with the learning data set is the most conventional type of evaluation and demonstrated that the random forests produced excellent predictions for all weed impact indicators.

Here, we completed this usual evaluation with a second step, running FLORSYS on a different set of real-life cropping systems to produce an independent set of virtual observations. We specifically chose cropping systems aiming at reducing herbicide use (Cellule d'animation nationale DEPHY Ecophyto, 2016) to check how far the trees and forests would give correct advices to design innovative cropping systems, particularly those aiming to reduce herbicide use. The random forests performed less well on the DEPHY data set, with higher prediction errors and a considerably lower modelling efficiency, indicating that the random forests are rather bad at predicting absolute indicator values. However, the random forests ranked the cropping systems satisfactorily, mainly for weed impact indicators assessing a weed function, thus answering to our main objective, i.e. discriminating systems with the better performance from those with a lower performance in terms of crop production, biodiversity and herbicide use.

The detailed analysis of the various weed impact indicators and cropping systems descriptors suggests several improvements. Even herbicide use intensity which, in FLORSYS, was directly computed from input variables without simulating effects of biophysical processes, was not predicted well in terms of absolute values in the DEPHY test data set. This means that the synthetic cropping system descriptors fed into the random forests were not sufficiently detailed to predict even the simplest weed impact indicator in innovative situations. Moreover, the DEPHY set included several cropping techniques and tools (e.g. alternate harrow with roller, alternate harrow, stubble cultivator) that were absent in the learning data set and could thus not be used to build the trees and forests. An initial screening of the cropping system inputs, with a particular focus on interactions, based on agronomical expertise, compensated with the addition of novel descriptors to assess the impacts of innovative techniques and tools might improve the prediction quality of the random forests.

The sensitivity analysis aimed to identify the key cropping techniques that drive weed impact. This was achieved here with the random-forest variable importance. However, neither the latter nor any other sensitivity indexes produce any information on how the output varies with the input (e.g. does the output increase or decrease with increasing input). Because of the complexity of the modelled processes and the many interactions among inputs, scatter plots of outputs vs inputs were usually useless as they showed huge clouds of data points without a general tendency. The combination of the random forests with decision trees was thus essential to produce information on interacting effects of variables, indicating how a given input changes outputs depending on other inputs. But the tree still gave no information on the direction of the relationship. This is where the random forests models are needed: they can test a given variation in an input (or a combination of inputs) very easily and quickly and thus identify relevant changes in cropping systems. It is by jointly using decision trees and random forests that we can extract the most information.

III.2.4.4 Where to go from here

The present methodology transformed and synthesized the biophysical knowledge and the testing abilities of FLORSYS into a simpler tool that contributes to give advice to farmers. Still, the models described here are not a tool or a decision support tool, and the insight and participation of future users are needed to develop a tool that can be useful and used by users (Prost et al., 2012). Users are essential to define which indicators to select and how to define performance profiles, depending on the objectives and constraints of the different farmers. Here, for example, we did not include indicators for weed-borne take-all disease risk or branched broomrape risk because they were specific to certain kind of farming systems and regions. But they would be relevant for cereal growers in Western France where take-all disease is frequent, or in oilseed rape crops in South-Western France which broomrape is invading. Using global scores as in (Colbach et al., 2017e) for the profiles regrouping indicators as we attempted could help analyse the tree results and force more extreme situations (i.e. only with optimum values of the indicators instead of a mix of good and bad). The cropping system descriptors also must be adapted, removing redundant and useless cropping techniques, and making them more understandable to users to avoid the risk on imposing the researcher point of view in spite of users (chapitre III, Colas et al., in prep.-a; Ravier et al., 2016).

Moreover, here, the cropping system was represented as a set of meta-decision rules and evaluated at a multiannual scale. Crop managers also need to manage their cropping systems at a short term, e.g. to adapt to weather hazards, treatment failures or the rapid change of regulations and prices. The methodology developed here should also be applied to design tools working at the annual scale, i.e. to predict weed impact in a given crop as a function of the same cropping system descriptors used here, combined with a set of new descriptors of the crop management planned for the current year and crop and possibly for the preceding crop year.

III.2.5 Conclusion

We combined here several data mining techniques to provide knowledge and tools for sustainable weed management, using the existing FLORSYS model as a virtual experimental platform. The sensitivity analysis combined a simulation plan exploring both real-life and virtual cropping systems with random forests to analyse the simulated output and showed that tillage and herbicide strategies are the most influential cropping techniques for multiperformant weed management. This use of random forests giving variance importance values was complemented with decision trees for contrasting production situations to identify key combinations of cropping techniques and allowed to identify other influential techniques such as frequency of rolling and sowing date in Burgundy. Trees and random forests are inseparable to provide knowledge for sustainable cropping system design to crop managers. Random forests indicate which techniques to change first, decision trees show how to combine the techniques and in which conditions, and, finally, random-forest models allow a quick and simple multicriteria evaluation of the novel cropping systems in terms of weed impact on crop production, herbicide use intensity and biodiversity. We went further than the conventional cross-validation associated to data mining and particularly checked the adequacy of the predictions on innovative integrated cropping systems. This complex methodology allowed us to extract the biophysical knowledge quantified and synthesized in FLORSYS and to feed it into a decision-support tool to help crop advisors and farmers design novel cropping systems. To make this tool usable and used, our team is now working on co-developping the structure of the tool with future users.

Acknowledgments

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Appendix

Table III.A. 1: List of all cropping systems descriptors, with explanation and basic summary for the cropping systems descriptors.

Short name	Description	Min	Median	Max
CropRotationLength	Length of crop rotation (years)	1	5	13
destructiveOperationsDuringBeeFeed	Number of weed-destructive operations (tillage, herbicides, mowing, mechanical weeding, harvest) per year during bee-feeding period, average over the simulation	0.77	3.68	15.06
DurationCropCover	Proportion of time with crop cover (including temporary and undersown crops) [0,1]	0.15	0.63	1.06
DurationCropCoverByBroomrapeHosts	Proportion of time with crop cover by temporary crops [0,1]	0	0.2	1.06
DurationCropCoverByTemporaryCrops	Proportion of time with crop cover by broomrape host crops (incuding temporary and undersown crops) [0,1]	0	0	0.28
harvestDate	Harvest date (Julian days), averaged over simulation. In case of associated crops, only the last cash crop harvest date is considered each year.	66	229	303
harvestDateSpringCrops	Harvest date (Julian days) of spring crops (= crops sown before or on July 31), averaged over simulation.	19	250	319
harvestDateWinterCrops	Harvest date (Julian days) of winter crops (= crops sown after July 31), averaged over simulation.	16	208	335
IVcoverCrops	Interannual variability in cover crops proportion of crop years where a year with a cover crop follows or precedes an "uncovered" year. E.g. 0 0 1 1 0 1 0 = 4/7. All years of a multiannual crop except the first are considered to be "uncovered"	0	0	1
IVdaysBetweenHarvests	Interannual variability of day between two harvest	278	370	1893
IVdaysBetweenSowingAndHarvest	Interannual variability of day between sowing and harvest	40	237	1742
IVdaysBetweenSowings	Interannual variability of day between two sowings	191	372	2024
IVdirectSowing	Interannual variability in direct sowing: proportion of crop years where a direct-sown year follows or precedes a tilled year. E.g. 0 0 1 1 0 1 0 = 4/7. All years of a multiannual crop except the first are considered to be directly sown	0	0	1
IVherbicides	Interannual variability in herbicides proportion of crop years where a sprayed year follows or precedes a herbicide-free year. E.g. 0 0 1 1 0 1 0 = 4/7. Each year of a multiannual crop is considered as a crop year	0	0	0.47

IVmanure	Interannual variability in manure spreading: proportion of crop years where a manured year follows or precedes a manure-free year. E.g. 0 0 1 1 0 1 0 = 4/7. Each year of a multiannual crop is considered as a crop year	0	0	1.01
IVmechWeeding	Interannual variability in mechanical weeding: proportion of crop years where a mech-weeded year follows or precedes a mech-weed-free year. E.g. 0 0 1 1 0 1 0 = 4/7. Each year of a multiannual crop is considered as a crop year	0	0	1.01
IVnbHerbicideOperations	Interannual variability of the number of herbicide operation	0	0	4
IVnbManureOperations	Interannual variability of the number of manure operation	0	0	4
IVnbMechanicalWeedingOperations	Interannual variability of the number of mecanical weeding operation	0	0	5
IVnbTillageOperations	Interannual variability of the number of tillage operation	0	0	5
IVPlough	Interannual variability in ploughig: proportion of crop years where a ploughed year follows or precedes an unploughed year. E.g. 0 0 1 1 0 1 0 = 4/7. All years of a multiannual crop except the first are considered to be unploughed	0	0	1.01
maxTillageDepth	Maximum tillage depth (cm) per year, averaged over simulation	0	20	29
MowingHeightCrop	Mowing height for crops (cm)	0	0	38.58
MowingHeightFallow	Mowing height during fallow (cm)	0	0	5
MultiannualCrops	Proportion of multiannual crops in the simulation [0,1]	0	0	1
nb ROTARY_HOE	Number of mechanical weeding operations per year carried out with a rotary hoe averaged over simulation. Operations carried out on the same day are counted individually	0	0	2
nbACTISOL	Number of operation with the tool actisol, averaged over simulation. Operations carried out on the same day are counted individually	0	0	0
nbALT_HARROW	Number of operations with an alternate harrow per year averaged over the simulation.	0	0	0
nbALT_HARROW_ROLLER	Number of operations with an alternate harrow and a roller per year averaged over the simulation.	0	0	0
nbBineuse	Number of mechanical weeding operations per year carried out with a BINEUSE, averaged over simulation. Operations carried out on the same day are counted individually	0	0	3
nbCHISEL	Number of operations with a chisel per year averaged over the simulation.	0	0	2.010465

nbDifferentCrops.species_x_variety.	Number of different species x variety combinations sown during the simulation, divided by the simulation legnth	0.03	0.13	0.47
nbDISC_HARROW	Number of operations with a chisel per year averaged over the simulation.	0	0.166575	1.998986
nbDISC_HARROW_ROLL	Number of operation with disc harrow, averaged over simulation. Operations carried out on the same day are counted individually	0	0	0
nbDISKING	Number of disking operation, averaged over simulation. Operations carried out on the same day are counted individually	0	0.17	3.3
nbFallowHerbicides	Number of herbicides per year sprayed during fallow (including cover crops), averaged over simulation. If several herbicides are applied on the same day (e.g. as a mixture), they are counted separately	0	0	1.37
nbFoliarOnlyHerbicides	Number of sprayed herbicides per year sprayed with only foliar entry mode, averaged over simulation. If several herbicides are applied on the same day (e.g. as a mixture), they are counted separately	0	0.2	4.06
nbHARROW	Number of mechanical weeding operations per year carried out with a harrow averaged over simulation. Operations carried out on the same day are counted individually	0	0	1.33
nbHerbicides	Number of applied herbicides per year, averaged over simulation. If several herbicides are applied on the same day (e.g. as a mixture), they are counted separately	0	1	7.39
nbHOEING	Number of hoeing operation, averaged over simulation. Operations carried out on the same day are counted individually	0	0	1
nbInCropHerbicides	Number of herbicides per year sprayed during cash crops (including pre-sowing root or pseudo-root herbicides), averaged over simulation. If several herbicides are applied on the same day (e.g. as a mixture), they are counted separately	0	1	6.79
nbMAGNUM_HARROW	Number of mechanical weeding operations per year carried out with a magnum harrow averaged over simulation. Operations carried out on the same day are counted individually	0	0	0
nbMechWeeding	Number of mechanical weeding operations per year, averaged over simulation. Operations carried out on the same day are counted individually	0	0	4.03
nbMIXER10	Number of operation with a tool that mix the soil up to 5 cm, averaged over simulation. Operations carried out on the same day are counted individually	0	0	2.01
nbMIXER5	Number of operation with a tool that mix the soil up to 10 cm, averaged over simulation. Operations carried out on the same day are counted individually	0	0	3.66
nbMowingCrop	Number of mowing operations during primary crops ("fauche") per year, with mowing height > 0 cm, averaged over simulation. Operations carried out on the same day are counted individually	0	0	3.01
nbMowingFallow	Number of mowing/cutting operations during fallow ("broyage") per year, averaged over simulation. Operations carried out on the same day are counted individually	0	0	1
nbMultipleHerbicides	Number of sprayed herbicides per year sprayed with multiple entry modes, averaged over simulation. If several herbicides are applied on the same day (e.g. as a mixture), they are counted separately	0	0.46	4

nbNonSystemicHerbicides	Number of applied non systemic herbicides per year, averaged over simulation. If several herbicides are applied on the same day (e.g. as a mixture), they are counted separately	0	0.46	3.13
nbPloughing	Number of mouldboard ploughing operations per year, averaged over the simulation	0	0.1	1.66
nbPseudoRootOnlyHerbicides	Number of sprayed herbicides per year sprayed with only pseudo-root entry mode, averaged over simulation. If several herbicides are applied on the same day (e.g. as a mixture), they are counted separately	0	0.17	2
nbRolling	Number of rolling ploughing operations per year, averaged over the simulation	0	0.1	3.33
nbRootOnlyHerbicides	Number of sprayed herbicides per year sprayed with only root entry mode, averaged over simulation. If several herbicides are applied on the same day (e.g. as a mixture), they are counted separately	0	0.1	2.8
nbROTARY_HARROW	Number of operation with rotary harrow, averaged over simulation. Operations carried out on the same day are counted individually	0	0.2	2.5
nbROTARY_HARROW_ROLL	Number of operation with rotary harrow and roller, averaged over simulation. Operations carried out on the same day are counted individually	0	0	0
nbROTAVATOR	Number of operation with rotavator, averaged over simulation. Operations carried out on the same day are counted individually	0	0	1.34
nbROTAVATOR_ROLL	Number of operation with rotavator with roller, averaged over simulation. Operations carried out on the same day are counted individually	0	0	0
nbSowings	Number of crop sowing operations per year, averaged over rotation	0.33	1	4.98
nbSTUBBLE_BREAKING	Number of operations with a stubble breaking per year averaged over the simulation.	0	0	0
nbSTUBBLE_BREAKING_SOFT	Number of operations with a stubble breaking with soft tines per year averaged over the simulation.	0	0	0
nbSTUBBLE_COULTER	Number of operation with stubble coulter, averaged over simulation. Operations carried out on the same day are counted individually	0	0	3.66
nbSystemicHerbicides	Number of applied systemic herbicides per year, averaged over simulation. If several herbicides are applied on the same day (e.g. as a mixture), they are counted separately	0	0.68	4.4
nbTillageOtherThanPloughOrRoll	Number of tillage operations (orther than mouldboard ploughing and rolling) per year, averaged over the simulation	0	1	11.66
nbWEED_HARROW	Number of mechanical weeding operations per year carried out with a weed harrow averaged over simulation. Operations carried out on the same day are counted individually	0	0	1.99
PropSpringCrops	Proportion of spring crops in the simulation [0,1]	0	0.4	1.01
PropTemporaryCrops	Proportion of temporary crops in the simulation [0,1] (number of cropping periods with at least one temporary crops/simulation length)	0	0	1
PropWinterCrops	Proportion of winter crops in the simulation [0,1]	0	0.5	1.02

rep.meteo	Repetition for the same meteo files, from 1 to 10	1	10	for all meteo/region
RotationDiversity	Interannual variability in rotation: proportion of crop years where previous and current crops differ in terms of winter, summer and multiannual crops. E.g. WWSS = 0.5, WSWS = 1, WWWW = 0. WWMm = 0.5 (and not 2/3 because the multiannual crop is 2-year long)	0	0.5	1.23
sowingDate.primaryCrops.	Sowing date (Julian days), averaged over simulation. Dates > 365 indicate spring sowings	233	372	560
sowingDateSpringCrops.primaryCrops.	Sowing date (Julian days) of spring crops (= crops sown before or on July 31), averaged over simulation.	1	110	211
sowingDateWinterCrops.primaryCrops.	Sowing date (Julian days) of winter crops (= crops sown after July 31), averaged over simulation.	212	283	365
std.harvestDate	standard-deviation of harvestDate	0	29	185
std.nbHerbicides	standard-deviation of nbHerbicides	0	0.01	7.62
std.nbMechWeeding	standard-deviation of nbMechWeeding	0	0	2.21
std.nbPloughing	standard-deviation of nbPloughing	0	0.03	1.5
std.nbRolling	standard-deviation of nbRolling	0	0.3	1.7
std.nbTillageOtherThanPloughOrRoll	standard-deviation of nbTillageOtherThanPloughOrRoll	0	5	411
std.sowingDate.primaryCrops.	standard-deviation of sowingDate.primaryCrops	0	86	170
std.tillageDepth	standard-deviation of tillageDepth	0	4.69	11.32
SummerPlough	Number of ploughing operations from April to Sept per year, averaged over the simulation	0	0	1.49
SummerTillage	Number of tillage operations (other than mouldboard ploughing and rolling) from April to Sept per year, averaged over the simulation	0	0.53	8.59
tillageDepth	Average tillage depth (cm) during simulation	0	10.56	29
tillDuringBirdFeed	Number of tillage and mechanical weeding operations per year during bird-feeding period, average over the simulation	0	0.67	5.6
tillDuringInsectFeed	Number of tillage and mechanical weeding operations per year during carabid-feeding period, average over the simulation	0	1.01	10.26

TimeHarvest1stRoll	Number of days from previous harvest to first rolling operation. Only crop years with tillage are considered	1	48	399
TimeHarvest1stTill	Number of days from previous harvest to first tillage (other than roll). Only crop years with tillage are considered	1	41	291
TimeHarvestPlough	Number of days from previous harvest to first ploughing. Only crop years with ploughing are considered	1	84	380
TimeLastherbicideHarvest	Time from last herbicide to last harvest. Only crop years with herbicides are considered	2	110	2779
TimeLastMechanicalWeedingHarvest	Time from last mechanical weeding operation to last harvest. Only crops with mechanical weeding are considered	1	95	345
TimeLastRollSow	Number of days from last rolling operation to first primary-crop sowing. Only crop years with tillage are considered	-267	40	434
TimeLastTillSow	Number of days from last tillage (other than roll) to first primary-crop sowing. Only crop years with tillage are considered	-0.5	29	360
TimePloughSow	Number of days from last ploughing to first primary-crop sowing. Only crop years with tillage are considered	0	58	340
TimeSow1stHerbicide	Time from first primary-crop sowing to first in-crop herbicide (including pre-sowing root or pseudo-root herbicides). Only crop years with in-crop herbicides are considered	-30	73	315
TimeSow1stMechanicalWeeding	Time from first primary-crop sowing to first mechanical weeding. Only crops with mechanical weeding are considered	1	92	399
WinterPlough	Number of ploughing operations from Oct to March per year, averaged over the simulation	0	0	1.5
WinterTillage	Number of tillage operations (other than mouldboard ploughing and rolling) from Oct to March per year, averaged over the simulation	0	0.5	4.02
YearsBetweenCoverCrops	Time between years with a cover crop (years). All years of a multiannual crop except the first are considered to be "uncovered". If time between "uncovered" years is required, this is 1/(1-1/time between "covered" years)	0.1	0.71	9.67
YearsBetweenDS	Time between years with direct sowing (years). All years of a multiannual crop except the first are considered to be directly sown. If time between tiled years is required, this is 1/(1-1/time between directly sown years)	0.12	1	10
YearsBetweenHerbicides	Time between years with herbicides (years). Each year o f a multiannual crop is considered as a crop year. If time between herbicide-free years is required, this is 1/(1-1/time between sprayed years)	1	1	14.5
YearsBetweenManure	Time between years with manure (years). Each year o f a multiannual crop is considered as a crop year. If time between manure-free years is required, this is 1/(1-1/time between manured years)	1	2.5	15
YearsBetweenMultiannualCrops	Time between years with multiannual crops (years). WWWMmmm = 7, the multiannual is sown every 7 years	0.97	6	15

YearsBetweenMW	Time between years with mechanical weeding (years). Each year o f a multiannual crop is considered as a crop year. If time between mech-weeding-free years is required, this is 1/(1-1/time between mech-weeded years)	1	1.3	15
YearsBetweenPlough	Time between years with ploughing (years). All years of a multiannual crop except the first are considered to be unploughed.If time between unploughed years is required, this is 1/(1-1/time between ploughed years)	0.97	3	15
YearsBetweenSpringCrops	Time between years with spring crops (years). WWSWW = 5, WSWSW = 2.333, WWSS = 2	0.97	2.31	15
The crop related descriptors are listed here, their description can be found in the above lines. The difference it is that the computation concern only the years where the crop associated to the descriptor is sown.				
Concerned cropping technique descriptors are (the global description can be found in previous rows, here the computation were adapted to the specific crop): nbRolling_CROP, cropCoverDuration_CROP, durationCoverCrop_CROP, durationHostCover_CROP, freqCoverCrop_CROP, Frequency_CROP, harvestDate_CROP, TFIh_CROP, MaxTillageDepth_CROP, MeanTillageDepth_CROP, mowingHeight_CROP, nbDISC_HARROW_CROP, nbSTUBBLE_CULTIVATOR_CROP, nbDifferentCrops.species_CROP, nbFallowHerbicides_CROP, nbFoliarHerbicides_CROP, nbALT_HARROW_CROP, nbHerbicides_CROP, nbROTARY_HARROW_CROP, nbIncropHerbicides_CROP, nbManure_CROP, nbMechWeeding_CROP, nbMowing_CROP, nbMultiHerbicides_CROP, nbNonSystemicHerbicides_CROP, nbPloughing_CROP, nbPseudorootHerbicides_CROP, nbResidueShredding_CROP, nbRootHerbicides_CROP, nbROTAVATOR_CROP, nbSuperficialTillage_CROP, nbSystemicHerbicides_CROP, operationDuringBeeFeeding_CROP, previousCereal_CROP, previousLegume_CROP, previousMixture_CROP, previousMultiCrop_CROP, previousOther_CROP, previousSpringCrop_CROP, previousWinterCrop_CROP, PrimaryCropSowingDate_CROP, shreddingHeight_CROP, summerPlough_CROP, summerTillage_CROP, tillageDuringBirdFeeding_CROP, tillageDuringInsectFeeding_CROP, timeHarvest1stManure_CROP, timeHarvest1stPlough_CROP, timeHarvest1stRoll_CROP, timeHarvest1stTill_CROP, timeLastHerbicideHarvest_CROP, timeLastManureSow_CROP, timeLastMechWeedingHarvest_CROP, timeLastPloughSow_CROP, timeLastRollSow_CROP, timeLastTillSow_CROP, timeSow1MechWeeding_CROP, timeSow1stHerbicide_CROP, winterPlough_CROP, winterTillage_CROP				
CROP can correspond to: Lucerne, Barley, Maize, Oilseed rape, Peas, Soya, Sugar beet, Sunflower, Wheat				

III.3Conclusion

Dans cette partie, nous avons identifié les techniques culturales, ainsi que leurs combinaisons, permettant de gérer les adventices afin de concilier la réduction de leurs impacts négatifs sur la production avec la promotion des services écosystémiques rendus par ces mêmes adventices. Cette étude, sans *a priori* sur les variables de description des systèmes de culture et utilisant, entre autres, des systèmes de cultures aléatoires, a fait ressortir les techniques connues du travail du sol et des stratégies d'usage des herbicides. C'est grâce à une analyse plus fine en fonction de la situation de production que nous avons pu identifier des techniques plus mineures et, surtout, des combinaisons de techniques. Par exemple, le rouleau ou la date de semis ont de l'importance selon le nombre de travaux du sol ou le nombre de traitements herbicides dans la rotation.

Cette partie a dû utiliser un grand nombre de variables pour décrire synthétiquement un système de culture, ce qui est nécessaire étant donné la complexité des systèmes de culture et des interactions entre techniques. En outre, notre but était de s'affranchir des préjugés sur les pratiques qui influencent les adventices lors de l'analyse de sensibilité. Ce travail ne remplace pas les études plus fines, qu'elles soient expérimentales ou virtuelles par simulation, pour identifier plus précisément l'effet de certaines techniques en interaction sur les adventices. Au contraire, il peut indiquer des pistes de réflexion à explorer plus particulièrement comme la relation entre le travail du sol en hiver, le peu d'usage d'herbicide et le passage de rouleau qui semblait bien contrôler la nuisibilité des adventices.

Certaines approches utilisées dans ce chapitre étaient inspirées des premières interactions avec les futurs utilisateurs de l'outil d'aide à la décision décrites au chapitre suivant, notamment le besoin d'un outil guidant dans la reconception de systèmes de culture basée sur des métarègles de décision ou bien l'identification de profils d'utilisateurs contrastés ("productiviste", "intégré", "agroécologique"). Cependant, même si la combinaison des arbres de décision et des forêts aléatoires permet d'identifier les techniques les plus influentes, de proposer des pistes pour combiner les techniques culturales les plus pertinentes et de rapidement évaluer des grands changements dans les systèmes de culture, nous sommes encore loin d'un outil d'aide à la décision à proprement parler. Par exemple, les descripteurs des systèmes de culture ne sont pas tous pertinents, d'autres sont redondants et d'autres encore insuffisants pour intégrer la complexité des effets et interactions des techniques dans les systèmes de culture et ils ne correspondent pas forcément aux usages, besoins et concepts des agriculteurs. Il reste aussi la question de comment présenter les arbres et forêts pour qu'ils deviennent faciles à comprendre et à utiliser. Ces questions sont primordiales pour que le futur outil d'aide à la décision devienne utile et utilisé et doivent être traités en interaction avec les futurs utilisateurs de l'outil. Ces différentes étapes de co-développement de l'outil sont présentées dans le chapitre suivant.

Chapitre IV : Implication des futurs utilisateurs dans le co-développement d'un outil d'aide à la décision

PARLER À DES HUMAINS, ÇA FAIT DU BIEN

IV.1 Introduction

Pour développer un outil d'aide à la décision (OAD) pour la gestion intégrée des adventices, nous avons, aux étapes précédentes, accéléré le modèle puis fait de la fouille de données afin d'identifier les techniques culturales les plus influentes et synthétiser leurs effets sur les indicateurs d'impacts des adventices. Pour planifier l'analyse de sensibilité, notamment au niveau des entrées, nous avons interagi avec des futurs utilisateurs de l'OAD : des conseillers agricoles et des agriculteurs. Cette interaction a eu lieu tout au long de la thèse, pour définir et tester la structure de l'outil d'aide à la décision. En effet, pour développer un outil utile et utilisé, il est essentiel d'intégrer les futurs utilisateurs au plus tôt du développement (Cerf *et al.*, 2012a). Comme les futurs utilisateurs et le modèle ont parfois des besoins et contraintes non compatibles, il est essentiel de les appréhender le plus tôt possible afin de trouver des solutions conciliant au mieux les besoins et contraintes des deux parties.

L'objectif de cette partie est de résumer toutes nos interactions avec des conseillers agricoles et des agriculteurs pour le développement de l'outil d'aide à la décision. Avec eux, nous avons défini quelles seraient les questions auxquelles l'outil devrait répondre, c'est-à-dire comment les conseillers et agriculteurs voient la gestion des adventices et comment ils appréhendent les stratégies de gestion à l'échelle du système de culture. Après avoir défini l'objectif de l'outil d'aide à la décision, nous avons testé différentes sorties possibles pour le nouvel outil, répondant à cet objectif, mais aussi réalisables avec le modèle FLORSYS. Nous avons également, avec les conseillers agricoles et les agriculteurs, amélioré et ajouté des variables d'entrées pour décrire les systèmes de culture de façon synthétique, afin de saisir au mieux, dans l'outil, la complexité d'un système de culture. Pour cela, l'implication des futurs utilisateurs s'est déroulée en quatre étapes :

- Enquêtes en ligne, avec des conseillers agricoles dans toute la France et quelques agriculteurs, pour définir l'objectif de l'OAD et, de façon préliminaire, les entrées et les sorties de l'OAD.
- Première réunion avec des agriculteurs, pour les confronter aux réponses des conseillers agricoles et pour compléter la vision des agriculteurs qui n'avait pu être que partiellement appréhendée dans les enquêtes précédentes.
- Deuxième réunion avec des agriculteurs, pour tester des formats pour le futur OAD, dont un format suggéré par les participants à l'étape précédente.
- Atelier avec des conseillers agricoles pour tester le prototype d'OAD dans une situation de conception de système de culture, pour identifier le format préféré de sortie et ajouter des entrées plus parlantes pour les utilisateurs et observer comment les utilisateurs utilisent l'outil.

Cette partie a fait l'objet d'un article qui sera soumis à Agronomy for sustainable development. Certains résultats de cette partie ont été présentés à différents congrès, notamment au COLUMA sous la forme d'un article de 10 pages dont de nombreuses parties ont été reprises ici.

Colas, F., Colbach, N., Cordeau, S., Jeuffroy, M.-H., Granger, S., Queyrel, W., Pointurier, O., Rodriguez, A., Villerd, J., (in preparation). Co-development of a decision support system for integrated weed managment: contribution from future users.

Colas F., Cordeau S., Jeuffroy M.-H., Granger S., Queyrel W., Pointurier O., Rodriguez A., Villerd J., Colbach N. (2016) Développement d'un outil d'aide à la décision pour la gestion intégrée des adventices. In: 23e Conférence du COLUMA - Journées internationales sur la lutte contre les mauvaises herbes, Dijon, France, 467-476 (poster).

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Colas F., Granger S., Villerd J., Darmency H., Colbach N. (2016) Which decision-support systems for sustainable weed management: why, how and when to use it? International Weed Science Congress, Prague (poster).

Colas F., Cordeau S., Jeuffroy M.-H., Villerd J., Colbach N. (2015) Which decision-support system for sustainable weed management: needs and constraints of crop advisors 17th European Weed Research Society Symposium, “Weed management in changing environments", 23-26 June 2015, Montpellier, France, 239 (poster).

IV.2 Co-developement of a decision support system for integrated weed management: contribution from future users

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Abstract

Integrated weed management consists in using several weed management techniques in a long-term approach. This makes it difficult to easily design such cropping systems, especially when needing to take into account weather events. Farmers and farm advisors need decision support systems (DSS) to develop multiperformant weed management strategies adapted to the economic, social and environmental stakes and to the constraints of farmers. Here, we developed such a DSS (1) by defining its goal, application field and structure from interactions with future users, (2) by feeding the DSS with knowledge on biophysical processes comprised in the mechanistic weed dynamics model FLORSYS. This model is a "virtual field" simulating the effects of cropping systems on crop and weed dynamics as well as the resulting crop production and other ecosystem services over several decades and in a large range of pedoclimatic situations. In a previous work, biophysical knowledge was synthesized and quantified with applying data mining methods (decision trees and random forests) to several thousand cropping systems simulated with FLORSYS. Here, we explain how we worked with future users to define the use and type of needed DSS, and then to transform the models produced with data mining into a decision support system. First, we interviewed crop advisors and farmers via an online survey and determined that two complementary tools were needed, i.e. a synthetic tool working with meta-decision rules to help with a complete overhaul of a cropping system for users facing a dead end, a precise and detailed tool for fine tuning of cropping systems for users that want to take advantage of biophysical interactions. For the latter, we proposed the initial FLORSYS preparameterized with regional, superfluous or complicated inputs. For the former, we developed the models from data mining. Then, we worked with farmers and crop advisors in group meetings and workshops, to (1) observe how they would use the models, feed the inputs and interpret the outputs, (2) test different model structures and output formats, proposed by both the users and ourselves. The feedback helped us to define the structure of the tool, the vocabulary for describing agricultural practices, and output formats displaying output values with a colour code for faster reading. The DSS will consist of (1) tables ranking cropping system practices to help users choose the most influential ones in terms of weed impact on crop production, herbicide use and biodiversity, (2) a set of decision trees for contrasting production situations to visually guide users when combining management practices depending on their weed management goals,

(3) predictors based on random forests for a quick and easy multicriteria evaluation of cropping system prototypes, and (4) the simplified FLORSYS to fine-tune the optimal solutions.

Keywords:

Workshop, decision trees, random forest, multivariate output display, conceptual framework

IV.2.1 Introduction

Weeds are harmful for crop production (Oerke, 2006) but important for plant and functional biodiversity (Marshall *et al.*, 2003). Global changes and herbicide policies compel farmers to reduce their herbicide use (Directive 2009/128/CE; Ecophyto, 2017) in order to limit the impact on human health and environment (Wilson and Tisdell, 2001). In response, farmers replace herbicides with a combination of multiple, mostly preventive and partially efficient practices (Bonin, 2009; Liebman and Gallandt, 1997; Wezel et al., 2014). The complexity of effects of cultural practices combined with climatic uncertainty on weeds makes these modifications difficult to plan and risky (Ingram, 2008). Understanding the impacts of agricultural practices, and their interactions, on weeds is critical to help farmers develop cropping systems that reconcile crop production, biodiversity and reduced herbicide use, and decision support systems can help to tackle this challenge.

Various tools or Decision Support Systems (DSS) exist to help farmers to take strategic or tactical decisions to manage their fields. DSS are of many forms, ranging from small in-field tests of weed species recognition as InfloWeb (Terres Inovia *et al.*) to complex software to test on a computer different herbicide treatments for weed management, e.g. Weed Manager (Parsons *et al.*, 2009) or WeedSOFT® (Neeser *et al.*, 2004). However, these tools focus on one particular technique and to date, no DSS assesses the impacts of a combination of multiple and detailed cultural practices on weeds in the long term cropping-system scale, and none considers the multicriteria impacts of weeds on production and biodiversity. A need for a new DSS integrating weed management at a strategic scale was identified (Dubrulle et al., 2014; GIS GC HP2E, 2011).

Conversely, process-based cropping system models can be considered as a "virtual field" for researchers to virtually experiment and evaluate cropping systems. Among these, the very detailed weed dynamics model FLORSYS (Colbach et al., 2014c; Gardarin et al., 2012; Munier-Jolain et al., 2013) assesses the impact of weeds on both crop production and biodiversity within cropping systems, translating detailed crop and weed state variables into indicators of weed impact on crop production and biodiversity according to the cropping system (Mézière et al., 2015d). The high level of details needed, the many possibilities and its simulation/computation time are limits to the use of FLORSYS by farmers and crop advisors. Its modification and simplification are an interesting way of making available to farmers and crop advisors the synthetic knowledge embedded in the model (Colas et al., in prep.-b; Colbach, 2010). To make the model useful to and actually used by non-researchers, future possible users should be involved during the design and development stages, not only to provide expert knowledge, but also to participate to define the needs and possible uses of the DSS and iteratively tests the prototypes (Cerf et al., 2012a; Prost et al., 2012; Voinov and Bousquet, 2010). In this case, future users correspond to farmers and crop advisors, actors that can actively help change a cropping system.

Participatory design is an efficient way to involve the future users in the design process of a possible tool for them (Cerf et al., 2012a). The model is tested, improved and validated by the users, whether it is a tool developed by researchers (Becu *et al.*, 2008) or a model co-designed with all participants (Bah *et al.*, 2006). Using surveys to develop a DSS is an easy way to collect user inputs, especially when using semi-open questions that encourage explanations by farmers (Merot *et al.*, 2008). But for a better contribution of users to the tool development, the practical application is necessary, with workshops to allow a better appropriation of the model, and to encourages interactions among participants as well as social learning (Figureau et al., 2015; Hossard et al., 2013; Patel et al., 2007).

Here we propose a conceptual framework of interactions with future users with the aim of developing a DSS from FLORSYS, based on previous methodology (Cerf et al., 2012a). Those interactions are putting milestones on our path to the final DSS, to define and understand why and how future users would use such a tool. We developed the DSS (1) by defining its goal, application field and structure from interactions with future users, (2) by feeding the DSS with knowledge on biophysical processes comprised in the mechanistic weed dynamics model FLORSYS (Figure IV. 2). Here, we explain how we worked with future users to define the use and type of needed DSS, and then to transform the models produced with data mining into a decision support systems.

Step 1 used online surveys to define what the tool should do. The results contributed to the choice of method to extract the scientific biophysical knowledge comprised in FLORSYS in step 2 where data mining was applied to a large set of contrasting cropping systems simulated with FLORSYS (step 2 methodology in in (Colas et al., in prep.-b) . The data mining methods were chosen considering their ability to extract and synthesize data as well as to communicate these results to outsiders. Classification And Regression Trees (CART) (Breiman *et al.*, 1984), were used to find the best management practices and combinations thanks to the classification of evaluated cropping systems as in (Mézière *et al.*, 2015a). For simplification purposes, CART trees are referred as “decision trees” in the following. The tree shape representation has the additional advantage of presenting the results in a format similar to what is already used for guiding farmers' decisions, e.g. for slug control (Bodilis *et al.*, 2017) or risk of run off in potatoes (Arvalis-Institut du Végétal and Bayer, 2016). The CART methodology later evolved to produce random forests (Breiman, 2001). Thanks to their good capacity of prediction, these can emulate models, even complex ones such as FLORSYS, and could potentially help to quickly evaluate cropping systems without using the original model (Hill *et al.*, 2014). The results from steps 1 and 2 produced a DSS prototype (step 3) which was then tested with the future users in group meetings and workshops, to (1) observe how they would use the models, feed the inputs and interpret the outputs, (2) test different model structures and output formats, proposed by both the users and ourselves. The feedback helped us to define the structure of the tool, the vocabulary for describing agricultural practices, and output formats

IV.2.2 Material and methods

To develop the decision support system, we interacted regularly with future users, i.e. crop advisors and farmers, to co-design the tool in terms of type of use and structure. These interactions took place in five case studies (Table IV. 1). First, we carried out an online survey aiming at both farmers and crop advisors to identify the type of tool in terms of use, inputs and outputs. This step was essential to determine what data and knowledge to extract from FLORSYS and in which form. Based on this, we ran sensitivity analyses of FLORSYS and used different data mining methods to quantify and synthesize effects of cropping techniques on weed impacts. The details of that study can be found in Colas et al (chapter III).

The next interaction with users consisted in group meetings to observe what farmers thought of the crop advisors' answers to the online survey (for the first group only), how users would handle different tools and interpret their output formats, ranging from the virtual field model FLORSYS to visual decision trees on paper. Finally, the user friendliness and applicability of a prototype of the DSS was tested in workshops. The various steps were detailed below, followed by a short presentation of the FLORSYS model and the components of the DSS prototypes used to interact the future users.

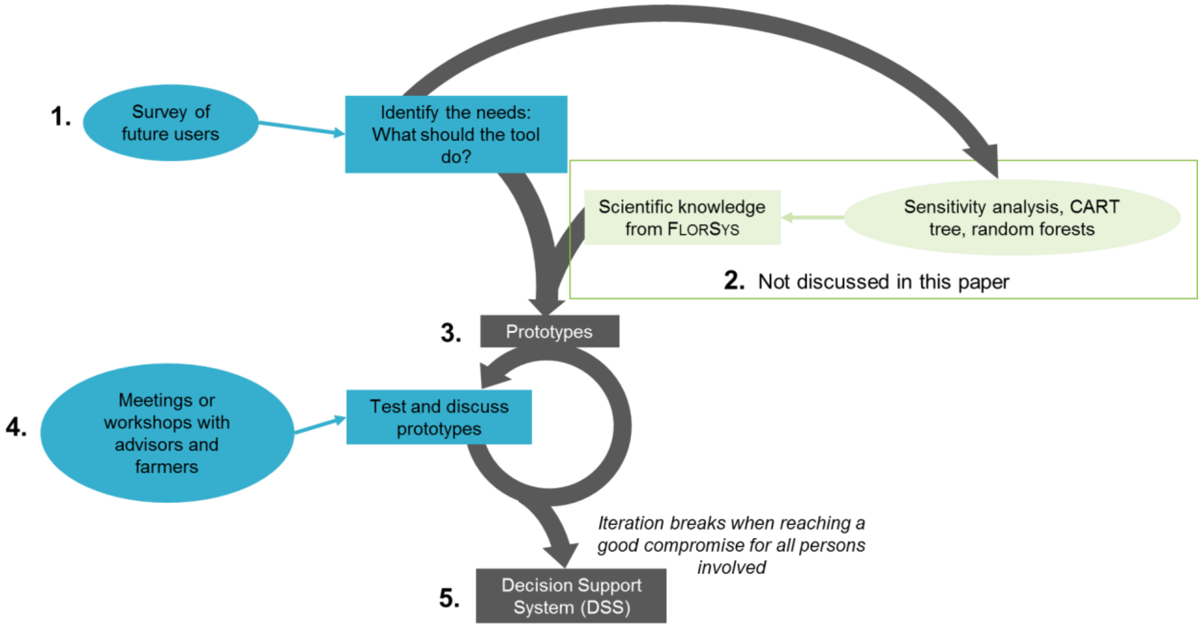

Figure IV. 1: Conceptual framework to co-design, with future users, a decision support system from an existing biophysical model. Ellipses represent the methods, rectangles the objectives, contents of the future tool are in light green, the structure and outline of the tool designed with the stakeholders are shown in blue, the different versions of the tool are shown in dark brown. (Floriane Colas © 2018)

IV.2.2.1 Online survey of crop advisors and farmers (step 1)

The first step was to identify the type of tool in terms of use, inputs and outputs. A survey was conducted with a semi-structured online questionnaire (example annex A8 section 2) sent in March 2015 via e-mail to 200 crop advisors from chambers of agriculture, technical institutes and agricultural cooperatives all over France. The online survey remained open during one month. The survey included four parts to identify: (1) the interviewed persons (e.g. which production system, which use of already existing DSS); (2) the aims, contents and structure of a DSS they would like to use for weed management advice: the criteria for evaluating cropping systems (*e.g.* weed harmfulness, food offer for pollinators), the temporal scale (*e.g.* one year, one rotation) and the description of farming practices (*e.g.* detailed list of cultural operations, meta decision rules); (3) the constraints for model use, *i.e.* the availability and difficulty to fill in the different types of input variables; (4) the functionality and readability of inputs and outputs of the future tool, *i.e.* the ability to understand why a given input leads to the resulting output. Questions on type and level of details of inputs and outputs were based on the kind of information fed into and provided by FLORSYS (section IV.2.2.4.1). Other questions were based on our need to better understand the way users would like to use a DSS and how they perceive weed management. Structured answers were analysed by counting occurrences for each proposal and compared to bring out the underlying crop advisor profile. For example, were the advisors that answered "Detailed list of operations" to the question "How much data are the users ready to provide for a decision-support system?" the same than the ones answering "Crop management sequences" to "Which decisions to take with the DSS?". Farmer's answers were analysed in a qualitative way, using their answers to illustrate some examples.

Table IV. 1: Summary of the case studies

Objectif (and correponding step)	Case studies	Numbers of farmers and advisors	Location	Methods of data collection	Farming systems:main productions
Identify the type of tool in terms of use, inputs and outputs (1.)	Crop advisors	40	All France	On line survey	Field crop and mixed cropping-livestock
	Farmers	4 full answers; 2 partial	All France	On line survey	Field crop and mixed cropping-livestock
	Group meeting with water agency	~15 farmers; 2 advisors	Picardie	Participant observations	Field crop
Identify how users would handle different tools and interpret their output formats (4.)	Group meeting with GRCETA* Aube	~ 50 famers; 2 technicians	Aube	Small survey and participant observation	Field crop
	Workshop	5 crop advisors	Champagne (Aube, Haute-Marne)	Workshop to test DSS prototypes	Mixed cropping-livestock

*GRCETA: Groupement Régional des Centre d'Etudes Techniques Agricoles, i.e. Regional group of a study center of agronomic techniques. Usually managed by one or two agronomical technicians.

IV.2.2.2 Group meetings with farmers and advisors (step 4)

We interacted with two groups of French famers and their advisors, first presenting the FLORSYS model and our aim in developing a DSS, and then requesting suggestions and improvements for the structure and outline. We also took advantage of the diverse public to compare their respective opinions, particularly to get farmers' reactions to advisors' opinions as recent studies have shown that advisors can sometimes hinder farmers moving toward more integrated practices (Pasquier and Angevin, 2017).

IV.2.2.2.1 First meeting: real-time feedback from farmers to crop advisors' answers at the survey

During the first meeting, we took advantage that the group was already acquainted with FLORSYS to present the advisors’ answers from the online survey of section IV.2.2.1 in order to collect the farmers' reactions. The group was composed of about 10 farmers from the Picardie region, with their two consultants from the water regulatory authority and a consulting company. The two consultants were using FLORSYS to test alternative practices proposed by farmers to control weeds with fewer herbicides.

We showed the farmers the answers from the online survey of what the crop advisors would like to have in terms of DSS and recorded their answers via a questionnaire and an open discussion. Only the answers to the following questions were shown: how much detail to describe a cropping system, which level of disruption in the existing cropping system level is acceptable or required, what are the constraints of weed management, which weed impact indicators are useful to evaluate weed management. In addition, we showed the farmers several options for displaying outputs (Figure IV. 3) as well as a decision tree to help define the outputs by recording what they thought of the different displays.

IV.2.2.2.2 Second meeting: testing formats for the visual decision guide

The objective of the second meeting was to test possible formats for the visual decision guide of the DSS. Based on past experience from both research and farming advice, we initially planned to work with decision trees, but following the suggestion of one of the Picardie farmers, we proposed a table format as an alternative (details in IV.2.2.4.3 and Appendix).

The meeting took place in the Champagne region, during the annual meeting of a GRCETA, a regional group of approximately 50 farmers aiming to innovate their farming practices, helped by two agricultural technicians. The members of the meeting were asked to answer a short questionnaire testing their understanding and the ease of handling these DSS output formats. Instead of answering individually the questionnaire, as it was originally intended, the farmers answered by spontaneous small groups of 3-4 farmers, resulting in 10 complete answers out of 50 farmers. First, we evaluated the farmers’ understanding in terms of decisions and weed impacts of the different output formats by grading their answers as entirely correct, partially correct (*i.e.* correct answer with additional wrong elements) or incorrect. Then, they were asked to evaluate how easy it was to handle and analyse the table (*e.g.*, finding a cropping system in the table is: really easy, easy, difficult and really difficult). After that analysis, the farmers were shown an example of a decision tree and their comparative reaction to this option was recorded. Finally, we wrote down farmers’ comments and suggestions for the development of the DSS.

IV.2.2.3 Workshops with future users of the decision support systems (step 4)

The surveys and group meetings gave us precious advice to develop the DSS, but the absence of “*in situ*” tests of a prototype limited the improvement of the tool. The actual manipulation of the tool can bring out the different use cases that users are susceptible to have and that we are not expecting (Cerf et al., 2012a). Hence, based on Lefèvre et al. (2014),, we proposed a workshop to design cropping systems with crop advisors, using the prototypes of the DSS (Figure IV. 2).

The workshop was organized in two days, with time in-between to build and simulate the cropping systems designed during the first day and to produce the prototypes. During the first day, the vocabulary used by the crop advisors was recorded to ensure that we used the same ways to describe and synthesise a cropping system. Moreover, a set of weed impact indicators to evaluate the tested cropping systems was chosen by the crop advisors among all the indicators available in FLORSYS.

During the second day, the results of the FLORSYS simulations were shown to evaluate the proposed cropping systems. Then, the DSS prototypes were tested, locating and evaluating the same cropping systems on the decision trees. These were preliminary trees built from the cropping-system data base for the production situation of the workshop participants (Colas et al., in prep.-b) and the ones designed during the first day and simulated with FLORSYS during step 2 (Figure IV. 2). At the end of the second day, participants were asked to assess their satisfaction using the different decision trees.

The workshop was held in spring 2017 in Champagne, with five crop advisors. We voluntarily worked with a small number of participants to make it easier for all participants to participate and not be intimidated by a larger crowd. The small group made it also easier to fully record all the reactions of crop advisors. In November 2017, the participants of the workshop were asked to use an online R-shiny application (Chang *et al.*, 2017) (see screenshots in supplementary material section 5, (Colas, 2017)) of the DSS prototype consisting of the decision tree shown during the workshop and a metamodel built from cropping-system data base (Colas et al., in prep.-b), during step 2 (Figure IV. 2) to quickly and easily predict the weed impact indicators from synthetic cropping sytem descriptors, using random forests (see section IV.2.2.4.4). To evaluate their experience with the prototype, a short online survey with a semi-structured question assed: (1) the ease of use of this prototype, i.e. of entering new data, (2) their confidence in the ranking of cropping systems descriptors and on the results of the prediction and (3) what improvements users would like to have.

IV.2.2.4 The models to interact with the future users

IV.2.2.4.1 The virtual field model FLORSYS

FLORSYS is a "virtual field" testing the impacts of cropping systems on weed dynamics depending on the pedoclimate (Colbach et al., 2016b; Colbach et al., 2014b; Colbach et al., 2014c; Gardarin et al., 2012; Mézière et al., 2015d; Munier-Jolain et al., 2014; Munier-Jolain et al., 2013). It is a dynamic model at a daily time step where cropping systems are described by a detailed list of operations with dates of occurrence and options, including the crop succession (i.e. species, variety, mix of species), sowing (e.g. seed density, row orientation, sowing depth), harvest and mowing (e.g. date, cutting height), tillage and mechanical weeding (e.g. tool, depth, speed), herbicides (e.g. product, dose, spraying conditions), mineral and organic fertilization, irrigation, and other pesticides. The soil is described in terms of physical and chemical characteristics (e.g. texture, depth, rate of stones). The initial weed flora present at the onset of the simulated is described via the seed bank, with weed species and seed densities at different soil depths. Finally, the weather for the length of the simulation is needed, usually daily weather station inputs (e.g. daily radiation, rainfall and temperatures).

Each day, these input variables influence weeds and crops. Pre-emergent stages (surviving, dormant and germinating seeds, emerging seedlings) are driven by soil structure, temperature and water potential. Post-emergent processes (e.g. photosynthesis, respiration, growth, etiolation) are driven by light availability and air temperature. At plant maturity, weed seeds are added to the soil seed bank; crop seeds are harvested to determine crop yield. Life cycle processes also depend on the dates, options and tools of management practices, in interaction with weather and soil conditions on the day the operations are carried out (annex A8 section 1).

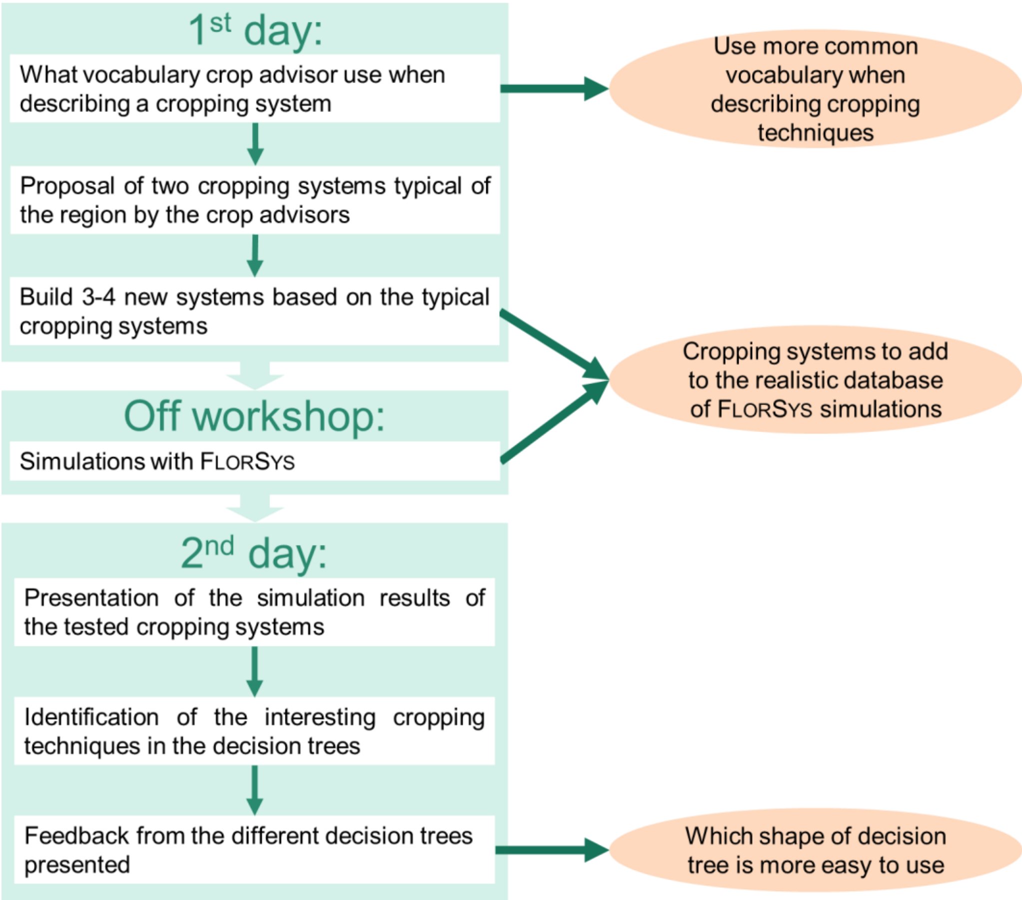

Figure IV. 2 : Framework of the workshop testing the future Decision Support Systems. (Floriane Colas © 2018)

IV.2.2.4.2 Indicators for assessing weed impacts on crop production and biodiversity

To simplify the evaluation of cropping systems, the many crop and weed state variables are transformed into weed impact indicators (Colbach et al., 2017a; Mézière et al., 2015c). The weed harmfulness indicators were developed with farmers and consider direct harmfulness for crop production (crop yield loss, harvest pollution by weed debris), technical harmfulness (harvesting problems due to green weed biomass blocking the harvest combine), and sociological harmfulness (field infestation by weed biomass during crop growth) which reflects the farmer's worry of being thought incompetent by his peers even if there is no effect on yield loss. We added two indirect harmfulness indicators due to pest survival and dispersal by weeds (increase in yield loss due to weed-borne take-all disease in cereals, parasite risk due to the holoparasitic plant *Phelipanche ramosa*) (Colbach et al., 2017a; Mézière et al., 2015c).

A second series of indicators concern weed-mediated ecosystem services. Functional diversity was assessed via weed-borne trophic resources for birds, granivore carabids and pollinators. Two further indicators assess weed contribution to wild plant biodiversity, via species richness and evenness

(Pielou's equitability index). A last set of indicators is still being developed and will assess the contribution of weeds to limiting environmental impacts of cropping systems e.g. reduction of soil erosion. These indicators were the outputs used in step 2 of Figure IV. 2 to evaluate cropping systems in both decision trees (section IV.2.2.4.3) and random forests (section IV.2.2.4.4).

IV.2.2.4.3 Visual guides for pinpointing pertinent changes in cultural practices

Based on the results of step 1 (section IV.2.3.1), the visual guides aim to support users in their choice of which cultural practices to change and how to combine them in order to reach a given weed-impact goal. These are based on the results of the CART data mining applied to a large and diverse cropping-system data base in step 2 (Colas et al., in prep.-b). Instead of detailed lists of operations as those used by FLORSYS (section IV.2.2.4.1), they are fed with synthetic cropping system descriptors as proxies for meta-decision rules.

IV.2.2.4.3.1 Format for cropping-technique combinations

The various format options were inspired by the results of the online survey of section IV.2.2.1, past research studies, feedback from technical institutes and cooperatives as well as participants in the group meetings. For instance, the results of FLORSYS simulations were often synthesized as decision trees (Appendix), identifying combinations of cultural practices resulting in different performances in terms of weed impact on crop production and biodiversity (Colbach and Cordeau, 2018b; Mézière et al., 2015a) and have already been used successfully to design innovative multiperformant cropping systems (Colbach et al., 2017d). Technical institutes and private companies propose a similar approach for various decisions related to crop protection (e.g. slug control (Bodilis *et al.*, 2017)) or environmental impacts (e.g. risk of run off in potatoes (Arvalis-Institut du Végétal and Bayer, 2016)).

These decision trees may not always be evident to read for everyone and indeed, participants of the first group meeting (section IV.2.2.2.1) proposed an alternative format based on tables. Consequently, we transformed the decision trees into a table showing the same information as the trees, with the first column showing the different performance profiles in terms of weed impact and the subsequent columns showing cultural practices (e.g. sowing date of cash crops, proportion of winter crops in rotation). Each line describes the complete list of combined cultural practices associated to a given performance profile. This format included many redundant information as two lines can have many practices in common, which, in the tree, are merged into a common branch segment. The table also comprised empty cells when practices have no significant effect on weed depending on the other cultural practices of the combination.

IV.2.2.4.3.2 Format for displaying the weed impact indicators

In previous studies using the indicators computed by FLORSYS, polar area diagrams (Mézière et al., 2015d) and barplots of multicriteria scores were used (Colbach and Cordeau, 2018b). Here, we wanted to keep the details of all indicators as experience with other multicriteria tools such as DEXiPM (Pelzer *et al.*, 2012) showed that users are often more interested in individual scores than in the final score. Consequently, we tested five kind of multi-criteria diagrams (Figure IV. 3): polar area diagrams (A), bar plots (B) and different kind of tables improved with colour gradients (C) or integrated bar plot (D).

Combining in a same ensemble values that need to be maximized with values needing to minimize was always harder to be understood by the crop advisors and farmers. This is why radar plot were not tested. A and B required rescaling the different indicators to a common [0,1] scale values to make them comparable.

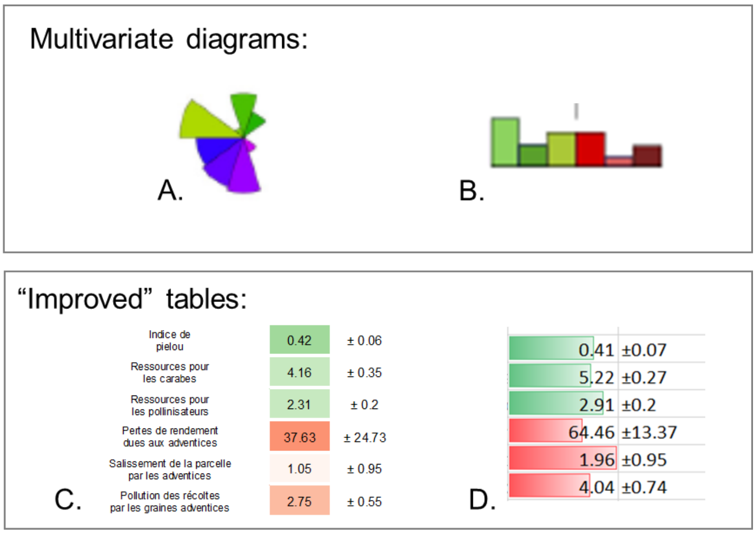

Figure IV. 3: Different output format that we tried to test the prototypes of the decision support system. (Floriane Colas © 2018)

IV.2.2.4.4 A meta-modelled FLORSYS for predictions: FLORSYS's random forest

Because of its complexity, FLORSYS is slow to simulate the cropping systems (e.g. 40 minutes for a 13-year long simulation and one weather repetition, chapter II, Colas *et al.*) and cannot be used in workshops for real-time evaluation of cropping systems. Moreover, step 1 (section IV.2.3.1) showed the need for a simpler tool that was fed by meta-decision rules instead of detailed list of operations. Thus, in step 2 (Colas et al., in prep.-b), we used the random forest method to produce a metamodel, i.e. a model of the model, prediction weed impact indicators from the same synthetic cropping system descriptors as the decision trees (section IV.2.2.4.3). Random forest are an ensemble data mining method based on classification and regression trees that improves their prediction capacities (Breiman, 2001). To all the weed impact indicators, the rfsrc package (Ishwaran and Kogalur, 2017) for multivariate forest was used to create random forest and compute the predictions. The resulting metamodel will emulate the behaviour of FLORSYS, i.e. predict weed-impact indicators from cropping system inputs. The prototype used in the workshops of step 4 (section IV.2.2.3) was built from the cropping-system data base of step 2, using the cropping systems corresponding to the same production situation (Colas et al., in prep.-b).

IV.2.3 Results

IV.2.3.1 Crop advisors' needs and constraints to use a decision support system

Forty crop advisors from all over France (16 regions) answered the online survey (annex A8 section 2). Weed harmfulness indicators were considered the most useful by crop advisors, especially grain yield loss, harvest pollution and field infestation (Figure IV. 4).Pest problems specific to certain regions or crops (i.e. weed-borne take-all disease and broomrape risks) interested fewer advisors. Ecosystem service indicators were judged less important, but still considered useful by 30 to 70 % of the respondents, with food offer for domestic bees scoring best. But in terms in weed benefits, advisors were much more interested in a potential contribution of weeds, particularly during summer fallow, to reducing other environmental impacts of cropping systems, i.e. pesticide transfer, nitrate leaching and soil erosion. When asked how many indicators the tool should have as output, 71% crop were interested in having multiple indicators, without any aggregation of the results, to and the same amount of crop advisors wanted also be able to choose from the pool of indicators. 91% said that they would be interested in two indicators summarizing, respectively, harmfulness and ecosystems services indicators. Only 25% said that they would be interested in a global value score aggregating for all indicator performances.

The major reason why crop advisors considered weeds difficult to manage was the lack of biological knowledge (*e.g.* how long do weed seeds persist in the soil? When and how fast do they emerge?) (Figure IV. 5). The lack of efficiency of some practices (*e.g.* mechanical weeding or the difficulty to know the actual efficiency of tillage) and the existence of particularly difficult species (like perennial plants) were two other frequently cited answers. The kind of issues the advisors had with weed control influenced the kind of data they wanted to provide to feed a DSS. The same was true when looking at the kind of decisions that the advisors would like to take with a DSS (Figure IV. 6). The combination of the two analyses led to the identification of different needs in terms of DSS: (1) users confronted with major problems such as herbicide resistance, highly competing weeds or the need to manage infestations at a multiannual scale preferred to focus on meta decision rules (*e.g.* a plough every two years) for the DSS (Figure IV. 5) and would be ready to radically change their practices (*e.g.* diversification of crop succession) (Figure IV. 6); (2) users deploring the lack of knowledge on how to combine a multitude of techniques and how to efficiently manage a diversity of weeds, both in terms of costs and weather robustness (Figure IV. 5), were ready to understand and modify their practices before reaching a dead-end and would provide a detailed description of the practices (*e.g.* crop succession, list of operations) to finely tune their system in terms of options and timings of operations (*e.g.* which practices, which mechanical weeding) (Figure IV. 6).

The few farmers that answered the survey confirmed these two contrasting needs for a DSS. A farmer from northern France stated that "*to find the best weather conditions to apply herbicides*" was the major obstacle to efficient weed management. A DSS should "*advise on the crops to avoid when the user wants to avoid the [weed infestation] problem*". He then declared that "*it is important to provide all management practices*" when asked the level of detail that he was ready to provide to the tool. A farmer from Picardie had different needs in terms of DSS. For him, a DSS should help on *"the effect of crop rotation in order to control a given weed species*" and it should use "*the major management rules*". Another farmer from Bretagne had similar views on a DSS and weed management constraints. He considered that weeds "*affect the whole crop management plan and [that] no technique is as efficient as herbicides*" and for that reason "*meta-decision rules*" were needed for the DSS.

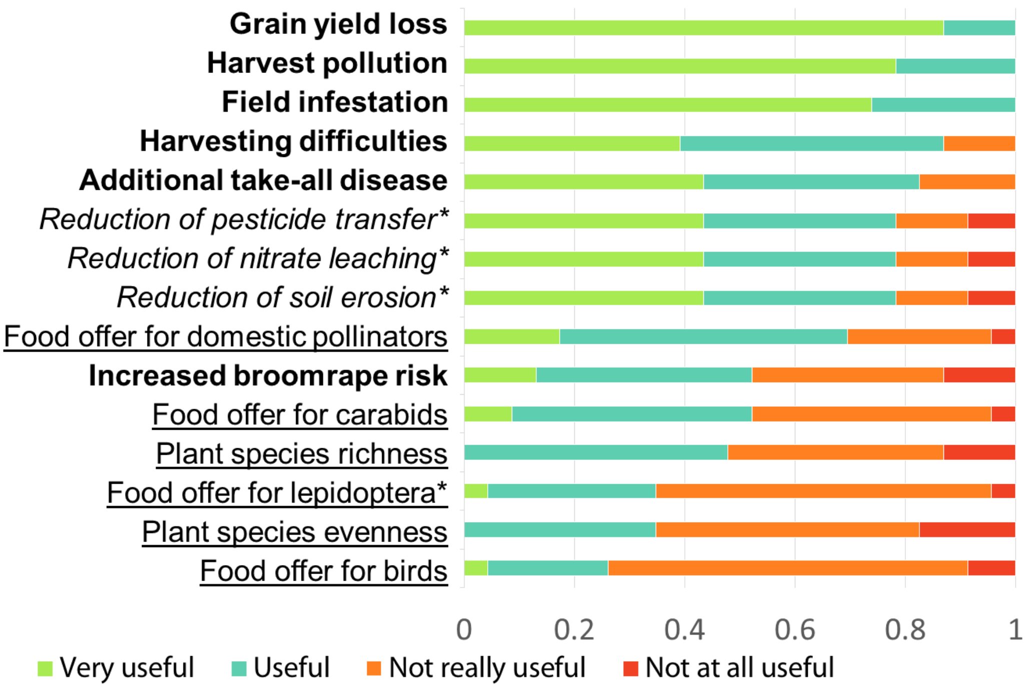

Figure IV. 4 : Which weed impacts interest crop advisors? Proportion of answers in the online survey assessing the usefulness of the weed impact indicators available in FLORSYS. Indicators of weed harmfulness for crop production (**in bold**), of weed contribution to limiting environmental impacts of cropping systems (*in italics*), of ecosystem services provided by weeds (underlined). (*) Shows indicators that are still in development. (Floriane Colas © 2018)

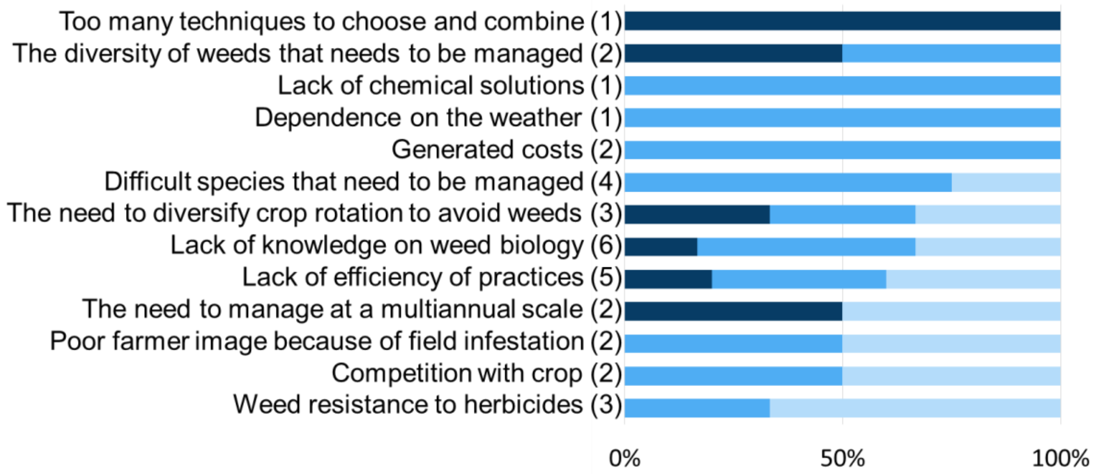

Figure IV. 5 : Willingness of crop advisors to provide complex data on cropping systems for a decision-support system depending on their perception of weed control issues. Percentage of advisors willing to provide detailed lists of operations (dark blue), synthetic meta-decision rules (light blue) or both (intermediate blue) depending on why they consider weeds difficult to manage (in brackets: number of advisors, of the 15 full answers, having mentioned the reason). Respondents who were left free to complete in their own but "weed resistance to herbicide" and "long persisting seeds in the soil" were given as an example. (Floriane Colas © 2018)

IV.2.3.2 Contributions of the group meetings

IV.2.3.2.1 Farmers' reactions to the advisors' responses to the online survey

Generally, the farmers of the Picardie group meeting agreed with the crop advisors' answers to the online survey. For example, when asked why weed management was difficult, they talked about the lack of active ingredients and of alternative solutions. The lack of information on species and biology was also stressed out, with precise examples, e.g. allelopathy. They also mentioned climate change and inter-annual weather variations.

Although, farmers were more open to innovation than the crop advisors thought by suggesting more and more diverse modifications of cropping techniques when asked what level of disruption in the existing cropping system to test with the DSS. However, they were less open to changes in crop rotation, because of missing outlet for the new production in the region. Farmers were also more sensitive to the weather influence and said it was difficult to project farther than three years because of the frequent change in policies.

The outputs presented (Figure IV. 3) were much discussed, saying that the display of inputs was hard to understand. The decision tree presented as an example was difficult to understand and confusing for some farmers, and they suggested a table format instead which was tested in the next group meeting (section IV.2.3.2.2). Finally, they stated that the future DSS needed both a detailed version of the inputs and a synthetic one "*depending on the user and the available time*".

IV.2.3.2.2 Farmers' feedback to improve the format of the decision support system

Farmers were presented FLORSYS and the project to develop a decision support system from it. First, the table-shaped visual guide for identifying pertinent changes in cultural practices based on feedback from the previous meeting (section IV.2.3.2.1) was presented (Appendix). The evaluation of the table was two-fold. First, it assessed whether the farmers were able to identify the correct combination of different cultural practices corresponding to a given cropping system in the table. The participants considered this to be difficult (70% of the answers) or very difficult (20%). Then, we assessed whether the participants understood the table correctly, i.e. whether they drew the correct conclusions in terms of decisions and weed impacts. There were only 20 % of correct answers, the rest being totally wrong (45 % ± 30 %) or comprising partially incorrect answers (35 % ± 30 %). Conversely, when a decision tree was shown, its principle was immediately understood and approved by all farmers.

During the questionnaire time, farmers were discussing together, helping each other to understand and propose interpretations. The majority of their feedback consisted of a discussion with us, asking questions and giving us their immediate thoughts. This recommends to encourage discussions in small groups of participants for a better understanding of the prototype for the future workshops.

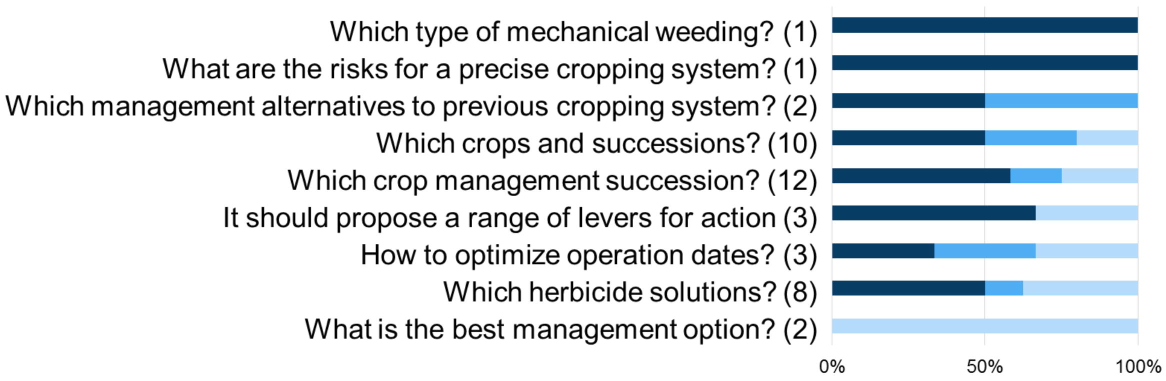

Figure IV. 6 : Percentage of answers of how much data crop advisors are willing to provide for a decision-support system depending on the decisions they would like to take with it. Dark blue: detailed list of operation, light blue: synthetic meta-decision rules, intermediate blue: both, in brackets: number of advisors, of the 15 full answers, having mentioned the decision. (Floriane Colas © 2018)

IV.2.3.3 Workshops results to improve the prototype of the DSS

The objective of the workshop was to use the prototypes in a cropping system design situation. Crop advisors were asked to design cropping systems, to use decision trees and rank the display of weed impact indicators. After the workshop, they could test on their own, via an online link, FLORSYS's random forest that can predict weed impact indicators depending on cropping systems descriptors values.

IV.2.3.3.1 Vocabulary to describe cropping systems

The design of cropping systems during the first day and the handling of the decision-tree prototype (annex A8 section 4.2) triggered a discussion on more efficient ways to describe cropping systems in a synthetic way. This resulted in: (1) new ideas for cropping system descriptors: e.g. crop rotation length, alternation of spring and winter crops, frequency of tool use (e.g. frequency of hoe), composition of the crop rotation (e.g. proportion of cereal crops or legumes crops), return time of ploughing. As crop advisors usually referred to cropping techniques in association with a given crop species, we subsequently computed cropping systems descriptors not only over the rotation and also crops species e.g. frequency of ploughing in wheat, number of herbicide operations in oilseed rape. (2) Other proposals were actually already included in the initial decision tree but their labelling was unclear, (e.g. the proportion of fodder crops in the rotation was labelled initially as the proportion of multiannual crops). (3) Some proposals were too vague to become serviceable inputs for the decision tree. For instance, the participants proposed an input qualifying whether sowing was early or late. But the decision tree and the underlying FLORSYS simulations require actual calendar dates to correctly predict effects. Moreover, the early or late character of a sowing (or any operation) not only depends on the crop but also on the region. To include this type of input, an additional layer is required on top of the DSS to transform qualitative inputs into quantitative ones, considering regional specificities.

IV.2.3.3.2 Display of weed impact indicators and use of decision trees

In order to choose the best way to display the weed impact indicators, the crop advisors were presented three different displays of the weed impact indicators values (B, C and D in Figure IV. 3). All five participants considered the format C to be the best, and the multivariate barplot B the worst. A colour blind participant found option D as good as option C because he could not discriminate the colour variation of C, in contrast to the bar heights of format D. The crop advisors also suggested an additional indicator assessing the dynamics of weed biomass over the years, to discriminate those branches that decreased weed infestation over time from those that were unable to avoid an increase. Overall, they evaluated that the use of decision tree when working as a group to be 50% quite easy and 50% not easy (Table IV. 2). When evaluating the use of the tree alone, it was only 60% not easy to 40% not easy at all. The reading direction of the table was not clear enough for farmers and they struggled with the different cropping systems descriptors.

Table IV. 2 : Are decision trees easy to use? Evaluation by the five crop advisors of the ease to use a decision tree to design new cropping system in a group or alone.

If used?	Really easy	Quite easy	Not easy	Not easy at all
In group	0	2.5[§]	2.5	0
Alone	0	0	3	2

[§] One participant hesitated between two answers

IV.2.3.3.3 Use of FLORSYS's random forest

After the workshop, the link to the R-shiny online prototype of FLORSYS's random forest (annex A8 section 5) was sent to the participants of the workshop. The application takes approximately three seconds to predict weed impact indicators for a set cropping system descriptors entered by the user. R-shiny. Only two of the workshop participants gave feedback on the easiness of use, both stating that they found it easy to fill in the inputs. As it is fastidious to change all cropping descriptors values in the app, because there are many, we used the mean value for all descriptors. This was satisfactory for one crop advisor but not for the other crop advisor.

IV.2.3.3.4 Overall use of the tool and trust in results

The crop advisors were asked their confidence in the tool results to see how the tool is perceived and what support to provide when giving the tool to users. In the workshop, the crop advisors estimated that the agronomical results from the decision trees and random forests were moderately interesting, one crop advisor saying in the comments section of the survey that "*Surprising results considering the diversity of the rotations which led here to an average performance*". The two crop advisors testing the R-shiny FLORSYS's random forest were surprised by the ranking of input variables in terms of multiple weed impacts, especially by the low importance of crop succession (in the model) of winter crops and multiannual crops.

However, the crop advisors are mostly encouraging for the development of the tool as three of them would use and recommend the future tool, only one would probably not recommend the tool and one did not respond (Table IV. 3). In the comment section of the survey, crop advisors ready to use and recommend the tool specified that "*the current version is too complicated to use and to understand*" but "*improved in terms of visual display*" and "*adapted according to end user*" it could be an interesting tool. One crop advisor specified how the decision trees and FLORSYS's random forest should be used with FLORSYS simulations; the decision tree should be "*tool to use within working groups aiming to [radically] change the system*" and the random forest should "*rather be used individually to test changes in a given system*". The group dynamic was important to help to use the tool (Table IV. 3).

Table IV. 3: Evaluation by the five crop advisors of the workshop, the results of the decision tree and the prototype of decision tree.

	No	Probably no	Moderately	Probably yes	Yes	Comments
Are the decision tree results agronomically interesting?	0	0	5	0	0	
Was the work as a group rewarding and beneficial for the reflection	0	0	0	5	0	
Would they use or recommend the tool?	0	1	0	3	0	One crop advisor did not respond

IV.2.4 Discussion

The present study proposed and applied a methodology to combine participatory tool design with data mining to transform an existing mechanistic research model into a decision support system (DSS). We interacted with crop advisors and farmers first to guide the kind of data to extract from the research model and how to quantify these data, and then to transform the resulting decision trees and random forests (produced in a previous study, chapter II, Colas et al., in prep.-b) into a prototype of the decision support system. For this purpose, we carried out an online survey aiming at both farmers and crop advisors to identify the type of tool in terms of use, inputs and outputs. The next interaction with users consisted in group meetings to observe what farmers thought of the crop advisors' answers to the online survey, how users would handle different tools and interpret their output formats, ranging from the virtual field model FLORSYS to visual decision trees on paper. Finally, the ergonomics and applicability of a prototype of the DSS was tested in workshops. During all the different steps, we not only collected technical data on how to organize inputs and outputs, but also assessed how crop advisors and farmers see weed and weed management, how far they are ready to go when innovating their practices etc.

IV.2.4.1 Weed management vision of crop advisors and farmers

A crucial first step of our approach was to evaluate how stakeholders think about weeds and their management. When asked why they considered weed management to be difficult, crop advisors focused on lack of knowledge, both their own and the current knowledge, whether on weed biology or on efficiency of techniques. Our online survey did not produce sufficient farmers' responses to directly compare their attitude to that of crop advisors, but the first group meeting which confronted the crop advisors' responses to a group of farmers did not identify any major dissension.

Conversely, other studies that specifically questioned farmers in face-to-face interviews on the probable causes of weed infestations in their fields came up with slightly different answers. Farmers often blamed their infested fields on events outside their control, e.g. weather events, neighbours and neighbouring fields (Pasquier and Angevin, 2017) as well as technical failures, e.g. herbicide failure, inefficient mechanical weeding or the existence of difficult weed species (Pasquier and Angevin, 2017; Wilson et al., 2008). The technical failure aspects were also cited by the crop advisors in our online survey but were considered less important.

The differences between our survey and literature studies cannot be attributed only to a different stakeholder type, i.e. crop advisors vs farmers, or questions that were differently formulated. The method of interview is another factor, as answers to anonymous online surveys tend to be more open than when facing a human interview partner or a group of peers. Moreover, diverse attitudes exist even within a given stakeholder group. Indeed, both our online survey and previous literature working with diverse interview methods reported farmers to have a more herbicide oriented vision, in contrast to crop advisors and farmers in the group meeting focusing on agronomical knowledge and techniques to the detriment of herbicides (Doohan *et al.*, 2010; Pasquier and Angevin, 2017). Conversely, some of our group meetings showed farmers to be more open to innovation in terms of changes in crop management than crop advisors. This is consistent with the many farmers group setting up all over France to test innovative practices, such as the GRCETA which participated in the present study or GEDAs (Groupe d'Étude et de Développement Agricole, i.e. study group on agricultural development) focusing on direct sowing (GEDA de la Tille). However, feedback from farmers also highlighted that cropping system innovation not only requires decision support also the necessary socio-economic environment, particularly, buyers for the resulting production (Meynard *et al.*, 2013).

IV.2.4.2 Contribution of future users for the type and format of the DSS

Identifying the different profiles and needs for a DSS of crop advisors, via the online survey and group meetings, led us to propose two types of DSS, depending on the situation (Figure IV. 7): (1) a synthetic one, with meta decision rules for a radical change in cropping systems when faced with a dead-end (due to herbicide resistance, high weed infestation…); (2) a detailed one, describing cropping systems with detailed list of crops and operations and aiming to adjust practices before reaching a dead end. The use of one or the other of the two types of DSS may depend on the advisor profile of the crop advisor as well as the context where the tool is used. When providing precise and individual advice for one particular situation, the detailed tool would be better, whereas the synthetic tool would be more adapted for group advice that needs to fit a larger range of goals and constraints. This correspond to the fact that farmers have different needs of decision support tools depending on where they are for the change of their cropping system (Prost, 2008). Either they want: to conceive and evaluate solutions; to explore the flexibility and robustness of a cropping system or adapt the cropping system to deteriorations in the cropping system. This tool was conceive to help farmers achieve the conceiving and evaluation part for changing their cropping system.

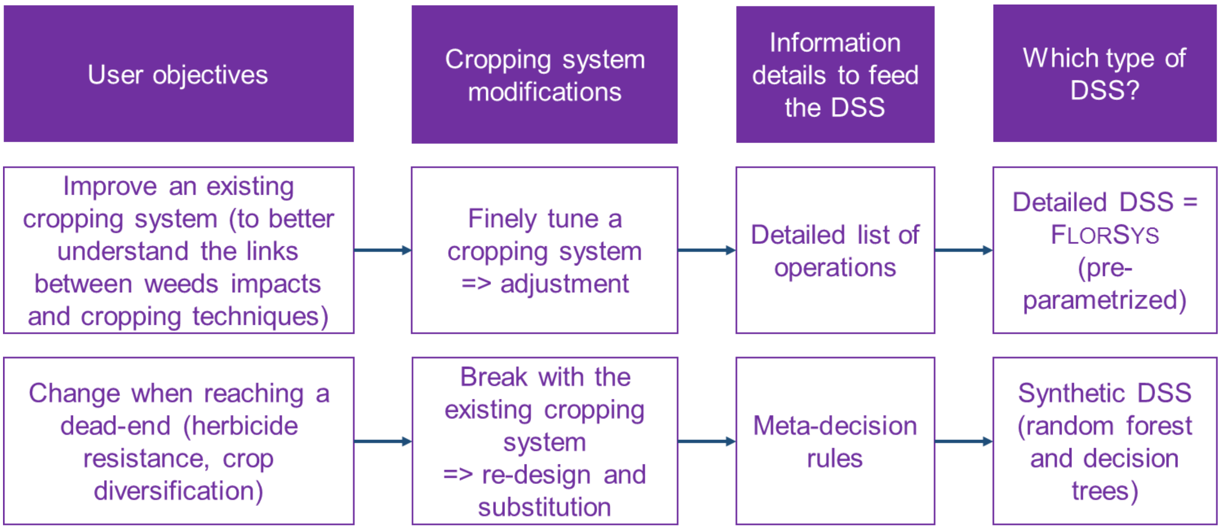

Figure IV. 7 : Schema representing the two types of decision support system (DSS) depending on the user objective and the level of details that the user is ready to feed to the DSS. (Floriane Colas © 2018)

The synthetic DSS is composed of charts of the most important cropping system practices, of decision trees, and FLORSYS's random forest, an emulator of FLORSYS based on random forests. The format of the new synthetic DSS tool was selected by the future users. For the visual guide, the tree format accommodated the majority of users, contrast to the table. For the display of weed impact indicator results in both the visual guide and FLORSYS's random forest, the users preferred a display showing values for all weed impact indicators, highlighting with colour codes, instead of bars or aggregated scores. The colour code was judged helpful to visually and faster extract the results, even though multivariate decision making based on colour seems to be only useful when the level of data complexity is low and mostly for females (Stella and Malcolm, 2002). Indeed, the red/green dichotomy is not adapted to colour-blind people, as we observed with one of the crop advisors in the workshops. Using different colours could help the 8% men and 0.5% women that are colour blind (Colour blind awareness, 2017). For a finishing touch of the development of the decision support system, intake from human-computer interaction specialist would be best.

IV.2.4.3 Towards the future DSS

User's advice is essential to design a decision support system but not all the suggestions of future users are relevant or possible to follow. For instance, the content of the DSS was derived from FLORSYS, with the sensitivity analysis performed on FLORSYS identifying the inputs essential for predicting weed impact on crops (chapter III, Colas *et al.*, in prep. b). These essential inputs must be included in the DSS, even if they are difficult to handle by the users. This applies even more to the pre-parameterized version of FLORSYS intended for fine-tuning cropping systems. It requires, for instance, an initial weed seed bank present at the onset of a FLORSYS simulation, a variable notoriously difficult to access, even for scientists (Dessaint *et al.*, 1986), let alone for farmers or crop advisors. In order to reconcile usability of the tool and quality of prediction, we propose to offer a regional set of options for these difficult variables from which the user the can choose. In the example of the weed seed bank, we thus already produced a list of regional weed seed bank estimated from regional weed flora assessments and checked the adequacy of this approach with independent field observations (Colbach *et al.*, 2016a). Ultimately, the pre-parameterization would transform FLORSYS into the more detailed tool requested for fine-tuning (Figure IV. 7).

The reaction of crop advisors to the ranking of cropping system descriptors in terms of multicriteria weed impact when testing the online FLORSYS's random forest demonstrates that it is essential to provide more instructions and support with the tool. This step is crucial to build the users' confidence in the tool. Here, for instance, R-shiny the online test illustrated that the testers were not sufficiently aware that the ranking was based on a multicriteria assessment of weed impacts, and not solely on weed-borne yield loss or field infestation, which explained the discrepancy between their perception of reality and the advice proposed by the tool. To remedy this lack of confidence, the input ranking could be completed by information on the causes of the different effects. This would also provide the kind of missing knowledge that many advisors required during the online survey (section IV.2.3.1). Moreover, the final DSS will let the user choose the kind of weed impacts that should be included when ranking the cropping system descriptors and running the predictions. This means, for instance, that advisors focusing solely on controlling weed harmfulness would find the kind of input ranking they are familiar with.

Rose et al (2016) produces a checklist for good design of decision support tool. In our study we worked on the first four parts of the checklist, i.e. performance (is the tool functioning and useful?), ease of use (are the user interface, the trees and forest easy to navigate?), peer recommendation (is it possible to encourage knowledge exchange with the tool?) and trust (is the tool evidence-based and do we have the trust of users?). These parts still need some work done, especially in the introduction to the tool to gain the trust of the users. Moreover, we still need to complete the rest of Rose et al's checklist (e.g. is the tool matching habits of farmers? how far is the tool applicable to all types of farming?) by running more workshops. Here, we voluntarily ran workshops with a small group of relatively homogenous participants to facilitate exchanges and individual expressions. This helped a great deal to uncover the limits and possibilities of the prototypes. The various group meetings and workshops also demonstrated the usefulness of group interactions, e.g. leading to a better understanding of the proposed tool formats and triggering ideas on novel tool formats. The importance of group dynamic is well known advantage of workshops, for instance to help farmers to distance themselves from their current situation and to explore new ideas thanks (Lefèvre *et al.*, 2014). or to help the learning of a new technology and help its adoption (Labarthe, 2010). So, we need to putting the tool through a broader range of future users to develop the plasticity needed for the different usages that users will have have (Cerf et al., 2012a). Especially since knowing that farmers may not use a model a tool as a global, but only using the part that they are interested in (Toffolini *et al.*, 2017). Only by including more and more users, we will refine the cropping system descriptors to the most useful variables and produce a real decision support system.

IV.2.5 Conclusion

The development of a Decision Support System (DSS), whether from existing models or *de novo*, needs many interactions with the future users. Here, we proposed and applied a methodology combining online surveys, group meetings and workshops to integrate crop advisors and farmers into this process, showing what they brought to the development of the tool. Based on the users' needs and objectives for the future DSS, we identified two different types of prototypes, depending on the users' openness to change, their willingness to invest in the use of the tool and the challenges they faced in terms of weed infestation. Together, we identified the structure of the tool and how to display outputs. The workshops helped us to test the prototypes and to improve the vocabulary to use in the tool. The study also identified the limits of the DSS, not only intrinsically in terms of user friendliness or quality; feedback from farmers highlighted that cropping system innovation also requires a suitable socio-economic environment, for instance outlet for novel crops. Further back and forth runs between users and developers (both scientists and software engineers) are still needed to polish the tool and satisfy both parties, i.e. crop advisors and farmers on one hand, and researchers on the other hand.

Acknowledgements

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Appendix

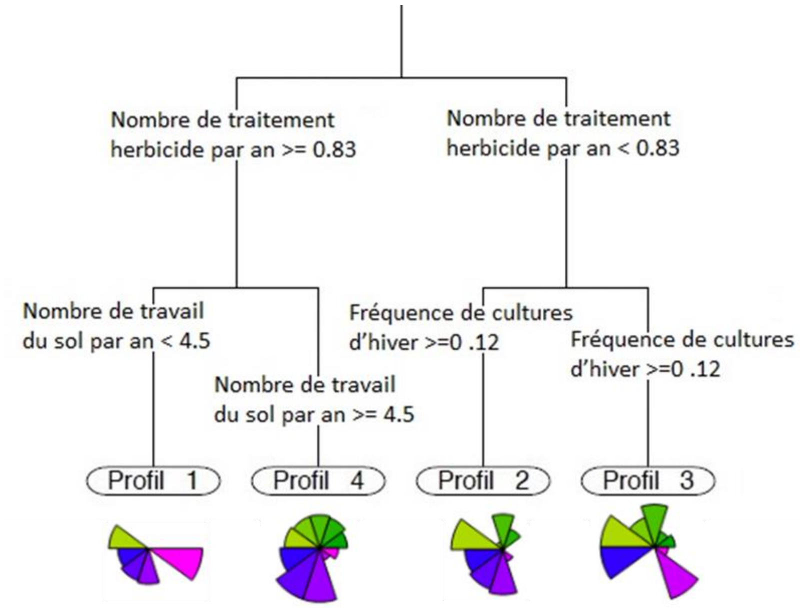
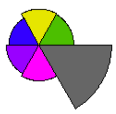
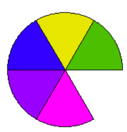


Figure IV.A. 1: Extract of a classification tree model as a possible visual guide of the decision support system for identifying innovative combinations of cultural practices. Polar area diagrams showing the weed impact indicators values (From Mézière *et al.*, 2015a)

Table IV.A. 1: Extract of the translated table given to farmers during the meeting in Aube (France) as a possible visual guide of the decision support system for identifying innovative combinations of cultural practices. Each row corresponds to a cropping system associated to a diagram presenting their performances in the form of weed impacts indicators; pink: yield loss, purple: field infestation, blue: harvest pollution, yellow: nitrate leaching limitation, green: food offer for domestic bees, gray: treatment frequency index for herbicides.

Profile (Cropping system performances)	Combinations of cultural practices				
	Diversity of crop species or varieties in the crop succession	Sowing date of cash crops	Harvest date of winter crops	Winter crop proportion in the succession	Mean tillage depth
	>= 1/30	after 15th January	before 10th July	< 1/3	no information
	< 1/30 : monoculture	after 15th January	before 10th July	< 1/3	no information
	no information	after 15th January	before 10th July	>= 1/3	no information
	< 1/30 : monoculture	after 15th January	before 10th July	< 1/3	no information
	no information	before 15th January	after 10th July	no information	< 11 cm
	no information	after 15th January	before 10th July	>= 1/3	no information

IV.3 Conclusion

Dans cette partie, nous avons décrit la participation des futurs utilisateurs de l'OAD au développement de l'OAD, et la manière dont nous avons fait la synthèse entre les travaux plus statistiques du chapitre II et III avec l'agronomie et la prise de décision stratégique par les conseillers agricoles et les agriculteurs. Nous avons pu identifier deux types d'utilisation pour l'OAD, ce qui se traduit en deux outils possibles : (1) un outil détaillé, correspondant au modèle FLORSYS actuel, mais étant pré-paramétré en prenant en compte les conditions locales pour faciliter son utilisation, et (2) un outil synthétique correspondant à une combinaison d'arbres de décision et de forêt aléatoires, vus au chapitre III. Nous avons également établi que le format arbre de décision était le plus approprié et le plus compréhensible par les utilisateurs pour faire ressortir les différentes combinaisons de techniques. En ce qui concerne la disposition des indicateurs, un tableau couplé à un jeu de couleur pour aider à une lecture rapide du niveau des indicateurs a été choisi. Des descripteurs ont été voulus et ajoutés quand c'était possible à l'outil. Ces descripteurs ont d'ailleurs été utilisés dans le chapitre précédent. Il ressort que les deux méthodes utilisées dans les chapitres III et IV : l'interaction avec les utilisateurs et la fouille de données, n'ont pas forcément donné le même classement d'importance, cette différence d'apports entre les utilisateurs et l'analyse de sensibilité sera discutée plus en profondeur dans le chapitre suivant de discussion générale. Cela montre qu'il faut combiner la modélisation et les interactions avec les utilisateurs pour développer un outil qui repose sur des connaissances scientifiques mais qui reste fonctionnel pour les utilisateurs.

Chapitre V : Discussion générale

Ce travail de thèse avait pour but de développer un outil d'aide à la décision (OAD), avec l'aide de conseillers agricoles et d'agriculteurs, les futurs utilisateurs de cet outil, à partir du modèle de recherche FLORSYS. Cet outil d'aide à la décision avait pour objectif de permettre la réflexion pour concevoir des systèmes de culture multiperformants permettant à la fois le contrôle de la nuisibilité de la flore adventice pour la production agricole et la promotion de services écosystémiques. Dans ce chapitre final, nous allons d'abord revenir sur les principaux résultats des chapitres II à IV en les mettant en parallèle. Les chapitres II et III (Figure V. 1) s'intéressent à des problématiques de l'analyse de sensibilité et de la méta-modélisation similaires mais à différentes échelles et degrés d'implication des futurs utilisateurs. Quand bien même si le chapitre IV vient en dernier, il est celui qui a ponctué toute la thèse (Figure V. 1) et, à chacune de ses étapes, a amélioré des analyses des autres chapitres, en particulier du chapitre III. Ensuite, nous reviendrons sur les apports méthodologiques de ce travail de thèse. Nous continuerons par les apports de ce travail à l'analyse multicritère et à la conception de systèmes de culture, pour enfin terminer sur les perspectives pour le développement de l'OAD.

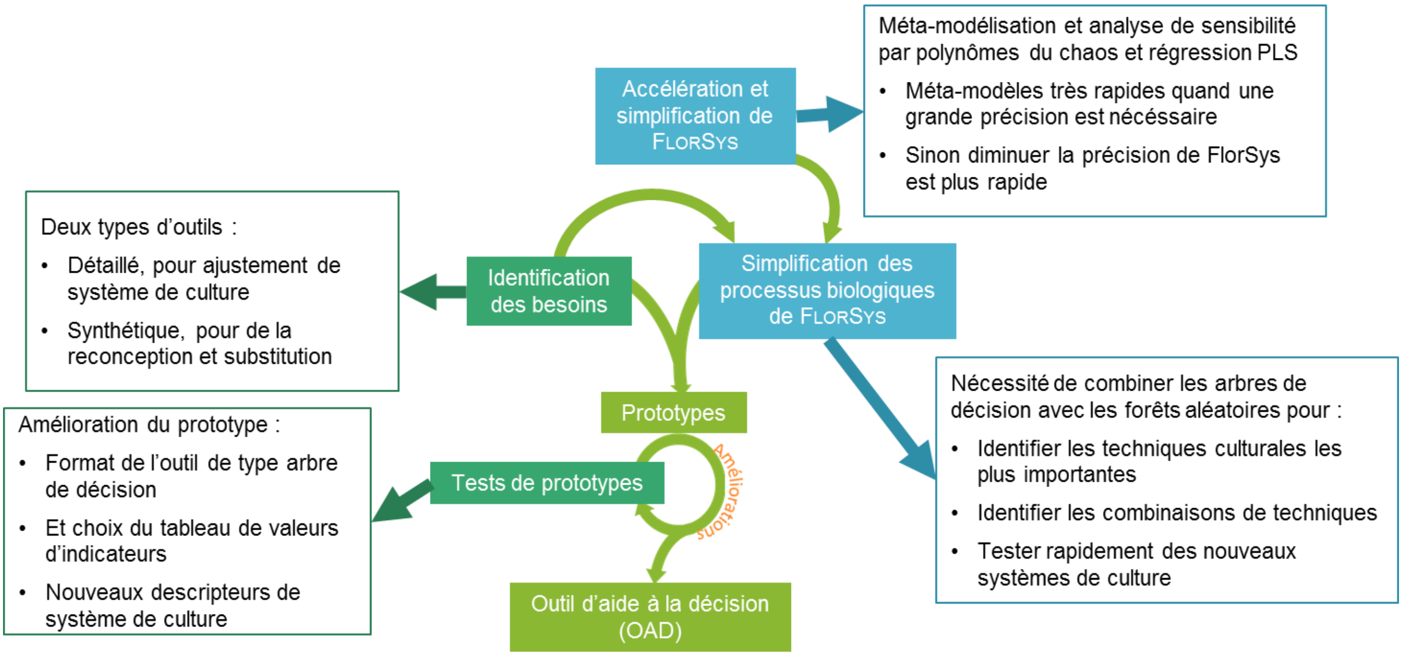


Figure V. 1 : Schéma des principaux résultats de cette thèse en fonction des différentes parties de la thèse pour le développement d'un outil d'aide à la décision à partir de FLORSYS

V.1 Imbrication des principaux résultats obtenus dans les différents chapitres

L'objectif de cette thèse était le co-développement d'un outil d'aide à la décision pour la gestion intégrée de la flore adventice à partir d'un modèle de recherche mécaniste complexe, c'est-à-dire FLORSYS. Cela faisait à la fois intervenir un développement avec les futurs utilisateurs de l'outil pour définir la structure et le format des sorties, mais aussi un développement lié à la simplification de modèle pour pouvoir utiliser les connaissances sur les processus de FLORSYS les plus essentielles pour l'aide à la décision (Figure V. 1). Nos principaux résultats sont :

- pour accélérer et simplifier un modèle complexe, il est possible d'utiliser les polynômes du chaos couplés avec de la régression PLS, mais pour intégrer le résultat dans un modèle plus large et le faire interagir avec d'autres modules, il est nécessaire de compléter les méta-modèles avec d'autres modèles et fonctions, réduisant ainsi l'avantage de gain de rapidité par rapport au module initial.
- en fonction de ce qui est identifié comme problématique pour la gestion intégrée des adventices, on peut observer différents profils en fonction des conseillers agricoles et aussi des agriculteurs, et deux cas d'usages se différencient : la reconception des systèmes de culture où la substitution de techniques requiert un outil synthétique, tandis que l'ajustement de systèmes a besoin d'un outil détaillé.
- pour l'outil détaillé, il est possible d'utiliser FLORSYS, mais en le pré-paramétrant pour les entrées les plus difficiles, en prenant en compte les spécificités régionales, pour en faciliter son utilisation.
- pour construire l'outil synthétique, il est nécessaire de combiner des arbres de décision avec des forêts aléatoires pour aider à identifier les techniques et les combinaisons de techniques les plus importantes et pour tester rapidement de nouveaux systèmes de culture.

La simplification et l'accélération du module d'interception du rayonnement lumineux au chapitre II a été complexe et n'a finalement pas eu les résultats escomptés qui étaient d'avoir un modèle FLORSYS méta-modélisé (FLORSYS-metaLight) qui permettrait de faire de nombreuses simulations très rapidement. Cette partie a tout de même permis de dégager une méthode pour méta-modéliser un modèle complexe et l'intégrer comme module dans un modèle mécaniste plus large. Ce chapitre a aussi permis d'augmenter la connaissance qu'on avait du processus d'interception du rayonnement lumineux par des plantes dans des couverts hétérogènes incluant des plantes sauvages, la hauteur de la plante est la variable la plus importante sur l'interception du rayonnement par rapport aux autres entrées environnementales qu'elles soient physiques, comme la latitude (et donc la longueur du jour et l'inclinaison du soleil), ou biologiques, comme l'influence des plantes voisines.

L'analyse de sensibilité et la méta-modélisation du module d'interception du rayonnement lumineux effectuées au chapitre II sont pertinentes pour des modèles (ou modules dans notre cas) ayant peu d'entrées, une dizaine environ. Pour l'analyse de sensibilité d'un modèle ayant beaucoup d'entrées, comme FLORSYS, les méthodes utilisées au chapitre II ne suffisent plus. En effet, il n'est plus possible de faire un plan d'expérience suffisamment équilibré, c'est-à-dire explorant tout l'espace des entrées en tenant compte de leurs corrélations, pour utiliser ces méthodes. Dans FLORSYS, les systèmes de culture sont décrits par une liste d'opérations détaillées. Le problème est le même pour établir le lien entre entrées et sorties, les polynômes du chaos ne pouvant pas gérer un nombre de variables aussi élevé. Nous avions certes déjà synthétisé les nombreuses entrées sous forme de descripteurs de systèmes de culture synthétiques, qui correspondent aux métarègles de décision réclamées par certains utilisateurs au chapitre IV. Cependant, le nombre final d'entrées reste très élevé (646). C'est pourquoi, dans le chapitre III nous avons exploré d'autres méthodes permettant de classer les entrées pour identifier celles ayant le plus d'influence sur la variation des sorties : les méthodes de classification et de régression issues de la fouille de données.

Les interactions avec les futurs utilisateurs au chapitre IV nous ont permis tout d'abord de définir deux cas d'usage de l'outil d'aide à la décision : (1) l'utilisation de précision, pour ajuster un système de culture qui respecte déjà les grandes règles d'un bon fonctionnement, et (2) l'utilisation synthétique pour reconcevoir des systèmes de culture ou substituer des techniques dans un système de culture qu'il faut repenser. L'outil détaillé, pour une utilisation de précision, existe déjà, FLORSYS permet de tester de façon très fine différents systèmes de culture. Un emballage pour les utilisateurs est cependant encore nécessaire car le modèle est à un état trop brut et demande la manipulation de fichiers textes et de remplir à la main toutes les options des outils utilisés. Pour l'outil synthétique, nous avons utilisé des métarègles de descriptions déjà employées pour décrire les systèmes de culture lors de l'analyse de sensibilité du chapitre III.

Les interactions avec les futurs utilisateurs ont aussi produit des connaissances, notamment sur l'effet de certains conseillers dans les freins au changement des pratiques culturales. Des enquêtes auprès d'agriculteurs ont déjà rapporté que le conseil et l'influence des techniciens dans ce conseil pouvaient freiner la réduction d'usage des herbicides (Pasquier and Angevin, 2017) ou avoir un effet de verrou vers l'utilisation de technologies moins consommatrices en intrants chimiques. En effet, le désengagement de l'État dans le conseil agricole a induit la privatisation et la commercialisation du conseil, ce qui a perturbé les services de conseils et de soutien financier, provoquant un décalage entre le conseil agricole et les agriculteurs (Labarthe, 2010). Ici, nous avons noté également quelques différences dans la réflexion entre conseillers agricoles et agriculteurs. Les agriculteurs étaient souvent plus extrêmes que les conseillers agricoles dans leur vision de l'innovation, soit en restant dans une réflexion principalement orientée herbicides (comme utiliser FLORSYS pour tester des mélanges d'herbicides), soit en poussant bien plus loin dans l'exploration des innovations (en proposant de nombreux changements qu'ils testeraient volontiers en virtuel avant de tenter en réel). Cela peut s'expliquer par le fait que les conseillers ont de plus en plus l'impression de s'occuper d'une diversité d'agriculteurs et qu'ils ne sont pas forcément bien accompagnés par leur organisation pour pouvoir adapter leur discours à cette diversité (Cerf et al., 2012b).

Pour développer un outil d'aide à la décision s'appuyant sur les connaissances concentrées dans FLORSYS, il était indispensable de combiner la simplification statistique/mathématique du modèle du chapitre III et la simplification par les utilisateurs du chapitre IV. Par exemple, pour la sélection des variables d'entrées et des sorties d'un outil d'aide à la décision, il est essentiel de combiner (1) les résultats de l'analyse de sensibilité, pour avoir les techniques et combinaison de techniques les plus importantes, et (2) les techniques auxquelles se rattachent les utilisateurs. Le choix de ces techniques s'est fait au chapitre IV, il est nécessaire pour que les utilisateurs ne soient pas perdus face à l'outil et qu'ils se rendent compte que leur classement *a priori* des techniques n'est pas toujours confirmé lors de la confrontation aux processus biophysiques révélée via l'analyse de sensibilité de FLORSYS. Par exemple, l'analyse de sensibilité globale a sélectionné le travail du sol en été, la profondeur du travail du sol et les herbicides comme étant les descripteurs du système de culture qui influencent le plus les impacts de la flore adventice sur la production agricole et la biodiversité. Les utilisateurs, focalisés sur la seule perte de rendement due aux adventices, s'attendaient à un effet majeur de la composition de la rotation (ex. proportion de cultures d'hiver) alors que cette variable est jugée mineure dans les analyses, une fois séparée de l'effet des techniques culturales associées aux cultures de la rotation.

L'outil synthétique défini au chapitre IV correspond aux arbres de régression et forêts aléatoires construits pour l'analyse de sensibilité au chapitre III. Cet outil s'appuie sur des entrées de type métarègles de décision pour décrire le système de culture. Il est constitué de trois éléments indissociables : (1) le classement des métarègles de décision aux effets les plus importants sur les impacts des adventices sur la production agricole et la biodiversité, (2) les arbres de décision qui sont des résultats visuels permettant d'identifier les combinaisons de pratiques et d'en tirer des conseils de modifications de pratiques à tester et (3) des forêts aléatoires permettant de prédire les indicateurs d'impacts de la flore adventice pour des nouvelles valeurs et combinaison de valeurs des entrées décrivant les systèmes de culture.

V.2 Contributions méthodologiques

V.2.1 Apports sur l'analyse de sensibilité et la méta-modélisation

Dans cette thèse, nous avons fait la démarche d'utiliser un modèle existant pour l'adapter aux besoins des utilisateurs, afin de conserver les fonctionnalités et les connaissances du modèle. Pour cela, le travail se situait à l'interface entre les statistiques et l'agronomie, deux disciplines assez éloignées, mais qui se sont alimentées mutuellement au long de ce travail. Même à l'intérieur des statistiques, nous avons exploré deux domaines différents et deux méthodes d'analyse de sensibilité et de méta-modélisation ont été testées. La première est la combinaison de polynômes du chaos avec de la régression PLS et la seconde est la combinaison d'arbres de classification et de régression (CART) avec des forêts aléatoires. Les deux approches sont complémentaires dans cette thèse car elles ne s'appliquent pas au même type de modèle. La première concerne un modèle relativement simple, avec un faible nombre d'entrées et un temps de simulation court, c'est-à-dire le module d'interception du rayonnement lumineux. La seconde concerne un modèle complexe avec de nombreuses entrées corrélées, ayant une large gamme de variation, des effets interactifs et un temps de simulation très long, c'est-à-dire FLORSYS. Dans le premier cas, les méthodes plus classiques d'analyse de sensibilité sont encore utilisables, car il est possible de préparer un plan d'expérience numérique et de faire toutes les simulations nécessaires. Pour le second cas, il fallait innover pour le plan d'expérience pour explorer au mieux l'espace des entrées, notamment en profitant de données déjà disponibles dans l'équipe. Dans le futur, combiner les deux méthodes, la fouille de données et la régression PLS pourrait être une piste intéressante à explorer pour améliorer la méta-modélisation. En effet, dans le cas de modèles biologiques dynamiques (par exemple, la modélisation de l'horloge circadienne des mammifères, ou des flux de régulation des gènes), Tøndel *et al.* (2011) ont utilisé le regroupement hiérarchique combiné à de la régression PLS pour développer des méta-modèles. En revanche, dans leur méthode, ils ne mentionnent pas l'analyse de sensibilité et la hiérarchisation des entrées les plus importantes.

Ce travail de thèse propose deux méthodes pour faire de l'analyse de sensibilité et de la méta-modélisation d'un modèle complexe en fonction du plan d'expérience réalisable et donc de son nombre d'entrées. Si le modèle possède un faible nombre d'entrées et qu'on peut construire un plan d'expérience équilibré, la méta-modélisation par polynômes du chaos couplée à la régression PLS est intéressante car elle permet d'identifier l'effet principal des entrées ainsi que leur effet total. Dès que le modèle a plus d'entrées (au-delà d'une vingtaine), CART et les forêts aléatoires deviennent intéressantes car moins contraignantes sur le plan d'expérience, mais elles ne permettent pas de discriminer l'effet principal d'une entrée de l'effet dû aux interactions avec d'autres entrées. Dans l'analyse de sensibilité par polynômes du chaos et régression PLS, comme les limites des plages n'ont pas été suffisamment représentées lors de la construction des polynômes lorsque nous avons cumulé les LHS, cela a posé des problèmes pour utiliser les méta-modèles aux limites des plages, montrant ainsi des limites pour extrapoler avec les polynômes du chaos. Pour les méthodes de fouille de données, les systèmes de culture issus de DEPHY n'appartenaient peut-être pas à la population des systèmes de culture du jeu de données d'apprentissage, ce qui n'est pas forcément une utilisation normale des forêts aléatoires, d'où des résultats de prédiction moindres. Mais les forêts permettent quand même de classer les systèmes de culture entre eux, ce qui est suffisant pour l'OAD.

Un autre parallèle à faire entre le chapitre II et le chapitre III est l'agrégation de variables pour limiter le nombre d'entrées. Dans le chapitre II, des variables de description des plantes voisines ont été agrégées pour avoir une valeur moyenne des plantes voisines, en attribuant une importance décroissante aux plantes voisines en fonction de leur éloignement à la plante cible. Dans le chapitre III, l'agrégation concernait le développement de métarègles de décision pour décrire un système de culture de façon synthétique réclamées par une partie des utilisateurs au chapitre IV. Cette agrégation d'entrées est recommandée par Marie et Simioni (2014) dans leur deuxième étape de méta-modélisation, inspirée de Kleijnen et Sargent (2000). En effet, pour optimiser le nombre d'entrées et éviter des redondances, il est possible d'agréger des entrées en fonction du niveau de généricité voulue par le méta-modèle. Dans le cadre du module d'interception du rayonnement lumineux, avoir une valeur moyenne pour caractériser les plantes voisines était amplement suffisant, tandis que pour pouvoir comparer plus facilement des systèmes de culture différents entre eux dans FLORSYS, il fallait passer par des métarègles de décision décrivant le système de culture. Les métarègles de décision ont l'avantage de rapprocher les entrées du modèle aux futurs utilisateurs, ce qui permet l'interaction entre analyse de sensibilité et co-développement avec les utilisateurs.

Si notre objectif est d'accélérer un modèle à faible nombre d'entrées, alors différentes étapes doivent potentiellement être suivies. Dans notre cas, pour l'accélération de FLORSYS, il aura fallu sélectionner le module le plus lent, explorer ce module pour savoir comment le méta-modéliser et faire une analyse de sensibilité de façon appropriée par rapport à ses spécificités. L'analyse de sensibilité visait à sélectionner les entrées les plus importantes du module et la méta-modélisation visait à faire un modèle du module plus rapide. Cette exploration s'est déroulée en différentes étapes : (1) travailler sur le cas le plus simple, une plante seule dans le champ, (2) identifier les entrées et les sorties essentielles pour l'interception de la lumière d'une plante seule, (3) vérifier l'influence de la plage de variation des entrées et définir la plage à sélectionner pour la suite, (4) évaluer l'effet des corrélations entre entrées sur la sensibilité des sorties pour sélectionner les méthodes d'analyse de sensibilité et de méta-modélisation appropriées, (5) méta-modéliser la plante seule et identifier les entrées les plus importantes, (6) passer au cas complexe de la plante cible entourée de plantes voisines, avec un travail préalable sur les entrées : sélectionner et agréger les entrées pour en réduire le nombre, (7) méta-modéliser la plante cible dans un couvert avec la méthode développée sur le cas de la plante seule, et identifier les variables les plus influentes à partir de nombreux couverts très variés que nous avons créé, (8) combiner les méta-modèles et ajouter des fonctions pour couvrir l'ensemble des situations biologiquement probables, (9) évaluer le modèle méta-modélisé (FLORSYS-metaLight), pour son ajustement au modèle mécaniste, sa capacité à reproduire des situations de terrain et pour sa vitesse de simulation.

Les étapes 8 et 9 sont assez innovantes car peu de méta-modèles vont jusqu'à ces étapes. Or, elles sont cruciales pour évaluer la performance du méta-modèle en prédiction dans la vraie vie. Classiquement, les méta-modèles sont évalués par validation croisée par rapport aux données de simulations qui ont servi à leur construction. Ici, dans l'étape 9, nous sommes allés bien plus loin, en comparant les prédictions des méta-modèles à des observations de terrain indépendantes, et donc dans des cas d'application réalistes et correspondants à l'objectif du modèle. L'étape 8 est également particulière dans la mesure où nous n'utilisons par directement le méta-modèle en tant que tel, mais nous le combinons avec d'autres modules existants. Cette étape de combinaison a demandé de nombreuses améliorations qu'il a fallu rajouter pour éviter d'utiliser les méta-modèles hors de la plage de variation utilisée lors de leur construction et donc de leur domaine de validité. Pour cela, des constantes et des lois écophysiologiques ont été combinées aux méta-modèles.

Au final, le méta-modèle issu des polynômes du chaos et régression PLS est intéressant pour des applications ayant besoin d'un niveau de discrimination très élevée en termes de localisation et volume des plantes (de l'ordre du cm), par exemple pour évaluer des systèmes de culture basés sur de l'agriculture de précision. En revanche, nous avons montré que diminuer le niveau de précision (en augmentant le voxel) dans la version initiale de FLORSYS est une alternative de simplification qui évite tous les désagréments de la méta-modélisation, comme la nécessité d'agréger les entrées, de rajouter des conditions pour utiliser un méta-modèle dans une situation ou d'utiliser une constante dans d'autres situations.

Afin de simplifier un modèle plus complexe, la méthodologie est plus grossière, mais reste efficace lorsqu'on s'intéresse à un modèle complexe dont les relations entre les entrées ne sont pas linéaires, comme dans notre cas ou dans le cas de dynamique de peupliers le long d'une rivière (Harper *et al.*, 2011). Dans notre cas, nous avons combiné des arbres de régression avec les forêts aléatoires pour extraire l'importance des entrées dans la variation des sorties, mais aussi les combinaisons de pratiques culturales. L'originalité de la méthode est ici de construire le jeu de données d'apprentissage en combinant des systèmes de culture réalistes avec des systèmes de culture aléatoires pour explorer des gammes de variations et des combinaisons non rencontrées dans les systèmes de culture réalistes et décorréler des pratiques fréquemment associées dans les systèmes actuels des agriculteurs. Comme à l'étape 9 du chapitre II, nous sommes allés au-delà de la validation croisée classique, en évaluant le méta-modèle, ici les forêts aléatoires, avec un jeu de données indépendant, réaliste et couvrant le futur domaine d'application du modèle, c'est-à-dire des systèmes de culture ciblant notamment la réduction de l'usage d'herbicides.

Cette évaluation montre certes que les forêts ne sont pas encore capables de prédire très bien les impacts de la flore adventice sur la production agricole et la biodiversité en termes de valeur absolue. Un méta-modèle reste dépendant du modèle qui en est à l'origine, dans notre cas FLORSYS. Ce dernier aussi est meilleur pour classer des situations en terme de flore adventice ou de rendement que d'en prédire les valeurs absolues (Colbach et al., 2016b). Nous n'avons cependant pas pu évaluer nos forêts directement à partir d'observations de terrain, sans passer par FLORSYS, puisque de telles mesures sur le terrain sont difficiles à obtenir comme les ressources pour les carabes ou les difficultés lors de la récolte. Mais la comparaison des forêts à la réalité virtuelle de FLORSYS montre que ces forêts répondent tout de même à notre objectif, c'est-à-dire de classer les systèmes de culture entre eux en fonction de l'impact des adventices. Or, classer des systèmes entre eux permet déjà de prendre des décisions (Loyce et al., 2002b). Les forêts répondent donc à notre objectif d'outil d'aide à la décision, puisqu'elles permettent en plus de tester rapidement une série de systèmes de culture, avec des allers-retours continus entre modifications des entrées décrivant les systèmes et analyses des sorties décrivant la performance de ces systèmes.

En outre, les modèles sont toujours faux, mais certains sont utiles (Box and Draper, 1986), et la question est de savoir quand et comment ils sont utiles. Les workshops et les réunions avec les agriculteurs dans le chapitre IV ont montré plusieurs pistes sur cette utilité. Par exemple, un mauvais modèle peut même être plus utile qu'un bon expert car le méta-modèle construit à partir de FLORSYS inclut les effets à long terme, les interactions entre pratiques et plusieurs pédoclimats, ce qui est difficilement réalisable par un expert. Ce sentiment est déjà ressorti de séminaires avec des conseillers et instituts techniques organisés par le GIS GC HP2E dans le passé (Journée de réflexion sur la création d'OAD pour la profession agricole, GIS GC HP2E, 2011). En outre, le modèle peut être un outil pédagogique et c'est là que réside la puissance des forêts, car elles permettent aux utilisateurs de tester rapidement des modifications pour voir par eux-mêmes quelles sont les techniques les plus intéressantes à modifier dans leur système et dans quel sens en testant de nombreuses situations. Nos workshops ont aussi montré toute la puissance de l'outil pour animer et diriger des discussions entre participants sur la conception de systèmes de culture.

Pour aller plus loin dans l'identification des techniques qui sont les plus intéressantes, nous avons utilisé la méthode de segmentation partitionnée (Lechenet et al., 2016; Ouellette et al., 2012) au chapitre III afin de dégager des combinaisons de descripteurs de système de culture plus détaillés et intéressants en fonction des situations de production, car les techniques culturales ainsi que leurs effets dépendent des situations de productions. En effet l'utilisation du labour ne peut se faire que dans certaines situations, par exemple, les agriculteurs du GRCETA de l'Aube participant aux réunions d'agriculteurs au chapitre IV avaient des sols riches en craie et le labour n'était pas envisageable pour eux.

V.2.2 Apports sur les interactions avec les utilisateurs

L'autre intérêt méthodologique de cette thèse est la constante interaction avec les futurs utilisateurs. En effet, l'évaluation des forêts grâce aux données du réseau DEPHY a contribué à savoir « quand » utiliser l'outil, tandis que les interactions avec les utilisateurs ont contribué à « comment » utiliser l'outil. Dans la littérature, il y a peu d'exemples de conception d'un outil d'aide à la décision, à partir d'un modèle, avec les utilisateurs. En revanche, il y a des exemples d'ateliers où il est question de conception de modèle *de novo* (Christen *et al.*, 2015) ou l'utilisation de modèle déjà fonctionnel (Figureau et al., 2015; Patel et al., 2007). Les articles existants sont surtout orientés sur l'intérêt d'utiliser un modèle avec différents acteurs pour un objectif donné, par exemple pour les faire échanger sur leurs idées et leurs problèmes entre eux ; ils ne traitent pas du développement à proprement parler de l'outil avec des utilisateurs. L'utilisation d'enquêtes est assez commune, par exemple pour identifier des critères d'évaluation et développer des indicateurs (Mézière et al., 2015d), ou bien pour définir des règles de décisions (par exemple, comment un agriculteur gère l'irrigation de sa ferme) et construire un outil basé sur ce processus de prise de décisions (Merot *et al.*, 2008). Nous avons testé différents types d'interactions avec les futurs utilisateurs et nous montrons ici chacun de ces apports. Les enquêtes nous ont permis de toucher un large public et d'avoir une vision globale de l'outil, les réunions et ateliers nous ont permis d'échanger plus facilement avec des groupes d'utilisateurs variés et de pouvoir approfondir sur pourquoi ce type d'outil est mieux que l'autre.

Si nous avons essayé de varier les origines des personnes consultées dans ce travail pour obtenir des avis différents, nous nous sommes limités au grand quart Nord-Est de la France. Seules les enquêtes en lignes nous ont permis de toucher des conseillers et quelques agriculteurs dans toute la France. Les deux groupements d'agriculteurs en Picardie et dans l'Aube et les conseillers agricoles en Haute-Marne nous ont fait travailler sur des systèmes de type grandes cultures céréalières ou commerciales. Des agriculteurs en monoculture de maïs dans le Sud-Ouest ou en production de lin dans le Nord de la France auraient peut-être eu des attentes différentes pour l'outil d'aide à la décision car ils ont d'autres besoins pour la conception de système de culture (Toffolini *et al.*, 2017). Nous avons choisi une situation de production familière (la Bourgogne) pour cette thèse, mais la méthodologie employée sera étendue à d'autres régions et d'autres situations de productions pour le futur OAD.

Le modèle à la base de l'outil d'aide à la décision a posé certaines limites sur le contenu de l'OAD, sur ce qu'on pouvait tester, sur les méthodes qu'on pouvait employer pour le simplifier. Il en est de même pour tout le travail avec les futurs utilisateurs. Par exemple, parmi les nouveaux descripteurs suggérés par les conseillers lors des ateliers, certains descripteurs ont pu être intégrés, comme le nombre d'opérations de travail du sol effectuées avec une bineuse, dans le but d'indiquer si cela vaut le coup d'investir dans une bineuse. D'autres ont besoin d'un travail supplémentaire pour les concilier avec FLORSYS, comme l'indication semis tardif ou précoce qui demande la transformation d'une variable qualitative en une variable quantitative, en intégrant les spécificités des cultures et des régions. Les propositions de descripteurs comme le semis tardif, montrent que certains utilisateurs préfèrent des catégories de descripteurs plus larges plutôt que des entrées précises, comme des dates calendaires. La méthode utilisée ici nous a permis d'identifier des profils d'utilisateurs variés, même en étant limitée géographiquement. Les profils identifiés se distinguaient autant au niveau des utilisations de l'outil qu'au niveau du choix des indicateurs pour évaluer les systèmes de culture, en lien avec les contraintes qu'ils rencontrent.

V.3 Contribution pour la conception de systèmes de culture multiperformants

Ce travail de thèse vise à aider à la conception de systèmes de culture multiperformants pour la gestion des adventices, avec le développement d'un OAD permettant de tester différents systèmes de culture et de les évaluer de façon multicritère. Les indicateurs d'impacts de la flore adventice nous permettent de faire une analyse multicritère du système de culture en termes d'impact de la flore adventice sur la production agricole et la biodiversité. La combinaison des indicateurs de nuisibilité des adventices et des indicateurs de services écosystémiques permet d'évaluer l'équilibre entre les impacts négatifs et positifs des adventices. Idéalement, il faudrait donner la main aux utilisateurs pour choisir le panel d'indicateurs qui les intéressent, notamment pour tenir compte de spécificités locales. Dans certains endroits il faut par exemple protéger la biodiversité dans les champs alors que dans d'autres régions, il y a suffisamment de zones refuges pour la biodiversité et les indicateurs de biodiversité au niveau des champs sont moins essentiels. Cependant, nos enquêtes au chapitre IV ont montré que manipuler de multiples indicateurs n'est pas forcément évident pour les utilisateurs et ces derniers préfèreraient deux indicateurs synthétiques, un pour la nuisibilité et un pour les services écosystémiques.

La construction des arbres de décision au chapitre III a montré que gérer trop d'objectifs en même temps réduit le nombre de combinaisons de pratiques et de profils de performances que l'on peut observer. Grace à l'analyse multivariée des indicateurs nous avons vu des limites à la multiperformance des systèmes, en effet il semble difficile de réconcilier production et ressources trophiques pour les abeilles domestiques. La réflexion autour de la multiperformance doit donc pouvoir s'inscrire à une échelle plus large et intégrer les espaces autour de la parcelle pour faire du « landsparing », donc réserver des zones dédiées à certains aspects de la biodiversité, à l'échelle de l'exploitation agricoles ou de la petite région (Colbach et al., 2018; Ekroos et al., 2016). Pour fouiller ces aspects à l'échelle paysage, il est envisageable d'utiliser une approche similaire à la nôtre en construisant des forêts aléatoires pour tester des scénarios de gestion de paysages (Viaud *et al.*, 2008).

Pour des fonctions de biodiversité moins contraignante que l'offre trophique aux abeilles, il est cependant possible de concilier différentes performances au niveau de la parcelle et donc au niveau du système de culture. En faisant l'analyse de sensibilité globale de FLORSYS au chapitre III, nous avons testé deux manières d'évaluer les techniques les plus influentes sur les impacts des adventices. D'un côté, nous avons utilisé des systèmes de culture réalistes pour se rapprocher le plus possible du raisonnement logique des techniques culturales cohérentes entre elles et avec la situation de production. De l'autre côté, nous avons utilisé des systèmes de culture aléatoires dont les techniques ont été choisies et combinées sans logique et sans cohérence avec la situation de production. Ces systèmes de culture permettent d'explorer un espace plus grand de valeurs et de combinaisons de pratiques culturales, sans *a priori* de notre part.

Malgré l'introduction de ces systèmes aléatoires, nous avons identifié que ce ne sont pas les techniques les plus innovantes comme l'utilisation de couvert, qui ressortent comme importantes, ce sont les techniques les plus classiques comme le travail du sol et les herbicides. Les systèmes de culture avec couvert n'étaient pas les plus représentés, mais la méthode de fouille de données aurait permis d'identifier les descripteurs de couvert même s'il y avait un faible nombre de cas, si ceux-ci avaient permis de bien différencier les impacts sur les indicateurs des systèmes de culture avec couverts. Cependant, les descripteurs utilisés n'étaient peut-être pas adaptés pour faire ressortir l'effet des couverts, ce n'est peut-être pas la durée du couvert ou la variabilité de sa durée, mais sa composition qui importe. Toutefois, derrière l'ajout de couvert, on retrouve des changements dans les techniques culturales, comme des changements des dates de travail du sol ou de fréquence du faux semis estival ou bien le passage au semis direct (Rodriguez, 2013). Cela met en lumière que la combinaison de techniques pour un système de culture multiperformant est primordiale. En effet, la gestion des adventices consiste à trouver l'équilibre entre protection de la culture et services écosystémiques et ce sont toutes les techniques qui sont mises en œuvre qui vont aider à atteindre cet équilibre équilibre (Liebman and Gallandt, 1997). Pour l'illustrer, nous avons trouvé que dans le cas d'un système de culture peu travaillé en hiver, sans usage d'herbicide, un semis après le 25 septembre permettait d'augmenter les ressources trophiques pour les oiseaux. Ou encore, dans un système avec un sol régulièrement travaillé en hiver et peu d'usage d'herbicide, passer le rouleau au moins 7 années sur 10 permettait de réduire fortement les nuisances des adventices. Cependant, dans les arbres de décision, le labour pouvait aussi expliquer les variations des indicateurs mais avec une moindre amélioration de l'erreur par rapport au passage du rouleau.

La conception de systèmes de culture multiperformants est aussi rendue possible ici grâce à l'OAD issu d'un modèle mécaniste qui permet de tester les effets de systèmes de culture sur différents indicateurs d'impacts de la flore adventice. Cela est différent d'une conception d'outil *de novo* où tous les processus sont mis en place et évalués avec les utilisateurs. Passer par FLORSYS nous a notamment permis d'inclure des connaissances difficilement accessibles sur le terrain comme les ressources trophiques pour les oiseaux ou les carabes (Colbach, 2010). Utiliser les forêts aléatoires permettant de prédire les indicateurs d'impacts de la flore adventice développées ici permettrait de faire de la conception de systèmes de culture par un processus d'optimisation multicritère.

Tout au long de ce travail, nous avons pris en compte les régulations biologiques via la compétition pour la lumière entre plantes et l'effet des plantes voisines, notamment dans le module d'interception et du rayonnement. Nous prenons également en compte les services écosystémiques qui dépendent des adventices, comme les ressources trophiques pour les oiseaux, les carabes et les abeilles domestiques. Ainsi, en prenant en compte à la fois la nuisibilité des adventices et les services écosystémiques qu'elles apportent nous allons au-delà de la conception multicritère de systèmes de culture en proposant une conception de systèmes de culture agroécologiques. En effet, notre démarche répond à la définition scientifique de l'agroécologie, où les interactions biologiques et les régulations biologiques des adventices sont prises en compte, mais aussi à l'agroécologie au sens des pratiques culturales, où une aide pour combiner des pratiques culturales économes en intrants chimiques est proposée (Wezel *et al.*, 2009).

V.4 Quelles perspectives pour aller vers une version finale de l'OAD ?

Les différentes limites identifiées tout au long de ce travail nous permettent d'envisager des perspectives de recherche et des améliorations à apporter à l'OAD. Dans cette thèse, des arbres de décision ont été construits pour une série de situations de production contrastées, déterminées par des variables pédoclimatiques et floristiques (via le stock semencier adventice initial), afin d'adapter les techniques culturales et leurs effets aux conditions locales. Cette approche limite en revanche la prise en compte des spécificités liées à des choix d'agriculteurs, par exemple des exploitations en bio ou en non travail du sol. Pour faire ressortir ces cas particuliers, un autre tri, non plus sur les situations de production, mais sur des grands types d'agricultures (par exemple, agriculture biologique, agriculture de conservation…) pourrait répondre à des problématiques plus spécifiques aux agriculteurs dans ces cas-là. Pour cela, il faudrait faire une typologie des systèmes de culture en s'appuyant par exemple sur des typologies existantes (Andersen *et al.*, 2007). Cela demandera aussi de compléter la base de données de systèmes de culture ayant servi à la construction des arbres et forêts par des simulations testant plus en détail les options de ce systèmes. Accessoirement, cela démontre encore une fois les limites des plans d'expérience LHS dans le cas de modèles à très grands nombres d'entrées où des plans combinant un ensemble de sous plans focalisés sur les situations les plus probables sont nécessaires.

Peu de systèmes obtenus dans les arbres de décision permettent de concilier services écosystémiques et protection de la culture. Dans la quantité des systèmes évalués, les quelques systèmes qui le permettent sont noyés dans les autres systèmes. Nous avons tenté de "pêcher" ces systèmes en utilisant des profils d'utilisateurs contrastés : le productiviste qui favorise la productivité et veut diminuer au maximum les indicateurs de nuisibilité, le profil de gestion intégrée qui veut en plus réduire le niveau d'usage herbicide, et celui qui favorise l'agroécologie qui veut minimiser les pertes de rendement tout en maximisant les services écosystémiques. L'utilisation de ces profils revenait à construire des arbres de décision multivariés à partir d'un panel différent d'indicateurs, mais ces arbres multivariés ne se sont pas distingués les uns des autres et n'ont pas souvent permis de discriminer des combinaisons de pratiques conduisant à la performance visée.

Dans le cas d'objectif multicritère, il faudra donc une méthode plus contraignante pour identifier des combinaisons de pratiques culturales permettant de concilier services écosystémiques et protection des cultures. Une alternative serait de forcer les arbres à rechercher des combinaisons de pratiques qui permettent d'atteindre une combinaison d'objectifs en termes d'impact de flore adventice (par ex : moins de 10% de perte de rendement, IFT herbicide < 1, biodiversité > 75% de l'optimum, (Colbach et al., 2017c)). Ici, les arbres étaient libres dans la construction et tendaient à discriminer des performances contrastées (ex. faible perte de rendement et forte biodiversité vs l'inverse), donc une typologie des pratiques en fonction des performances comme l'ont déjà fait Mézière *et al.* (2015b). Cependant, le forçage des arbres passe par l'usage d'une note unique qui est plus adapté à la recherche qu'à l'utilisation en OAD. En effet, le chapitre IV a montré que les conseillers agricoles sont assez peu nombreux à être intéressés par un indicateur global en sortie à l'OAD. Une alternative pourrait être de combiner deux notes synthétisant respectivement la nuisibilité et les bénéfices des adventices, comme suggéré par certains participants des enquêtes en lignes du chapitre IV.

L'outil d'aide à la décision développé dans ce travail de thèse ne s'intéresse qu'aux services et disservices de la flore adventice. Il n'aborde pas la question des impacts économiques et sociaux, même si cela était parfois demandé, surtout les aspects économiques, par les utilisateurs dans les enquêtes, réunions ou ateliers. Nous avons pris le parti de développer un outil se concentrant uniquement sur la gestion et les effets des adventices par une réflexion stratégique du système de culture car la réflexion au niveau système de culture est le moyen d'aller vers une agriculture durable (Hill and MacRae, 1996). D'autant plus que, si des outils existent, peu permettent d'évaluer des systèmes de culture contrastés, sur plusieurs années, en prédisant la variabilité d'une technique en fonction des autres techniques culturales et des conditions pédoclimatiques. La flore adventice est également un frein majeur à la gestion intégrée car elle est le bioagresseur le plus nuisible et difficile à gérer de façon intégrée (Bastiaans *et al.*, 2008).

Pour intégrer l'ensemble des besoins des utilisateurs, il faudra coupler notre outil dans le futur avec d'autres outils, comme DEXiPM (Pelzer *et al.*, 2012), qui se chargent déjà très bien des besoins sociaux et économiques. Il faudra aussi lier vers des sites comme Infloweb (Terres Inovia et al.) qui sont des sources d'information sur la biologie des adventices qui a été un point identifié, dans le chapitre IV, comme bloquant par les utilisateurs pour la gestion des adventices. Au final, l'outil d'aide à la décision que l'on développe ne fera que participer à l'un des éléments pris en compte lorsque l'agriculteur raisonne son système de culture, au même titre que ses expériences précédentes ou les échanges avec les autres agriculteurs (Doré *et al.*, 2011). Ce sera à l'agriculteur de décider s'il suit les conseils prodigués et de faire la balance entre ce qu'il compte privilégier : les conditions de travail, les conditions de production ou le budget.

Ce nouvel OAD vient s'ajouter à de nombreux autres OAD existants qui, chacun, a sa spécificité et spécialité. Chaque outil ne sera pas utilisé pour le même objectif et de la même manière. Par exemple, des outils comme MASC (Sadok et al., 2009b), DEXiPM (Pelzer *et al.*, 2012) et Systerre® (Arvalis) font une évaluation globale pour les trois piliers du développement durable, en traitant les questions de consommation d'énergie, de temps d'intervention et de marges. Un outil comme IPSIM (Aubertot and Robin, 2013b; Robin et al., 2013) est un outil large permettant de prédire un profil d'infection/infestation avec une vision globale de l'agroécosystème car comprenant les décisions des agriculteurs et les facteurs socio-économiques. En comparaison, l'OAD développé ici ne traite qu'une petite partie de la durabilité, mais permet de répondre précisément à un problème spécifique qui est l'impact du système de culture sur la gestion des adventices.

Dans cette thèse nous avons posé un prototype d'outil d'aide à la décision fonctionnel qui a déjà été utilisé dans des ateliers de conception de systèmes de culture et qu'il faut encore améliorer. Bien que nous ayons travaillé dans un seul cas d'étude, uniquement des conseillers agricoles de Champagne, c'est une preuve de concept que la méthodologie employée est efficace pour aider au développement de l'OAD. Pour continuer à améliorer l'OAD, il suffit d'utiliser cette méthodologie dans d'autres cas d'étude. Confronter FLORSYS à des potentiels utilisateurs est nécessaire pour trouver ce qui doit être pré-paramétré pour aider les conseillers agricoles et les agriculteurs dans leur utilisation de FLORSYS. Pour identifier quels éléments de FLORSYS pré-paramétrer en premier, il suffit d'utiliser les résultats de l'analyse de sensibilité du chapitre III, qui nous donnent l'ordre d'importance des paramètres. En combinant les deux, nous obtenons le pré-paramétrage à faire en premier. Pour l'OAD synthétique, nous avons déjà commencé au chapitre III à compléter les descripteurs de système de culture existants. Cependant, il y a encore un travail d'interfaçage entre utilisateurs et descripteurs avec des améliorations comme une traduction en date calendaire en fonction des régions, du sol, des cultures et des systèmes de culture afin d'intégrer des descripteurs de semis précoce et semis tardif. Il faut donc continuer ces allers-retours, d'autant plus que chaque interaction est spécifique du type d'utilisateur, de ses objectifs et de ses problèmes. Pour rôder au maximum l'outil, en plus de s'assurer que toutes les utilisations possibles de l'outil ont été envisagées et au besoin améliorées, il faudra s'assurer d'avoir une proportion représentative d'utilisateurs différents susceptibles d'utiliser l'OAD.

Une autre amélioration nécessaire est le développement d’une interface conviviale et plus intuitive pour encourager l’utilisation par de futurs utilisateurs. Cela demandera des compétences en ergonomie et en sociologie pour bien ajuster le développement. Il reste encore à valider les derniers points de la checklist proposée par Rose *et al.* (2016) sur le développement et la livraison efficace d’un OAD. Il s'agit des points dépassant le cadre de la recherche proprement dit, comme le coût de l’outil, s’il est adapté aux bénéfices qu’il apporte, si l’outil est conforme aux législations et aux demandes du marché des outils. Ceci est du ressort de l'ingénierie accompagnant la distribution future de l’outil.

V.5 Conclusion

Ce travail a permis de valoriser le contenu biophysique de FLORSYS et de le simplifier pour en tirer un prototype d’outil d’aide à la décision (OAD) afin d'assister à la reconception de systèmes de culture moins consommateurs en herbicide et multiperformants. La combinaison de méthodes statistiques et d’interactions avec des conseillers agricoles et des agriculteurs dans ce travail a permis de faire ressortir l’importance de faire le lien entre le développement statistique et les utilisateurs car chacun alimente l’autre de ses connaissances et de ses points forts. Deux méthodes pour faire de l’analyse de sensibilité et de la méta-modélisation sur un modèle ont été utilisées dans ce travail, soulignant les intérêts et limites de chacune. Pour des modèles complexes comme FLORSYS, seules les méthodes empruntées à la fouille de données permettent de simplifier le modèle mécaniste pour rendre son contenu biophysique utilisable par des conseillers agricoles et des agriculteurs. Grâce aux interactions avec des futurs utilisateurs nous avons défini un OAD double, (1) un OAD synthétique basé sur des méta-règles de décision pour la reconception de systèmes de culture, (2) un OAD plus détaillé en termes de description du système de culture et des effets de la flore pour le réajustement de système de culture. La méthodologie pour faire intervenir les futurs utilisateurs dans le développement de l’OAD est une preuve de concept qui a permis d’arriver à un prototype d’outil fonctionnel. Cet outil peut déjà être utilisé lors d’atelier de conception de systèmes de culture multiperformants. L’OAD n’est pas dans sa version finale, mais nous avons proposé de nombreuses idées pour l’améliorer et le rendre encore plus fonctionnel.

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Annexes

Annexe 1

Metamodelling and global sensitivity analysis for computer models with correlated inputs: a practical approach tested with a 3D light interception computer model.

L'article qui fait suite présente la méthode de méta-modélisation et d'analyse de sensibilité combinant régression PLS et polynômes du chaos :

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Position Paper

Metamodeling and global sensitivity analysis for computer models with correlated inputs: A practical approach tested with a 3D light interception computer model

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ABSTRACT

Models of biophysical processes are often time-consuming and their inputs are frequently correlated. This situation of non-independence between the inputs is always a challenge in view of simultaneously achieving a global sensitivity analysis of the model output and a metamodeling of this output. In this paper, a novel practical method is proposed for reaching this two-fold goal. It is based on a truncated Polynomial Chaos Expansion of the output whose coefficients are estimated by Partial Least Squares Regression. The method is applied to a computer model for heterogeneous canopies in arable crops, aimed to predict crop:weed competition for light. We now have fast-running metamodels that simultaneously provide good approximations of the outputs of this computer model and a clear overview of its input influences thanks to new sensitivity indices.

1. Introduction

Many techniques exist today for metamodeling a computer model output (Gasca and Sauer, 2000; Bates et al., 2003; Rasmussen and Williams, 2006; Wang and Shan, 2007; Stanfill et al., 2015). On the other hand, several methods exist for defining and estimating the Sensitivity Indices (SI) of computer (nonlinear) model inputs on the computer model output, based on the variance of this output. According to the technique used, even an effective metamodel can lead to very wrong estimates of the SI because the main goal of a metamodel is generally not to provide estimates of the SI but, instead, for prediction purposes. Similarly, correct estimates of the SI can be obtained by Monte Carlo techniques but they cannot lead to an effective metamodel.

The mathematical definition of this SI type, based on the variance of the output, was given by Sobol' (Sobol', 1993; Lemieux, 2009), and is referred to as the Sobol' Sensitivity Indices (SSI). It is based on the Hoeffding-Sobol decomposition of the total functional variance of an output (Hoeffding, 1948; Sobol', 1993), i.e., a generalization for nonlinear models of the usual decomposition of the total variance for linear models. The estimation of these SSI leads to a Global Sensitivity Analysis (GSA) (Saltelli et al., 2000, 2004; Saltelli, 2002) of the output.

It therefore remains a difficult two-fold challenge to *simultaneously* obtain an effective metamodel and correct SI estimates of this type. In order to meet this two-fold challenge, methods based on a truncated Polynomial Chaos Expansion (PCE) of the response (Sudret, 2008; Crestaux et al., 2009; Blatman and Sudret, 2011) where the coefficients are estimated by Ordinary Least Squares Regression (OLSR), were proposed. However, these methods are relevant only if the random inputs of the computer model are continuous and independent because the SSI are rigorously defined only in this situation (Sobol', 1993). They are not mathematically founded in the case of correlated inputs because the Hoeffding-Sobol decomposition no longer holds in this case. We therefore propose new SI in this paper that are not based on the Hoeffding-Sobol decomposition, which are different from the SSI.

The need for metamodels is crucial today in many applications in several scientific areas, including the agronomical and ecological sciences (Colbach, 2010; Marie and Simioni, 2014) because

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computer models very often take too much computing time to run, whereas an adapted metamodel takes a short time to run. It is true that several methods already exist where the inputs are correlated (Jacques et al., 2006; Li and Rabitz, 2012; Mara and Tarantola, 2012; Kucherenko et al., 2012), but these methods are not always convenient to use or applicable to our agronomical concerns. Below, we give a single disadvantage of each of these methods in order to understand why they are not really convenient and easy to use.

The method proposed by Jacques et al. (2006) leads to SI that are not decomposable to first-order effects and interaction effects. The method proposed by Li and Rabitz (2012) is based on very heavy mathematical tools (tensor product spline bases) and is consequently poorly adapted to many inputs (more than five or six). Moreover, their method does not lead to a single functional decomposition because the latter particularly depends on the number and choice of some approximating functions. The method proposed by Mara and Tarantola (2012) is based on a first step of decorrelation of the correlated inputs by means of a classical Gram-Schmidt orthogonalization (that lead to orthogonalized inputs). In a second step, relevant SI can then be obtained but these SI are interpretable only via the orthogonalized inputs and not via the natural inputs, which represents an obvious disadvantage. The method proposed by Kucherenko et al. (2012) is very heavy because it is based on the generation of conditional densities of Gaussian inputs (the case of uniformly distributed inputs is not mentioned) via the sophisticated copula techniques. This leads to a considerable number of samplings and, furthermore, no clear meaningful SI are obtained for separating first-order and total effects.

We propose a simpler and more practical alternative method here where the continuous inputs are correlated. This method simultaneously provides sensitivity indices of a new kind, as well as a metamodel. It is based on a truncated PCE of the response whose coefficients are estimated by Partial Least Squares Regression (PLSR), whereas Sudret (2008) used OLSR. This method is particularly well-adapted when the continuous inputs - in moderate number (typically ≤ 15) - are stochastically linked (correlated) or even deterministically (functionally) linked, on the one hand, and when a single computer run is moderately time-consuming (typically less than one minute), on the other. These input numbers and time-consuming values obviously depend on the type of computer used. They are given for a Pentium IV desk computer (with a clock speed of about 3 GHz) equipped with a 12-giga RAM. More details are given on this subject in the Discussion section.

In this paper, this method is applied to a biophysical computer model in the field of agroecology. Models that describe and predict biophysical processes that occur in the field are needed for agroecological crop management, but often require a significant number of inputs and are time-consuming (Lô-Pelzer et al., 2010; Vos et al., 2010; Colbach et al., 2014). If the inputs are considered as independent, a first approximation is used to make simulations faster by replacing these models with emulators or parsimonious metamodels that depend only on the most important inputs (Colbach, 2010; Marie and Simioni, 2014). This method was applied to a 3D individual-based light interception model (Munier-Jolain et al., 2013) whose aim was to predict crop:weed competition for light in heterogeneous canopies. This model is a central component of the multi-annual weed dynamics model, FlorSys, aimed at testing agroecological cropping systems (Colbach et al., 2014). A crucial difference in the present paper is that it considers non-negligible and even strong correlations between the inputs.

The rest of the article is organized as follows. Section 2 is devoted to a persuasive illustration of the influence of the input correlation on the sensitivity indices obtained by PCE (and OLSR) of the response, for two well-known academic models used as test functions in GSA (the so-called Ishigami and Sobol' functions). Section 3 presents our new method. Section 4 is devoted to an application to the two preceding academic models. Section 5 is devoted to the application to a case study with a process-based light interception model, revealing the effectiveness of this new approach. Section 6 contains the discussion and conclusions. Section 7 gives details about software/data availability. An appendix provides a list of the numerous abbreviations used in our paper.

2. Influence of the input correlation

This study on the influence of input correlation was a motivation for proposing new sensitivity indices adapted to the management of correlated inputs present in computer models (e.g., biophysical models), as well as to innovation using metamodeling techniques. Sobol' defined the First Order Sobol' Sensitivity Indices, referred to in this paper as the FOSSI, and the Total Sobol' Sensitivity Indices, referred to as the TSSI (Sobol', 1993; Lemieux, 2009). These FOSSI and TSSI are estimated by a classical method based on a truncated PCE whose coefficients are computed by OLSR (Sudret, 2008). Note that the inputs must be independent for the mathematical validity of the FOSSI and TSSI, as well as that of their estimations: the PC$_d$-PESI(OLS) and PC$_d$-TSI(OLS), defined at the end of Subsection 3.1, where d is the degree of the truncated PCE.

In this section, we only provide a simple illustration, obtained by a simulation study, of the influence of the correlations between the inputs on the value of these PC$_d$-PESI(OLS) and PC$_d$-TSI(OLS), for two very well-known academic models in the GSA domain: the Ishigami function (Saltelli et al., 2000; Chap. 2) and the Sobol' function (Sobol', 2003). The advantages of using these two functions are two-fold: (a) They are strongly nonlinear (this is the reason why the FOSSI and the TSSI are so different from each other; their analytical values are compared below), and it is therefore a challenge to obtain good respective estimations; and (b) The quality of any estimation method can always be evaluated because the FOSSI and TSSI *analytical values are known* (Saltelli et al., 2000) for these two functions.

The Ishigami function has three inputs $\mathbf{X} = (X_1, X_2, X_3)$ that are linked to the output Y according to:

$$Y = \sin(X_1) + \theta_1[\sin(X_2)]^2 + \theta_2 X_3^4 \sin(X_1) \tag{1}$$

where $\theta_1 = 7$, and $\theta_2 = 0.1$, given in Ishigami and Homma (1990). Each X_j is a uniform random variable on the interval $[-\pi; \pi]$. The analytical values of the FOSSI for the independent X_1, X_2 and X_3 are 0.3138, 0.4424 and 0, respectively, and the analytical values of the TSSI for X_1, X_2 and X_3 are 0.5574, 0.4424 and 0.2436, respectively.

The Sobol' function has eight inputs that are linked to the output Y according to:

$$Y = \prod_{j=1}^{8} \frac{|4X_j - 2| + a_j}{1 + a_j} \tag{2}$$

where $\mathbf{a} = (1, 2, 5, 10, 20, 50, 100, 500)$, given in Sudret (2008). Each X_j is a uniform random variable on the interval $[0; 1]$. Since the last four FOSSI$_j$ and TSSI$_j$, $j = 5, \ldots, 8$, are close to zero, we consider only the first four inputs, $X_j, j = 1, \ldots, 4$, in this paper, whereas $X_j, j = 5, \ldots, 8$ were set to the value of 1/2 (i.e., their mean value). The analytical values of the FOSSI for the independent X_1, X_2, X_3 and X_4 are then 0.6037, 0.2683, 0.0671 and 0.0200, respectively, and the analytical values of the TSSI for X_1, X_2, X_3 and X_4 are then 0.6342, 0.2945, 0.0756 and 0.0227, respectively.

For both functions, a simulation study made it possible to perceive the influence of correlation between the inputs according to four increasing correlation ranges: cor1 = [0.1; 0.3], cor2 = [0.3; 0.5],cor3 = [0.5; 0.7],cor4 = [0.7; 0.9]. The sequential procedure for both functions was the following: (a) In the p-input space, a large primary Space Filling Design (SFD) of $N = 20000$ rows was constructed by means of a Sobol' quasi-random sequence (Lemieux, 2009). An alternative way for forming this SFD could be to use a Latin Hypercube Sampling (LHS) (McKay et al., 1979); (b) On the basis of this SFD, 30 consecutive correlated SFD were constructed by sampling values of the correlation coefficients inside each correlation range, and the Iman and Conover technique (1982) was used to form the correlated inputs; (c) The PC$_d$-PESI(OLS) and PC$_d$-TSI(OLS) were computed with $d = 6$, a value that led to a $R^2 > 0.99$, for the Ishigami function, and $d = 5$, a value that led to a $R^2 > 0.99$, for the Sobol' function. This computation was done for each correlated SFD, leading to $4 \times 30 = 120$ computation sets for both functions. An additional set for the primary non-correlated SFD was computed (cor0 in Figs. 1 and 2). The results are shown in Figs. 1 and 2, for the Ishigami and Sobol' functions, respectively.

Figs. 1 and 2 clearly show a reasonable robustness of the PC$_d$-PESI(OLS) and PC$_d$-TSI(OLS) when the correlation level is moderate (typically < 0.5). This is useful information for practitioners because it is very easy to use the PCE method based on OLSR (e.g., with the "polychaosbasics" R package described in Section 7). However, the robustness of these indices can be very poor if the correlation level is high, i.e., in the Cor4 = [0.7; 0.9] range. For the Ishigami function, even the Cor3 = [0.5; 0.7] range led to a wrong estimation of the SSI, even if the metamodel accuracy did not significantly change (see the evolution of R^2 in Table 1). In this succinct simulation study, we showed that correct estimations of SSI cannot be reached if the inputs are moderately or strongly correlated.

3. A new method

In the context of correlated continuous inputs, our approach is to build a metamodel also based on a multivariate Legendre truncated PCE, as in Sudret (2008), *but* we propose to use the Partial Least Squares Regression (PLSR) to estimate the regression coefficients of this PCE, whereas Sudret (2008) used OLSR. These estimates lead to new SI defined in Subsection 3.2.1. In the next two subsections, we provide backgrounds on PCE and PLSR, respectively, because these techniques are not very frequently encountered in environmental research.

3.1. PCE background

Let M be the computer model, typically a "black box" type. Let $\mathbf{X} = (X_1, \ldots, X_p)$ be the design matrix formed by the p inputs, X_j, $j = 1, \ldots, p$. Assume that for $\mathbf{x}_i = (X_{i1}, \ldots, X_{ip})$, one point in the p-dimensional space of the p inputs (i.e., a row of $\mathbf{X}$), an M run leads to a value, y_i, of the Y output. We can therefore write $y_i = \mathrm{M}(\mathbf{x}_i)$. In this paper, we assume that the Y output can be approximated by a full (specific) polynomial metamodel (surrogate or emulator model) of degree d, referred to as M_d, built from the p continuous inputs, X_j. Each monomial of this polynomial is defined by a specific function of the $(X_1^{d_1}, X_2^{d_2}, \ldots, X_p^{d_p})$ terms, $0 \le d_j \le d$, $\sum_{j=1}^{p} d_j \le d$. The number of these monomials (without the constant term) is:

$$P = [(p + d)!/(p!d!)] - 1 \tag{3}$$

We can write:

$$y_i = \mathrm{M}(\mathbf{x}_i) = \mathrm{M}_d(\mathbf{x}_i) + \varepsilon_i \tag{4}$$

where ε_i is a deterministic model error because M_d is a deterministic polynomial approximation of M. For M_d, we chose a polynomial metamodel based on a PCE of the response (Wiener, 1938; Cameron and Martin, 1947) because this expansion proved its efficiency for metamodeling a computer output if the X_j are independent random variables that strongly interact nonlinearly (e.g., Sudret (2008)). According to this theory, any second-order random variable, Z, may be expanded as follows:

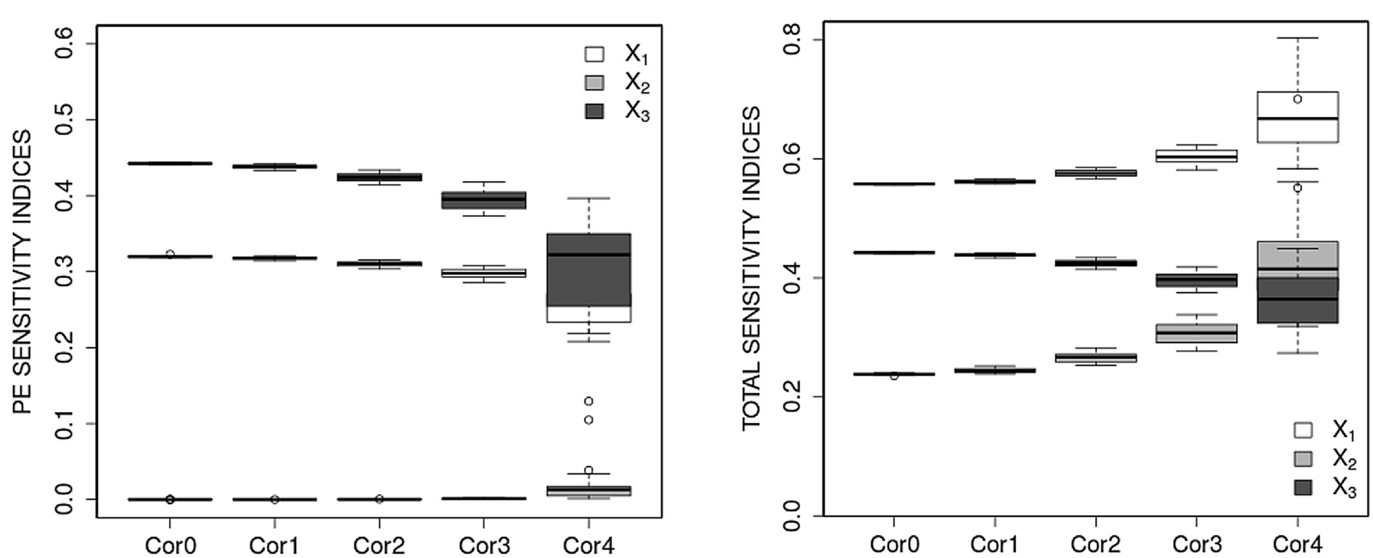

Fig. 1. Ishigami function: influence of the correlation between the inputs on the three PC$_6$-PESI(OLS) (left panel where the y-axis "PE Sensitivity Indices" represents the three PC$_6$-PESI(OLS)), and the three PC$_6$-TSI(OLS) (right panel where the y-axis "Total Sensitivity Indices" represents the three PC$_6$-TSI(OLS)). On the x-axis, the four correlation ranges, Cor1–Cor4, are indicated (see text for details). Cor0 = 0 stands for non-correlated inputs, and correct estimations of the analytical solutions of SSI are then obtained in this case. We recall these analytical solutions here: the First-Order Sensitivity Indices for the independent X_1, X_2 and X_3 are 0.3138, 0.4424 and 0, respectively, and the Total Order Sensitivity Indices for X_1, X_2 and X_3 are 0.5574, 0.4424 and 0.2436, respectively.

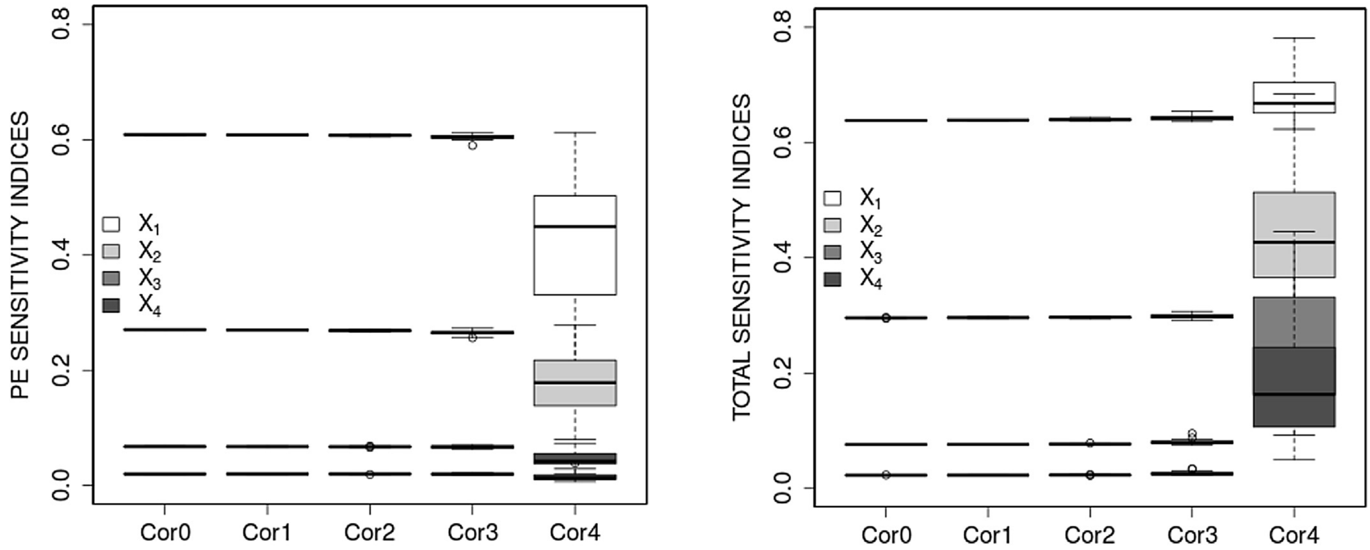

Fig. 2. Sobol' function: influence of the correlation between the inputs on the four PC_5-PESI(OLS) (left panel where the y-axis "PE Sensitivity Indices" represents the four PC_5-PESI(OLS)), and the four PC_5-TSI(OLS) (right panel where the y-axis "Total Sensitivity Indices" represents the four PC_5-TSI(OLS)). The same comment about the x-axis as in Fig. 1 applies here as well. Cor0 = 0 stands for non-correlated inputs, and correct estimations of the analytical solutions of SSI are then obtained in this case. We recall these analytical solutions here: the First-Order Sensitivity Indices for the independent X_1 , X_2 , X_3 and X_4 are 0.6037, 0.2683, 0.0671 and 0.0200, respectively, and the Total Order Sensitivity Indices for X_1 , X_2 , X_3 and X_4 are 0.6342, 0.2945, 0.0756 and 0.0227, respectively.

Table 1
Estimation of the Sensitivity Indices for the three-input Ishigami function, for $d = 6$, at two different correlation levels between the three inputs. The SFD size was $N = 10000$. R^2 is the usual determination coefficient of the regression, and Q^2_{cum} (h^*) is the PLS criterion computed with h^* significant PLS components. See Appendix for the other abbreviations.

Inputs	Analytical	cor = 0		cor = 0.8	
	FOSSI	PC_6 -PESI(OLS)	PC_6 -PESI(PLS)	PC_6 -PESI(OLS)	PC_6 -PESI(PLS)
X_1	0.314	0.314	0.321	0.252	0.269
X_2	0.442	0.444	0.443	0.311	0.394
X_3	0.000	0.000	0.000	0.008	0.015
Inputs	TSSI	PC_6 -TSI(OLS)	PC_6 -TSI(PLS)	PC_6 -TSI(OLS)	PC_6 -TSI(PLS)
X_1	0.557	0.555	0.557	0.669	0.574
X_2	0.442	0.448	0.443	0.372	0.451
X_3	0.244	0.241	0.236	0.435	0.323
R^2		0.984	0.982	0.987	0.986
$Q^2_{cum}(h^*)$			0.982 (3)		0.987 (22)

$$Z = \sum_{k=0}^{\infty} Z_k \Psi_k\left(\{\xi_p\}_{p=1}^{\infty}\right) \tag{5}$$

where Z_k are coefficients, $\{\xi_p\}_{p=1}^{\infty}$ is an infinite sequence of independent standard normal random variables, and the $\Psi_k(.)$ are the mutivariate Hermite orthogonal polynomials (generalization of the classical univariate Hermite orthogonal polynomials) (e.g., Abramowitz and Stegun, 1970). The $\Psi_k(.)$ are orthogonal with respect to the Gaussian measure.

When the X_j have independent uniform probability distribution functions – which is always the case in this paper – this former theory was generalized using multivariate Legendre orthogonal polynomials formed from univariate Legendre orthogonal polynomials (Abramowitz and Stegun, 1970). In practice, the infinite expansion of Eq. (5) will be truncated for computational purposes, and the computer code output, Y, can then be approximated by a Legendre truncated PCE with a polynomial degree, d, chosen beforehand:

$$Y \approx \mathrm{M}_d(\mathbf{X}) = \sum_{k=0}^{P} \beta_k \Psi_k(\mathbf{X}) \ , \ \mathbf{X} \sim \ \mathscr{U}([-1,+1]^p) \tag{6}$$

where the β_k are unknown (scalar) coefficients (β_0 is the constant term), forming a β vector. The P monomials, $\Psi_k(\mathbf{X})$, are now elements of a multivariate Legendre orthogonal polynomial. If we have N results, y_i, of the computer code output Y, forming the $(N \times 1)$-vector, Y_N, and if we note $\mathbf{\Psi}(\mathbf{X})$ the $(N \times (P+1))$-matrix formed by the vertical concatenation of $\Psi_{N,0}(\mathbf{X})$ (a $(N \times 1)-$ vector of ones) and the $\Psi_{N,k}(\mathbf{X})$ $(N \times 1)$-vectors, $k = 1, \ldots, P$ (each corresponding to the values of the $\Psi_k(\mathbf{X})$ for $\mathbf{x}_i, i = 1, \ldots, N$), we can then write in matrix notation:

$$Y_N = \mathbf{\Psi}(\mathbf{X})_{N \times (P+1)} \beta_{P+1} + \Sigma_{N \times 1} \tag{7}$$

where $\Sigma_{N \times 1}$ is the error vector whose elements are the $\varepsilon_i, i = 1, \ldots, N$.

In the context of independent inputs, a classical way to estimate the β vector is to use OLSR (Sudret, 2008). A good value for d is selected by sequential operating, from $d = 1$ to a value of d that simultaneously leads to a good value (reasonably close to 1) of the determination coefficient (the so-called R^2) of OLSR and a weak Root Mean Square Error in Prediction (RMSEP) (see Eq. (26)). We finally obtain the estimated metamodel, in the sense of Ordinary Least Squares (OLS):

$$\widehat{M}_d(\mathbf{X}) = \sum_{k=0}^{P} \widehat{\beta}_k^{[OLS]} \Psi_k(\mathbf{X}) \tag{8}$$

where $\widehat{\beta}_k^{[OLS]}$ is the *kth* element of the $((P+1)\times 1)$-vector $\widehat{\beta}^{[OLS]}$, or in matrix notation:

$$\widehat{Y}_N = \mathbf{\Psi}(\mathbf{X})\widehat{\beta}^{[OLS]} \tag{9}$$

To illustrate this, we give an example of a $\Psi_k(\mathbf{X})$ term of the Legendre-PCE:

$$\Psi\left(X_1^4 X_2^3 X_3^2\right) = \frac{1}{8}\left(35X_1^4 - 30X_1^2 + 3\right)\frac{1}{2}\left(5X_2^3 - 3X_2\right)\frac{1}{2}\left(3X_3^2 - 1\right) \tag{10}$$

Thanks to the orthogonal decomposition of the variance of Eq. (8), we obtain the P Individual Monomial Sensitivity Indices, IMSI$_k$, $k = 1, \ldots, P$, defined by:

$$\mathrm{IMSI}_k = \left(\widehat{\beta}_k^{[OLS]}\right)^2 E\left\{\Psi_k^2(\mathbf{X})\right\} \Big/ D_{PC} \tag{11}$$

where D_{PC} is defined by:

$$D_{PC} = \sum_{k=1}^{P} \left(\widehat{\beta}_k^{[OLS]}\right)^2 E\left\{\Psi_k^2(\mathbf{X})\right\} \tag{12}$$

where $E\{\Psi_k^2(\mathbf{X})\}$ is the variance of $\Psi_k(\mathbf{X})$ because $\Psi_k(\mathbf{X})$ is centered by the Legendre construction.

The two classical FOSSI$_j$ and TSSI$_j$ for every input X_j, defined in Sobol' (1993), were then estimated in Sudret (2008) for every input X_j, by the following SU$_j$ and SUT$_j$ formulas

$$\mathrm{SU}_j = \sum_{k \in \Omega_{j1}} \mathrm{IMSI}_k \quad \text{and} \quad \mathrm{SUT}_j = \sum_{k \in \Omega_{j2}} \mathrm{IMSI}_k \tag{13}$$

where Ω_{j1} is the indice set formed by the k values corresponding to the $\Psi_k(X_j^\lambda)$ functions, $\lambda = 1, \ldots, d$ (see example below), and Ω_{j2} is the indice set formed by the k values corresponding to the $\Psi_k(.)$ functions where X_j^λ, $\lambda = 1, \ldots, d$, appear in a monomial (see example below).

Therefore:

- A SU$_j$ is a Sensitivity Index, that represents the (estimated) Polynomial Effect of an input, X_j, obtained by cumulating the X_j, $X_j^2, \ldots, X_j^d$ effects based on a truncated PCE of degree d, and estimated by OLSR, more explicitly referred here to as PC$_d$-PESI(OLS)$_j$.
- A SUT$_j$ is a Sensitivity Index, that represents the (estimated) Total Effect, obtained by cumulating the X_j, $X_j^2, \ldots, X_j^d$ effects as well as the monomials where X_j appears based on a truncated PCE of degree d, and estimated by OLSR, more explicitly referred here to as PC$_d$-TSI(OLS)$_j$.

According to the formulas (13), each of these indices is obtained by an appropriate grouping of the P IMSI$_k$. In order to avoid additional complicated notations in this paper, we illustrate this grouping with only one example.

For example, for $d = 3$:

- PC$_3$–PESI(OLS)$_1$ is obtained by summing the three IMSI$_k$ corresponding to $\Psi_1(X_1)$, $\Psi_2(X_1^2)$, $\Psi_3(X_1^3)$, among the 19 IMSI$_k$ (for $d = 3$, we have $P = 19$), i.e., all of the $\Psi_k(.)$ where *only* X_1 appears.
- PC$_3$–TSI(OLS)$_1$ is obtained by summing the seven IMSI$_k$ corresponding to $\Psi_1(X_1)$, $\Psi_2(X_1^2)$, $\Psi_3(X_1^3)$, $\Psi_4(X_1X_2)$, $\Psi_5(X_1X_3)$, $\Psi_6(X_1X_2^2)$, $\Psi_7(X_1X_3^2)$, among the 19 IMSI$_k$, i.e., all $\Psi_k(.)$ where X_1 appears (*but not only* X_1).

3.2. PLSR background

3.2.1. Principle

PLSR is a bilinear regression method - therefore, a particular type of nonlinear method - for linking inputs to outputs and that has been very popular in the chemometrics field for many years (e.g., Martens and Naes, 1992; Tenenhaus et al., 1995; Tenenhaus, 1998; Wold et al., 2001). This regression method is very different - particularly from the algorithm point of view - from the familiar OLSR in that *no matrix inversion* is needed, on the one hand, and that it is based on the construction of some latent variables (the so-called PLS components, the t_h), on the other. For the sake of clarity, we use bold characters for the matrices below.

The general goal of PLSR is to model, via linear combinations, the link between P explanatory variables and L ($\geqslant 1$) responses (outputs) Y_l, $l = 1, \ldots, L$, both observed on the same N objects. In the context of this paper, we consider only one output at a time and, hence, $L = 1$. Keeping the same notations as in the preceding subsection, we can represent the estimated PLSR model, in matrix notation, by:

$$\widehat{Y}_N = \mathbf{\Psi}(\mathbf{X})\widehat{\beta}_{h^*}^{[PLS]} \tag{14}$$

where the $((P+1))$-vector $\widehat{\beta}_{h^*}^{[PLS]}$ is a PLS estimation of the β vector in Eq. (7), obtained with h^* optimal (significant) PLS components (see Subsections 3.2.3 and 3.2.4 for the meaning of the optimal number of PLS components, h^*). The PLSR algorithm is based on a very specific iterative algorithm, the NIPALS algorithm (Wold, 1966; Tenenhaus, 1998) whose main idea is to compute only simple regressions alternatively in the input space and the data point space. Following are some formal elements to help us understand PLSR.

Let $\mathbf{E}_0$ be the centered and scaled $\mathbf{\Psi}(\mathbf{X})$ matrix (i.e., mean $= 0$ and variance $= 1$ for each column); F_0, the centered and scaled Y vector; $\mathbf{E}_h$, the residual matrix from the decomposition of $\mathbf{E}_0$ using h PLS components, t_h; and F_h, the residual vector from the decomposition of F_0 using h *PLS* components. The PLSR objective is therefore to construct a linear combination, $u_1 = F_0c_1$, and a linear combination, $t_1 = \mathbf{E}_0w_1$ (the first PLS component) with the columns of $\mathbf{E}_0$, by the maximization of the covariance between the t_1 and u_1 components, subject to the constraints $\|w_1\|_2 = \|c_1\|_2 = 1$. Hence, we obtain two variables, u_1 and t_1, as correlated as possible, and best summing up E_0 and F_0. The following regressions:

$$\mathbf{E}_0 = t_1p_1^T + \mathbf{E}_1 \tag{15}$$

$$F_0 = t_1r_1^T + F_1$$

are then performed. The $\mathbf{E}_0$ and F_0 are deflated by $t_1p_1^T$ and $t_1r_1^T$, and second linear combinations, u_2 and t_2, are computed, and so on. We finally obtain:

$$F_0 = t_1 r_1^T + \ldots + t_h r_{h^*}^T + F_{h^*} \quad (16)$$

where the *PLS* components, the t_h, are orthogonal between them. We can develop the vectorial form of a t as:

$$t_h = \left[\sum_{j=1}^{P} cov^2\left(F_{h-1}, E_{h-1,j}\right)\right]^{-1/2} \sum_{j=1}^{P}\left[cov\left(F_{h-1}, E_{h-1,j}\right)\right] E_{h-1,j} \quad (17)$$

We can observe in Eq. (17) that PLSR deals with **partial covariances** for constructing the t_h components, $h = 1, \ldots, h^*$. The term $cov(F_{h-1}, E_{h-1,j})$ is a covariance between F_{h-1} and $E_{h-1,j}$, both residual vectors at the h step, and, this term is therefore a **partial** covariance by definition. This is the reason why Eq. (17) explains that the multicolinearity among the explanatory variables (X_j inputs and their monomials in this paper) is efficiently and iteratively taken into account.

On the basis of (16), we can deduce the following norm decomposition, i.e., an empirical decomposition of the output variance (because F_0 is centered and scaled), on the one hand:

$$\|F_0\|^2 = var(F_0) = r_1^2\|t_1\|^2 + \ldots + r_{h^*}^2\|t_{h^*}\|^2 + \|F_{h^*}\|^2 \quad (18)$$

and obtain the PLSR equation, on the other hand, as:

$$\widehat{Y}_{h^*} = \widehat{\beta}_{h^*,0}^{[PLS]} + \widehat{\beta}_{h^*,1}^{[PLS]}\Psi_1(\mathbf{X}) + \ldots + \widehat{\beta}_{h^*,P}^{[PLS]}\Psi_P(\mathbf{X}) \quad (19)$$

where the $\widehat{\beta}_{h^*,j}^{[PLS]}, j = 1, \ldots, P$, are the natural PLS estimates, elements of the $\widehat{\beta}_{h^*}^{[PLS]}$ vector.

Moreover, PLSR leads to the approximation $\widehat{F}_0 = \sum_{h=1}^{h^*} t_h r_h^T$, and we therefore obtain, for the Y output:

$$var\left(\widehat{Y}\right) = var(Y)\sum_{h=1}^{h^*} r_h^2 var(t_h) \quad (20)$$

which is an empirical **orthogonal** decomposition of the total variance of $\widehat{Y}$. Moreover, since $Y \approx \widehat{Y}$, Eq. (20) gives an approximation of an empirical orthogonal decomposition of the Y output variance.

Therefore, Eq. (11) and Eq. (12) are computed with $\widehat{\beta}_{h^*,k}^{[PLS]}$ instead of $\widehat{\beta}_k^{[OLS]}$. Two types of sensitivity indices, based on PLSR, are then obtained for every input X_j, by an appropriate grouping of the P new IMSI_k, (see end of Subsection 3.1). They are referred to, in a fairly obvious manner (OLS is replaced by PLS in the notation), as PC_d-PESI(PLS) and PC_d-TSI(PLS).

3.2.2. Two fundamental properties

3.2.2.1. Property #1. For situations with only one output Y (the case in this paper) and the $\mathbf{\Psi}(\mathbf{X})$ orthogonal model matrix, the one-component PLSR and OLSR give the same regression coefficients (Martens and Naes, 1992), i.e., $\widehat{\beta}_h^{[PLS]} = \widehat{\beta}^{[OLS]}$, where h, the number of PLS components, is equal to 1. Therefore the PC_d-PESI(PLS) and PC_d-TSI(PLS) have exactly the same values as the PC_d-PESI(OLS) and PC_d-TSI(OLS), respectively. See Tables 1 and 2 (cor = 0 columns).

3.2.2.2. Property #2. Let $\mathbf{\Psi}(\tilde{\mathbf{X}})$ be a non-orthogonal model matrix (where $\tilde{\mathbf{X}}$ is a correlated design matrix), of full rank, i.e., $A = P + 1$, or not full rank, i.e., $A < P + 1$. Then, it was proven that $\widehat{\beta}_h^{[PLS]}$ tends to $\widehat{\beta}^{[OLS]}$ when h tends to A (see de Jong (1995) and Tenenhaus (1998) for technical details of the proof). The consequence of this property is that the PC_d-PESI(PLS) and PC_d-TSI(PLS) converge to the PC_d-PESI(OLS) and PC_d-TSI(OLS), respectively, under these conditions, because the PC_d-PESI(PLS) and PC_d-TSI(PLS) are positive functions of squared PLS coefficients (the IMSI_k).

3.2.3. Validation of the PLSR model

The most frequently encountered validation methods of the significance of the PLSR model are based on cross-validation. Hence, a very popular criterion is the Q^2_{cum} (Tenenhaus, 1998; SIMCA-P9 software, 2001; Lazraq et al., 2003) constructed with the Q^2_h, $h = 1, \ldots, h^*$ (refer to the next subsection to see how h^* is obtained). It is a PLS-specific fitting-prediction criterion. Q^2_h is defined for the PLS component, t_h, by:

$$Q^2_h = 1 - \frac{\text{PRESS}_h}{\text{RSS}_{h-1}} \quad (21)$$

where:

$$\text{RSS}_{h-1} = \sum_{i=1}^{N}\left(y_i - \widehat{y}_i^{[h-1]}\right)^2 = \sum_{i=1}^{N} e^2_{h-1,i} \quad (22)$$

and

$$\text{PRESS}_h = \sum_{i=1}^{N}\left(\frac{e_{hi}}{1 - \Gamma_{h,ii}}\right)^2 \quad (23)$$

proposed in Lazraq et al. (2003), where:

- $e_{hi} = y_i - \widehat{y}_i^{[h]}$, y_i is an output result obtained with M, the computer model (see Eq. (4)), and $\widehat{y}_i^{[h]}$ is the h-component PLSR model prediction;
- $\Gamma_{h,ii}$ is the *ith* diagonal element of the $\Gamma_h = T(T^T T)^{-1} T^T$ matrix where T is the $(N \times h)$ matrix formed by vertical concatenation of the first h PLS components: $T = [t_1 \| t_2 \| \ldots \| t_h]$.

Since the computing time of a classical leave-one-out cross-validation procedure should be totally prohibitive (typically because P can be very large), it is instead possible to use Eq. (23) to obtain a (pseudo)-leave-one-out cross-validation that is well-known in the statistical theory to be a good approximation of a classical leave-one-out crossvalidation (Miller, 1990, pp. 13–14).

When a t_h component is associated with a Q^2_h value $>$ 1, it means that some potential supplementary predictive ability is contained in this t_h component because, in this case, $\text{PRESS}_h < \text{RSS}_{h-1}$. On the contrary, when a t_h component is associated with a Q^2_h value $<$ 0, it means that no potential supplementary predictive ability is contained in this t_h (because, in this case, $\text{PRESS}_h > \text{RSS}_{h-1}$) and Q^2_h is then set to zero. Note that Q^2_h does not have a monotonic behavior according to the h value.

Finally, with the h^* retained PLS components, the $Q^2_{cum}(h^*)$ cumulated index is defined by:

$$Q^2_{cum}(h^*) = 1 - \prod_{h=1}^{h^*}\left(1 - Q^2_h\right) \quad (24)$$

Note that $Q^2_{cum}(h)$ is a monotonic increasing function of h until $Q^2_{cum}(h^*)$ is reached; it is bounded between 0 and 1. It is a fitting-prediction-type criterion typically designed for a PLSR model. Its major advantage in comparison to a classical R^2 is that it avoids overfitting. If it is close enough to one, then $\widehat{M}_d(h^*)$ will be a useful estimated approximation, a metamodel, of the computer model for both fitting and prediction.

Table 2
Estimation of the sensitivity indices for the four-input Sobol' function for $d = 5$ at two different correlation levels between the three inputs. The SFD size was $N = 10000$. R^2 is the usual determination coefficient of the regression, and $Q^2_{cum}(h^*)$ is the PLS criterion computed with h^* significant PLS components. See Appendix for the other abbreviations.

Inputs	Analytical	cor = 0		cor = 0.8	
	FOSSI	PC_5-PESI(OLS)	PC_5-PESI(PLS)	PC_5-PESI(OLS)	PC_5-PESI(PLS)
X_1	0.6037	0.6123	0.6123	0.5266	0.5703
X_2	0.2683	0.2701	0.2701	0.2610	0.2551
X_3	0.0671	0.0675	0.0675	0.0683	0.0626
X_4	0.0200	0.0200	0.0201	0.0213	0.0076
Inputs	*TSSI*	PC_5 -TSI(OLS)	PC_5 -TSI(PLS)	PC_5 -TSI(OLS)	PC_5 -TSI(PLS)
X_1	0.6342	0.6391	0.6391	0.6319	0.6223
X_2	0.2945	0.2935	0.2935	0.3653	0.3409
X_3	0.0756	0.0750	0.0750	0.1021	0.1094
X_4	0.0227	0.0224	0.0225	0.0697	0.0434
R^2		0.981	0.981	0.996	0.996
$Q^2_{cum}(h^*)$			0.981 (4)(4)		0.996 (29)(29)

3.2.4. Stopping rule

The PLSR model is iteratively built and the PLS components are computed step-by-step until $h = h^*$. These iterations are stopped by means of a stopping rule, different from those found in Tenenhaus (1998) or in SIMCA-P9 software (2001) that are adapted for real experimental noisy data (where the error variance has its usual meaning). For computer models, there are no definitive relevant stopping rules. Instead, in our computer model context, we propose the following stopping rule: to retain h^* significant components, i.e., $h^* = h - 1$ when $\left|Q^2_h - Q^2_{h-1}\right| \leq 10^{-4}$. This threshold value was empirically chosen after several trials and is low enough to always be adapted, regardless of the situation. The $Q^2_{cum}(h^*)$ is then computed with Formula (24), and the new indices are computed (corresponding to the vertical line in Figs. 5 and 7). $\forall h > h^*$, Q^2_h is then set to zero and $Q^2_{cum}(h > h^*) = Q^2_{cum}(h^*)$.

Note that for $h = h^*$, the PC_d-PESI(PLS) and PC_d-TSI(PLS) are different from the PC_d-PESI(OLS) and PC_d-TSI(OLS), respectively. This a crucial point in the method: generally, we have $h^* \ll A$, the rank mentioned in Property #2. Therefore, in Figs. 5 and 7, the optimal values of the sensitivity indices are obtained at $h = h^*$(at the vertical lines) and not when $h = 80$ (Fig. 5) or $h = 50$ (Fig. 7). We let the iterations on h continue to 80 and 50 only for the purpose of illustrating Property #2: indeed, for these latter h values, the PC_d-PESI(PLS) and PC_d-TSI(PLS) values are close to the PC_d-PESI(OLS) and PC_d-TSI(OLS) values, respectively.

3.2.5. Root Mean Square Error in Prediction

For illustration purposes - not for a stopping rule - we also computed the Root Mean Square Error in Prediction ($RMSEP_h$), defined in the PLS context by:

$$RMSEP_h = \sqrt{\frac{PRESS_h}{N}} \tag{25}$$

and in the OLS context by:

$$RMSEP = \sqrt{\frac{PRESS}{N}} \tag{26}$$

where the usual PRESS is defined by:

$$PRESS = \sum_{i=1}^{N} \left(\frac{e_i}{1 - P_{ii}}\right)^2 \tag{27}$$

where P_{ii} is the *ith* diagonal element of the usual OLSR projector.

3.3. Steps of the method

The practical implementation of this method is based on the following six-step procedure.

Step #0: $h = 1$.Set N, p, $h_{\max}$, $d_{\max}$, TH (threshold for $Q^2_{cum}(h)$; see comment at the end of this subsection).
Step #1: An initial independent SFD of N rows and p columns (p inputs are involved) is generated, referred to as *N-SFD*, which leads to a first **X** design matrix once the column ranges of the SFD have been calibrated to the input ranges we have to analyze. This SFD can be made of a Sobol' quasi-random sequence (Lemieux, 2009) or, in an alternate way, made of a Latin Hypercube Sampling (LHS) (McKay et al., 1979). Therefore, in **X**, the inputs are (approximately) independently and uniformly sampled (inside their own ranges) and, hence, (approximately) not correlated. There is not a general rule for deciding the value of a SFD size, N. However, there are some publications that give a rule of thumb about this N. See, for example, Loeppky et al. (2010) and Levy and Steinberg (2010). In GSA, it seems that the results are acceptable with N approximately equal to $100 \times p$. However, it is also true that the results actually become more stable and more relevant if $N \geq 1000 \times p$. This value of N depends on the nonlinearity, generally not known, of the computer model. For instance, the Ishigami model analyzed in the next section requires at least $N = 10000$ to obtain good estimations of the (analytical) SSI, whereas $p = 3$ only. However, it should be emphasized that the N value may be very small if some optimized SFD are used (see, for example, the sequential approach in Sudret, 2008).
Step #2: Once a target correlation matrix is chosen (by simulation or by the experts of the scientific problem; see Subsection 5.4), the inputs in **X** are correlated using the Iman and Conover technique (Iman and Conover, 1982). The clever Iman and Conover technique works by sorting the values of the inputs in the initial **X** to correlate the inputs as closely as possible to the correlation matrix target, while the original input uniform distributions remain unchanged. The resulting correlated matrix design, $\tilde{\mathbf{X}}$, has the same dimensions as **X**.
Step #3: The N runs, described by the respective N rows of $\tilde{\mathbf{X}}$, are achieved by the computer model, M, and the response output values are stored in the $Y_{N\times 1}$ vector.
Set$d = 1$.
Step #4: The model matrix $\boldsymbol{\Psi}(\tilde{\mathbf{X}})_{N\times P}$ corresponding to the truncated Legendre PCE of degree d with P monomials is built (see Subsection 3.1).

Set $h = 1$
Step #5: The metamodel, $M_d(h)$, is computed by using $\boldsymbol{\Psi}(\tilde{\mathbf{X}})_{N\times P}$ and the $Y_{N\times 1}$ vector, by means of PLSR.
Bounding: if $Q_h^2 < 0$ then $Q_h^2 = 0$.
Beginning of the Tests:

- If $h = 1$, then do $h = h + 1$, and go to Step #5.
- If $h > 1$, then do:
  - If $\left|Q_h^2 - Q_{h-1}^2\right| > 10^{-4}$, then do:
    - If $h < h_{\max}$, then $h = h + 1$, and go to Step #5.
    - If $h = h_{\max}$, then do:
      - If $Q_{cum}^2(h) \geq$ TH, then $h^* = h_{\max}$; $d^* = d$; the procedure is successful: an optimal metamodel, $M_{d^*}(h^*)$, is obtained, characterized by $Q_{cum}^2(h^*)$. In this case, go to Step #6.
      - If $Q_{cum}^2(h) <$ TH, then do:
        → if $d = d_{\max}$, then the procedure stops: no metamodel is obtained and, hence, no SI can be computed.
        → if $d < d_{\max}$, then do: $d = d + 1$ and go to Step #4
  - If $\left|Q_h^2 - Q_{h-1}^2\right| \leq 10^{-4}$, then do:
    - If $Q_{cum}^2(h) \geq$ TH, then $h^* = h - 1$; $d^* = d$; an optimal metamodel, $M_{d^*}(h^*)$, is obtained, characterized by $Q_{cum}^2(h^*)$. In this case, go to Step #6.
    - If $Q_{cum}^2(h) <$ TH, then do:
      - If $d = d_{\max}$, then the procedure stops: no metamodel is obtained and, hence, no SI can be computed.
      - If $d < d_{\max}$, then do: $d = d + 1$ and go to Step #4.

End of the Tests
Step #6: The $\widehat{\beta}_{h^*}^{[PLS]}$ vector of $M_{d^*}(h^*)$, leads to the P IMSI$_k$ (see Eq. (11)) and, consequently, to the PC$_d$-PESI(PLS) and PC$_d$-TSI(PLS) obtained by the grouping of these IMSI$_k$, as explained at the end of Subsection 3.1. The procedure is over.

Note that if the procedure converges to STOP (see Fig. 3), it is possible to re-run this procedure after a forward momonial selection, as described in Subsection 3.5. If $Q_{cum}^2(h^*)$ is less than TH when d reaches $d_{\max}$, a less ambitious TH value can be proposed by the user, typically 0.90, and the procedure is run once again. If a TH value of 0.75 is never reached, then it is not possible to obtain a good metamodel or reliable SI for the available dataset. Fig. 3 gives a scheme of the method steps.

3.4. Summary of the advantages of the method

- a) The P monomials, the $\Psi_k(\mathbf{X})'s$, can be highly correlated or even functionally linked but the $\widehat{\beta}^{[PLS]}$ estimate of β remains computable because *no matrix inversion* is used in *PLSR* (e.g., see the very well-illustrated example in Kettaneh-Wold (1992) where the inputs add up to one at each row of the design matrix).
- b) P can be larger than N, the row size of $\tilde{\mathbf{X}}$; this property can be very useful if only a reasonable number of runs is affordable in the case of an excessively time-consuming run and, therefore, the number of runs, N, will be less than the total number of monomials, P.
- c) Information about the probability distributions of the inputs is not needed (it is considered to be a so-called distribution-free method) and, therefore, it should be possible to consider non-uniform distributions for the p inputs.

In the situation (a) (in the case of functionally linked inputs) and (b), it is obviously impossible to use OLSR because the so-called information matrix of the OLSR is consequently singular. In addition to these benefits, fundamental mathematical justifications for using PLSR in the context of GSA based on a polynomial metamodeling rely on Properties #1 and #2 given in Subsection 3.2.2.

3.5. Improvement of the method: a forward monomial selection

Since the total number of monomials, P, can become very large when d and/or p increase - that should lead to intractable huge matrices in the computed memory - we propose to decrease P to P' by a forward monomial selection. The principle of this selection is very simple: the P (ordinary) simple regressions of the output function of only one monomial are performed, while the P values of R^2 are stored. This task is very fast, i.e., one million simple regressions can be performed in approximately 20 h on a standard Pentium desk PC. The stored P values of R^2 are sorted, and the user then decides to select the P' ($\ll P$) monomials corresponding to the P' highest R^2. Finally, the metamodel is estimated with these P' ($\ll P$) monomials with a shorter computing time (see Tables 6 and 7). The choice of P' is a compromise depending on d and TH. This approach was applied for the biophysical application and the results are given in Tables 6 and 7

4. Application to two academic models

4.1. Application to the Ishigami function

We used a SFD of size $N = 10000$. The results of the method applied to the Ishigami function are given in Table 1.

When the inputs are not correlated (cor = 0 in Table 1), we can observe a clear illustration of Property #1: the results based on OLS and PLS are very close, and very close to the analytical values as well, even if the significant PLS component number, h^*, should have been 1 according to Property #1, not 3. Indeed, the inputs in $\mathbf{X}$ are not strictly orthogonal because some very weak correlations can exist due to the SFD generation procedure: correlation coefficients between the three inputs were $\rho_{12} = 0.0027$, $\rho_{13} = -0.0066$, $\rho_{23} = -0.0061$, all very close to zero. Therefore, the lines in Fig. 4 vs. h, corresponding to the three inputs, are always practically flat. For the correlated case (cor = 0.8 in Table 1), $h^* = 22$ because $Q_h^2 = 0$ for $h > 22$.

Otherwise, note that the metamodel accuracy practically did not change regardless of the correlation level (cor = 0 or cor = 0.8). From a theoretical point of view, in the context of OLS, the correlation between the inputs does not affect the metamodel accuracy (R^2 changes very little, from 0.984 to 0.987) because the projection operator is not affected: the projection of the output vector on the space spanned by the input vectors remains an orthogonal projection. This is the fundamental reason. Moreover, in this case, the metamodel accuracy does not really change in the PLS context. However, in some application cases, it has been observed that the metamodel accuracy can be improved (in the presence of a strong correlation between the inputs) if PLSR was used to estimate the coefficients of the metamodel (based on a PCE or not). The reason is that the projection operator in PLSR is not the same as in OLSR (see Tenenhaus, M., 1998; pages 115–116). This specific projection operator leads to the well-known high predictive ability of the PLS regression.

Finally, we recall that the (ambitious) objective of our method is to provide accurate estimations of sensitivity indices in the case of correlation between the inputs, as well as *simultaneously* obtaining a good metamodel. This is the crucial point: correctly doing both simultaneously.

Fig. 4 displays the evolution of the PC$_6$-PESI(PLS) and the PC$_6$-TSI(PLS) for the non-correlated case, respectively, vs. the current PLS component number, h.

Fig. 5 displays the evolution of the PC$_6$-PESI(PLS) and the PC$_6$-TSI(PLS) for the correlated case, respectively, vs. the current PLS component number, h.

To the contrary of Fig. 4, we can observe a strong variation of the

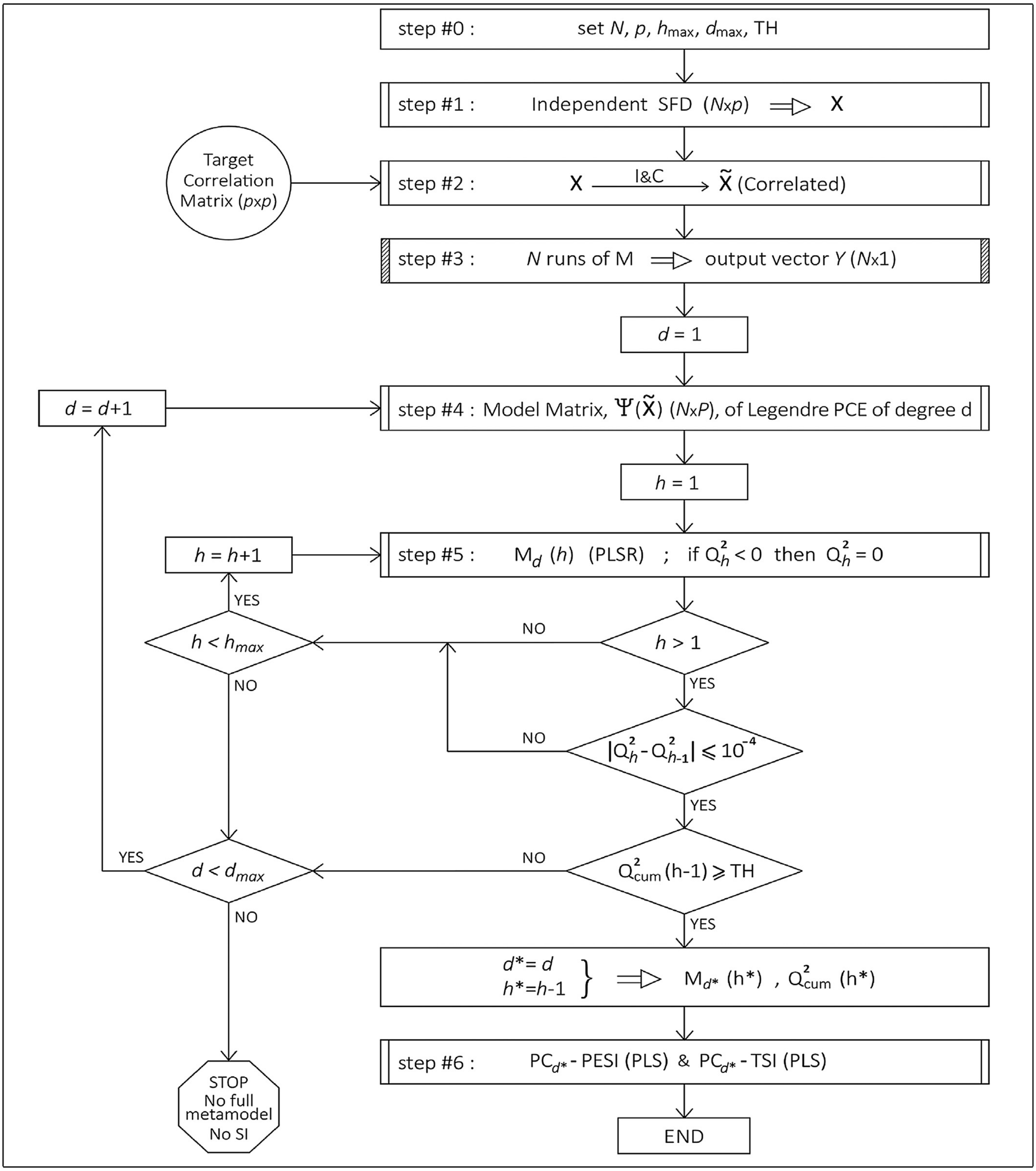

Fig. 3. Scheme of the method steps. If the procedure converges to STOP, it is possible to re-run this procedure after a forward monomial selection, as described in Subsection 3.5.

three lines in Fig. 5, corresponding to the three inputs vs. h when $h > h^*$. This is an expected behavior due to the deflation process (see Eq. (15)) that continues until the h_{max} value decided by the user beforehand is reached.

4.2. Application to the Sobol' function

We used a SFD of size $N = 10000$. The results of the method applied to the Sobol function are given in Table 2.

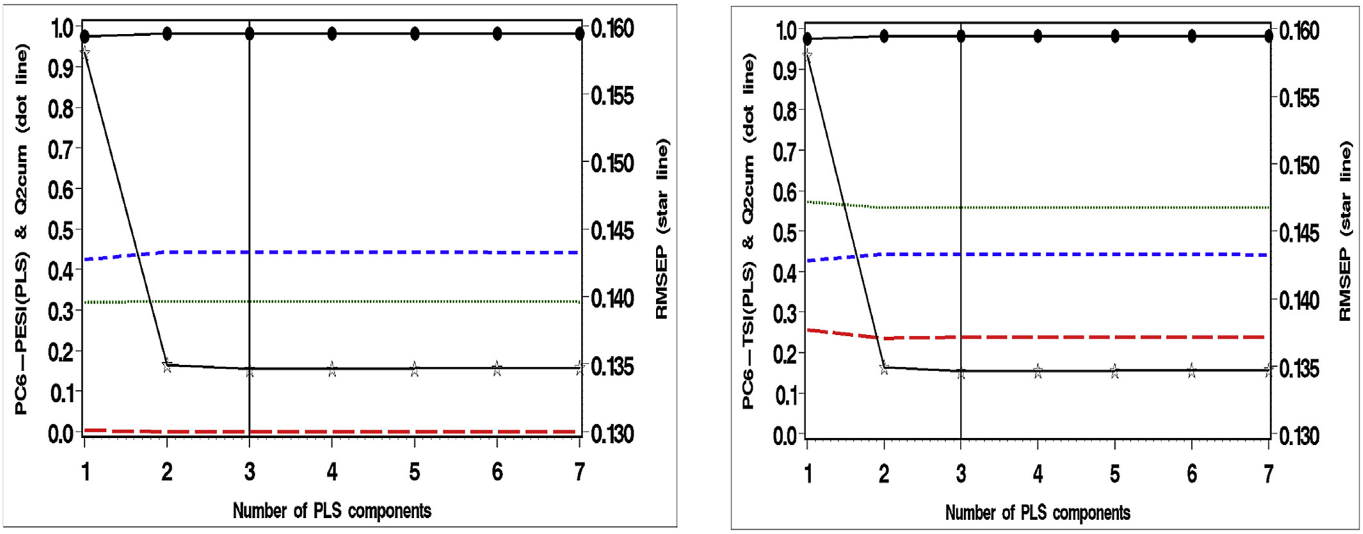

Fig. 4. Ishigami function, NON-CORRELATED case, for a 10000 -SFD. The evolution of the three PC_6-PESI(PLS) in the left panel (small dashed line for X_1 , medium dashed line for X_2 , large dashed line for X_3) and the three PC_6-TSI(PLS) in the right panel, vs. the PLS component number, *h*. The dotted line stands for the $Q^2_{cum}(h)$ evolution, and the starred line stands for the $RMSEP_h$ (see Eq. (25)). The values of $RMSEP_h$ are on the same scale as that of the output. The vertical line, $h^* = 3$, indicates the optimal values of the SI.

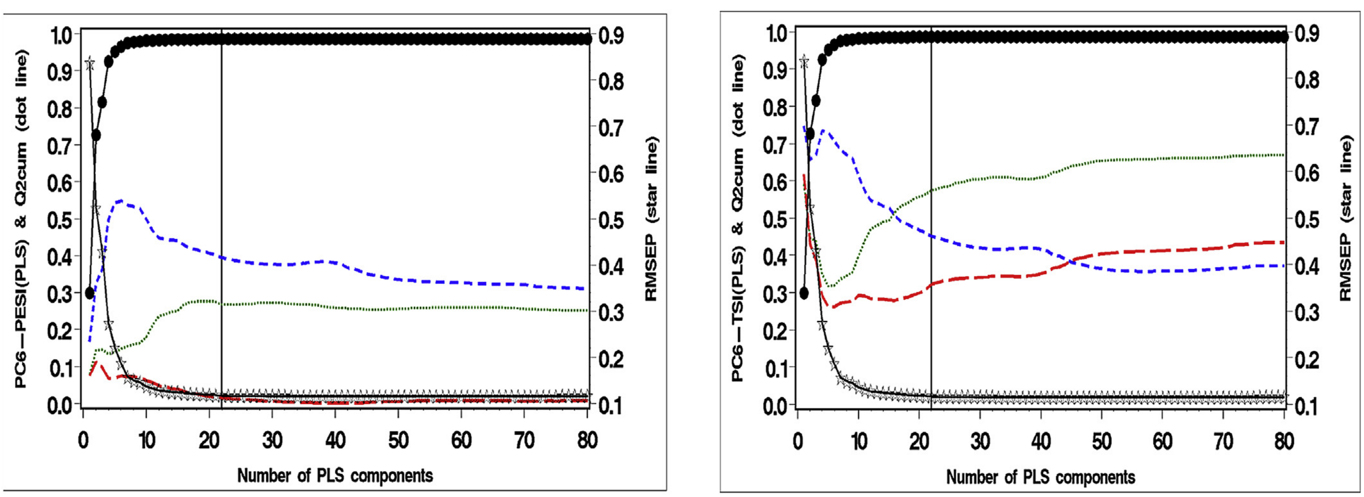

Fig. 5. Ishigami function, CORRELATED case (cor = 0.8), for a 10000 -SFD. Evolution of the three PC_6-PESI(PLS) in the left panel (small dashed line for X_1 , medium dashed line for X_2 , large dashed line for X_3) and the three PC_6-TSI(PLS) in the right panel, vs. the PLS component number, *h*. The doted line stands for theQ^2_{cum} (h) evolution, and the starred line stands for the $RMSEP_h$ (see Eq. (25)). The vertical line, $h^* = 22$, indicates the optimal values of the SI.

We can make the same comments about Table 2 as for Table 1. Figs. 6 and 7 display the evolution of the PC_5-PESI(PLS) and the PC_5-TSI(PLS) for the noncorrelated and correlated cases, respectively, vs. the current PLS component number, *h*.

The same comments as for Fig. 5 can be made about Fig. 7. In the next section, our method is applied to a real world case.

5. A case study with a 3D-light interception computer model

5.1. Presentation of the problem

F LORS YS is a mechanistic weed dynamics computer model (coded in C/C++) that can be applied to current and prospective cropping systems. Testing numerous cropping systems and combinations of agricultural practices can help to predict the impacts of agricultural practices and their interactions on weeds. Weeds are both harmful for crop production and important for biodiversity, so it is critical to help farmers to design cropping systems that reconcile these two aspects. We need a faster version of F LORS YS in order to develop a decision support system to reach this goal.

Building a metamodel of the 3D light interception computer model is a solution to simplify and accelerate F LORS YS. We began by analyzing light interception by a single plant, depending on its morphology, as well as day, latitude and field parameters. The effect of neighborhood canopies will be treated in a future paper.

5.2. Inputs

Three types of input variables were used in the sensitivity analysis and metamodeling, resulting in a total of 11 inputs (Table 3): (a) the variables determining the position of the solar angle, i.e., the latitude (Lati) of the simulated field and the Julian day; (b) the variables describing the field sample, i.e., its dimensions in the north-south and in the east-west directions, as

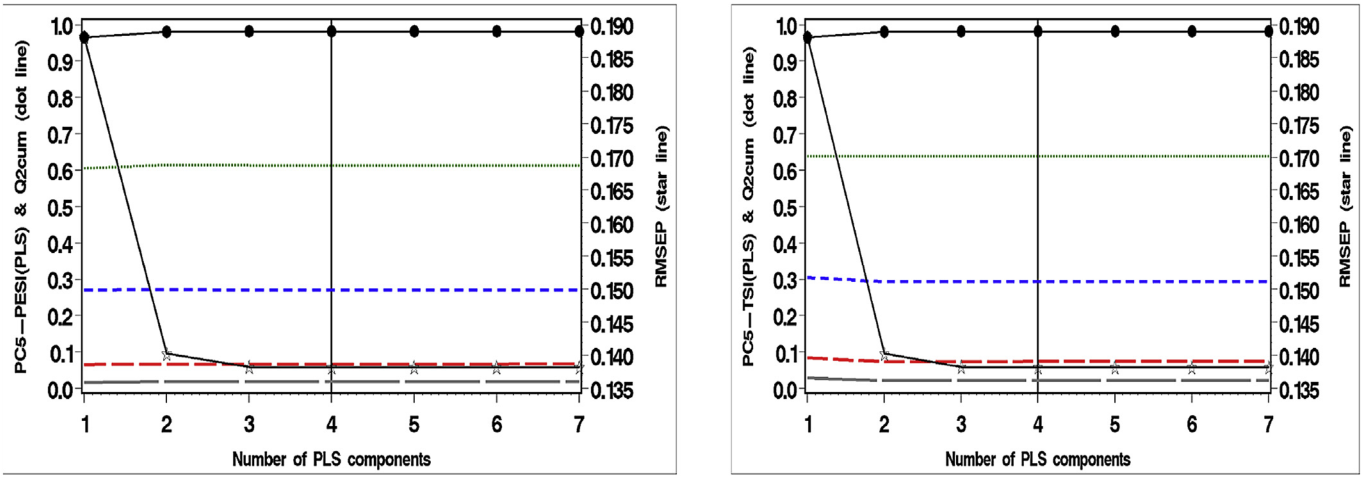

Fig. 6. Sobol' function, NON-CORRELATED case, for a 10000 -SFD. The evolution of the three PC_5 -PESI(PLS) in the left panel (small dashed line for X_1 , medium dashed line for X_2 , large dashed line for X_3 , very large dashed line for X_4) and the three PC_5 -TSI(PLS) in the right panel, vs. the *PLS* component number, *h*. The dotted line stands for the Q^2_{cum} (h) evolution, and the starred line stands for the $RMSEP_h$ (see Eq. (25)). The values of $RMSEP_h$ are on the same scale as that of the output. The vertical line, $h^* = 4$, indicates the optimal values of the SI.

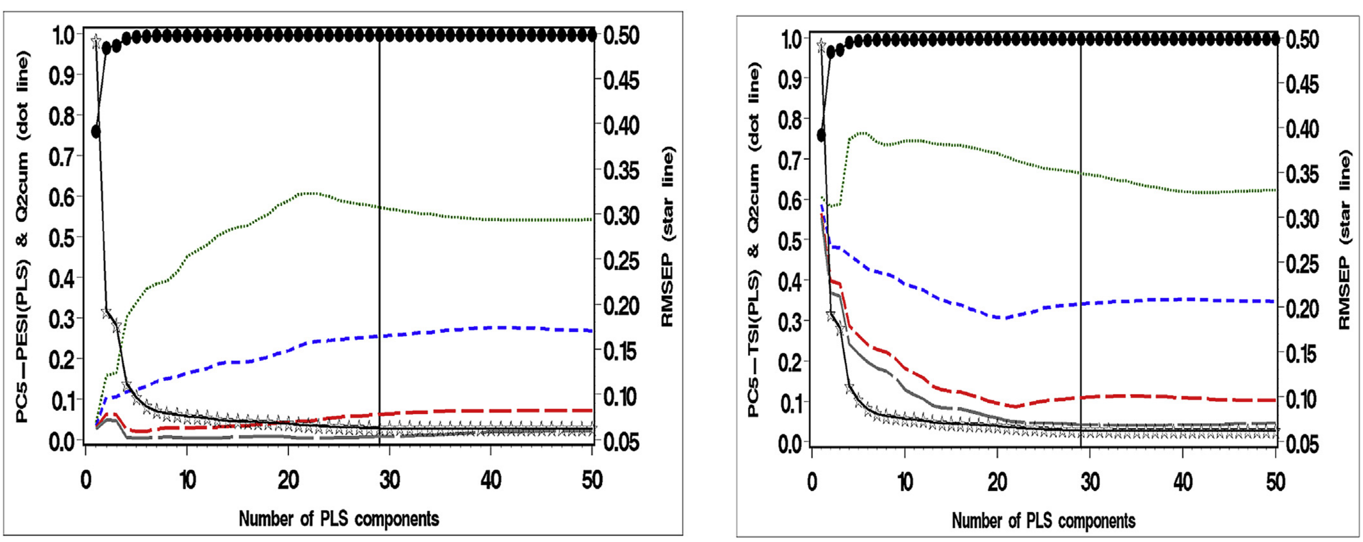

Fig. 7. Sobol' function, CORRELATED case (cor = 0.8), for a 10000 -SFD. Evolution of the three PC_5 -PESI(PLS) in the left panel (small dashed line for X_1 , medium dashed line for X_2 , large dashed line for X_3 , very large dashed line for X_4) and the three PC_5 -TSI(PLS) in the right panel, vs. the PLS component number, *h*. The dotted line stands for the Q^2_{cum} (h) evolution, and the starred line stands for the $RMSEP_h$ (see Eq. (25)). The vertical line, $h^* = 29$, indicates the optimal values of the SI.

Table 3
Range of variation and unit of the 11 inputs in the 3D light interception computer model. Note that the value of 1.1 for k is a possible value for an extinction coefficient, as it was found in the literature for Trifolium repens (Monteith, 1969).

Input Name	Short explanation	Ranges of variation	Units
Lati	Latitude of the simulated field	[−66 ; +66]	angle degree
Day	Julian day	[1 ; 365]	
Xmax	Xmax: Field sample size in the east-west direction	[1 ; 4]	*m*
Ymax	Ymax: Field sample size in the south-north direction	[1 ; 4]	*m*
Voxel	Voxel edge size	[1 ; 20]	*cm*
Height	Height of the plant	[1 ; 250]	*cm*
Width	Width of the plant	[1 ; 200]	*cm*
LA	Cumulated leaf area of the plant	[1 ; 10^5]	cm^2
k	Light extinction coefficient	[0.01 ; 1.1]	no unit
RH50	Relative plant height below which half of the cumulated leaf area is located	[0.01 ; 1]	cm/cm
b	Shape parameter for leaf distribution vs. plant height	[0.01 ; 6]	no unit

Note that we can consider the "Day" input as a continuous input because it has a large number of levels (365).

well as the grain of the discretization, i.e., the voxel edge size; (c) the variables describing the plant morphology. A plant is

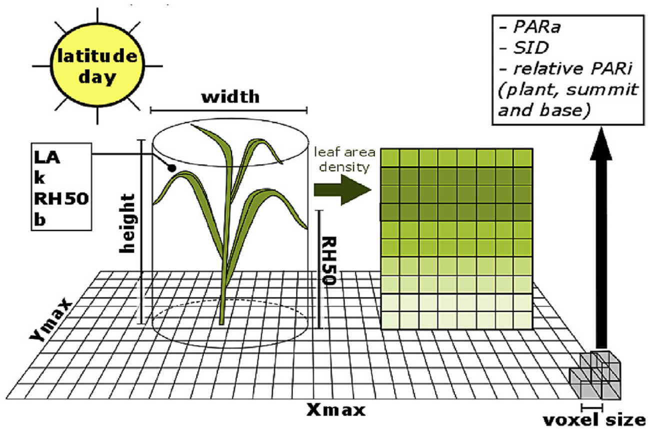

Fig. 8. Schematic representation of the 11 **inputs** (see Table 3 for a short explanation), and the five **outputs** (PARa, SID, rPARi, rPARiS(ummit), rPARiB(ase)) of the 3D light interception computer model. Voxels may be empty or may include a variable leaf density. Only PARa is analyzed in this paper.

represented as a cylinder bounded by its height and width (Fig. 8). The cumulated leaf area (LA) of the plant is distributed in the successive voxel layers of the cylinder, with 50% of the cumulated leaf area below relative height RH50 of the plant and its distribution governed by the shape parameter, b. The light extinction coefficient, k, determines how the incident light is absorbed by the leaves. The terms used are defined in Table 3.

5.3. Outputs

Each day, the 3D light interception computer model computes several output variables (see Fig. 8) for the target plant, which are all expressed as a proportion of the incident photosynthetically-active radiation arriving on top of the canopy (in this case, it is reduced to the target plant). In this paper, for reasons of space, only the PARa (normalized range $= [0, 100]$) will be analyzed and simply referred to as output (or response) below. The PARa is the photosynthetically-active radiation, i.e., the wavelength range of sunlight that is usable by plants.

5.4. Construction of the correlated ***design matrix***

This construction is the objective of Steps #1 and #2 (see details in Subsection 3.3 and Fig. 3). A first independent 10000-SFD of 11 columns was generated (Step #1) that lead to an $\mathbf{X}$ design after calibrating the SFD values in the input ranges of Table 3. The values of the correlation coefficients between the 11 inputs were then chosen according to the following rationale. The Voxel input and the four inputs, Latitude (Lati), Day, Xmax and Ymax, describing the solar angle and field sample, were considered to be independent and uncorrelated. In order to identify correlations between input variables (except field sample variables), we achieved the following simulation design. We randomly sampled plants occurring in 12 diverse cropping systems of past simulations run with 13 crop species and 25 weed species (Colbach et al., 2016). More precisely, the 12 (real) cropping systems are from 11 to 28 years long (four are 11 years long, five are 13 years long, one is 32 years long, and the last two are 27 years long). For each one, we sampled at least 100 plants a month. In theory, we should have 234,000 plants, but some months we had less than 100 plants on the field (i.e., non-cultivated months, etc.). Hence, we finally obtained 221,288 plants. Correlation coefficients between the 11 input values were computed for these simulated plants. These correlations and expert knowledge

Table 4
Target correlation sub-matrix (part of the 11 × 11 target correlation matrix) needed for the Iman and Conover technique, for the six inputs, Height, Width, cumulated leaf area (LA), k, RH50, and b. The other five inputs, Voxel, Lati, Day, Xmax, and Ymax, are assumed not to be correlated.

	Height	Width	LA	k	RH50	b
Height	1	0.60	0.20	−0.2	0.20	0.30
Width	0.60	1	0.20	0	0.20	0.30
LA	0.20	0.20	1	0	0	0
k	−0.20	0	0	1	0.2	−0.10
RH50	0.20	0.20	0	0.20	1	0.10
b	0.30	0.30	0	−0.10	0.10	1

were used to construct a target correlation matrix for the 11 inputs. The non-diagonal 6× 6 sub-matrix is given in Table 4.

Step #2 lead to the correlated $\mathbf{X}$, the $\tilde{\mathbf{X}}$ characterized by the resulting correlation matrix given in Table 5 (very close to the target correlation matrix).

In Step #3, the 10000 runs were computed with the 3D light interception computer model. Therefore, the primary dataset was formed by a matrix of 10000 rows and 12 columns: 11 columns for the 11 inputs (the $\tilde{\mathbf{X}}$) and column #12 for the vector of the corresponding 10000 output values. This primary dataset was divided into two datasets: a learning dataset of 9500 rows, on one hand, and a validation dataset of 500 rows (randomly sampled in the 10000 rows of the primary dataset), on the other.

6. Results

We now emphasize a crucial aspect of the method. Assessing correlation between inputs is not trivial. In the likely case that correlations exist but are not known, we compare the results based on an independent $\mathbf{X}$ design here, therefore not corrected for correlations. Results for the correlated and non-correlated cases are given below. Steps #4 and #5, detailed in Subsection 3.3 and Fig. 3, were iteratively achieved on the learning dataset in two different ways: (a) by considering a full metamodel, i.e, with P monomials; or (b) by considering a partial metamodel according to the forward monomial selection described in Subsection 3.5, i.e., with $P'(<P)$ monomials. The results for the correlated case are given in Table 6, and for the non-correlated case in Table 7.

By observing Table 6, the final choices could be made either for the full metamodel, M7, which leads to a fairly good metamodel ($R^2 = 0.96$ and $Q^2_{cum}(22) = 0.96$), or for the partial metamodel, M#5, which leads to a roughly equivalent good metamodel ($R^2 = 0.94$ and $Q^2_{cum}(15) = 0.93$) based on less monomials (2000 instead of 4367), leading to predictions that are approximately two times faster. The sensitivity indices corresponding to M#7, the PC_5-PESI(PLS) and the PC_5-TSI(PLS) are given in Table 8. CTB is the Computing Time for Building a metamodel, i.e., the time required to build a PLS-metamodel with its h^* significant components,

Table 5
The resulting correlation sub-matrix obtained by the Iman and Conover technique for the six inputs, Height, Width, cumulated leaf area (LA), k, RH50, and b. The other five inputs, Voxel, Lati, Day, Xmax and Ymax, have correlation coefficient estimations very close to zero, as expected.

	Height	Width	LA	k	RH50	b
Height	1	0.58	0.19	−0.19	0.20	0.29
Width	0.58	1	0.19	0	0.19	0.30
LA	0.19	0.19	1	0	0	0
k	−0.19	0	0	1	0.20	−0.11
RH50	0.20	0.19	0	0.20	1	0.09
b	0.29	0.30	0	−0.11	0.09	1

Table 6
CORRELATED CASE. Results of the 13 PLS-metamodels for the PARa output, according to their degree d. See Appendix for definitions of h^*, $Q^2_{cum}(h^*)$, R^2 and $RMSEP_{h^*}$. CTB# (Computing Time for Building) is the time required for a PLS-metamodel to be built with its h^* significant components (this time includes the computing time of its associated sensitivity indices). P stands for the number of monomials in a full metamodel of degree d, while P' stands for the number of selected monomials in a partial metamodel (see Subsection 3.5) of degree d.

M#	d	Monomial number	h^*	$Q^2_{cum}(h^*)$	R^2	$RMSEP_{h^*}$	CTB#
1	1	$P = 11$	3	0.56	0.56	0.662	3 s
2	2	$P = 77$	6	0.80	0.80	0.450	24 s
3	3	$P = 363$	8	0.87	0.87	0.358	2 min
4	4	$P = 1364$	12	0.91	0.92	0.290	10 min
5	5	$P' = 2000$	15	0.93	0.94	0.250	20 min
6	5	$P' = 3000$	18	0.94	0.95	0.224	1 h
7	5	$P = 4367$	22	0.96	0.96	0.195	4 h
8	6	$P' = 2000$	17	0.94	0.95	0.241	28 min
9	6	$P' = 3000$	20	0.95	0.96	0.212	1 h 18 min
10	6	$P' = 4000$	24	0.96	0.97	0.186	3 h 30 min
11	7	$P' = 2000$	19	0.93	0.94	0.246	43 min
12	7	$P' = 3000$	22	0.95	0.95	0.215	1 h 42 min
13	7	$P' = 4000$	28	0.96	0.97	0.186	5 h

Table 7
NON-CORRELATED CASE. Results of the 13 PLS-metamodels for the PARa output, according to their degree d. See Appendix for definitions of h^*, Q^2_{cum}, R^2 and $RMSEP_{h^*}$. CTB# (Computing Time for Building) is the time required for a PLS-metamodel to be built with its h^* significant components (this time includes the computing time of its associated sensitivity indices). P stands for the number of monomials in a full metamodel of degree d, while P' stands for the number of selected monomials in a partial metamodel (see Subsection 3.5) of degree d.

M#	d	Monomial number	h^*	$Q^2_{cum}(h^*)$	R^2	$RMSEP_{h^*}$	CTB#
14	1	$P = 11$	2	0.49	0.49	0.713	3 s
15	2	$P = 77$	2	0.72	0.72	0.528	15 s
16	3	$P = 363$	3	0.83	0.83	0.407	1 min 14 s
17	4	$P = 1364$	6	0.90	0.90	0.316	6 min
18	5	$P' = 2000$	9	0.92	0.92	0.275	12 min
19	5	$P' = 3000$	12	0.94	0.95	0.224	33 min
20	5	$P = 4367$	16	0.94	0.96	0.209	2 h 15 min
21	6	$P' = 2000$	10	0.94	0.95	0.241	17 min
22	6	$P' = 3000$	12	0.95	0.96	0.212	38 min
23	6	$P' = 4000$	16	0.96	0.97	0.186	1 h 45 min
24	7	$P' = 2000$	11	0.90	0.93	0.267	30 min
25	7	$P' = 3000$	14	0.89	0.94	0.238	57 min
26	7	$P' = 4000$	15	0.87	0.95	0.213	1 h 47 min

Table 8
Sensitivity Indices: the PC_5-PESI(PLS) and PC_5-TSI(PLS) corresponding to the metamodels M#7 and M#20 given in Tables 6 and 7, respectively, for the correlated and non-correlated cases.

	Correlated Case		Not-Correlated Case	
Inputs	PC_5-PESI(PLS)	PC_5-TSI(PLS)	PC_5-PESI(PLS)	PC_5-TSI(PLS)
Latitude	0.005	0.112	0.007	0.090
Day	0.000	0.084	$\simeq 0$	0.058
Xmax	0.000	0.051	$\simeq 0$	0.034
Ymax	0.000	0.053	$\simeq 0$	0.036
Voxel	0.087	0.234	0.105	0.229
Height	0.289	0.508	0.358	0.507
Width	0.154	0.376	0.171	0.305
LA	0.016	0.108	0.023	0.099
k	0.019	0.108	0.021	0.091
RH50	0.001	0.069	0.001	0.044
b	0.003	0.074	0.001	0.042

including the computing time of its associated sensitivity indices. Other elements about computing times are given in the Discussion section.

In Table 8 and Fig. 9, the total effect indices in both cases are much larger than the polynomial effect indices, so we can deduce that the inputs act in a very interactive nonlinear way on the response via some complex interactions represented by particular $\Psi_k(\tilde{\mathbf{X}})$ monomials. These $\Psi_k(\tilde{\mathbf{X}})$ play a strong role in the construction of the total indices.

In this case study, it did not appear to be reasonable to compute these indices by ignoring input correlations because, in this case:

- the order between some SI can be changed,
- the PC_5-PESI(PLS) of the height input is increased,
- all the SI are modified even if they were only slightly modified (we however recall that the SI of the academic models of Subsections 4.1 and 4.2 were strongly modified when correlations were ignored).

By considering the total effect indices, the most relevant indices, we can now clearly deduce the input influences on the response from Table 8 and Fig. 9. Inputs that determine plant volume were shown to present the strongest total effect (i.e., height and width), followed by the discretization grain of the 3D plant representation (i.e., voxel). Plant inputs that determine light absorption ability (cumulated leaf area, LA and extinction coefficient, k), as well as the variable that determines the maximal solar angle (Lati) have similar medium influences. Finally, inputs that determine cumulated leaf area inside the plant volume (RH50 and b), actual solar angle (i.e., day) and field sample area (Xmax and Ymax) have similar weaker effects.

Fig. 10 (left panel) is the observed-predicted scatter plot of the 3D light interception computer model output vs. the M#7 metamodel output. The R^2 value of the corresponding regression line on this plot is 0.96, which means that the metamodel is an acceptable fitting of the computer output. For a more rigorous and severe test, M#7 was then used to predict the 500 output values of the validation dataset. The result is represented in Fig. 10 (right panel) where the R^2 value of the regression line is 0.789, which means that the metamodel has a fairly good predictive ability for such a sophisticated real case study. For the non-correlated case, the corresponding scatter plots are not given in this paper because they appear to be very close.

7. Discussion and conclusions

7.1. Methodological aspects

The powerful practical method we propose makes it possible to obtain both estimations of sensitivity indices and metamodel construction when the continous inputs of a computer model are correlated, regardless of the correlation level between the inputs, the type of computer model and the input distributions. To achieve this goal, we used a truncated PCE of the computer output, but by estimating its coefficients with PLSR rather than with OLSR. Properties #1 and #2 provide a strong rationale for the use of PLSR. Notably, Property #1 guarantees that our PC_d-PESI(PLS) and PC_d-TSI(PLS) are equivalent to the PC_d-PESI(OLS) and PC_d-TSI(OLS) if the inputs are independent. They are therefore correct estimations of the SSI if the input distributions are uniform. When the inputs are correlated, these new indices are not estimations of SSI because the SSI are mathematically defined only for independent continuous inputs. However, the PC_d-PESI(PLS) and PC_d-TSI(PLS) can correctly reflect the sensitivity of the output relative to the correlated inputs, thanks to the best well-known management of the multicolinearity by PLSR (see the comment about Eq. (17) in Subsection 3.2.1). We also emphasize that a crucial aspect of the method is to have rather good correlation estimations beforehand.

Note that we cannot really compare our results with those of Marie and Simioni (2014) who studied a case similar to ours

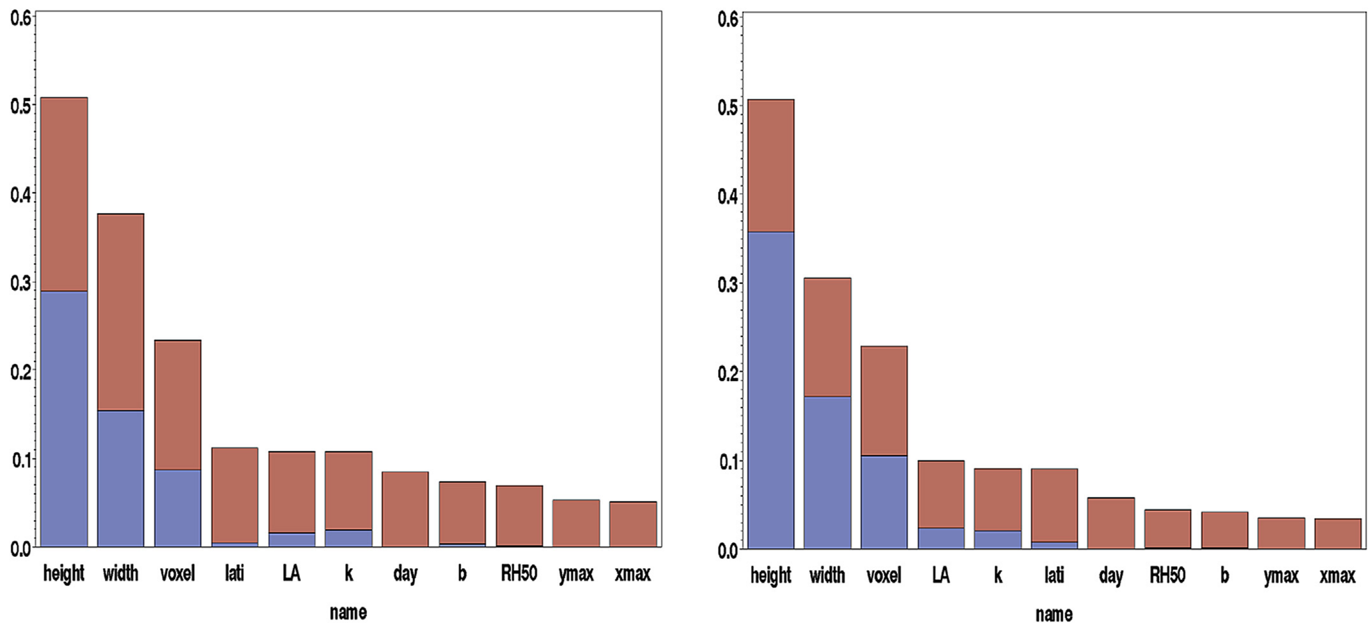

Fig. 9. Stacked bar plots of the sorted sensitivity indices (the PC_5-PESI(PLS) in blue, and the PC_5-TSI(PLS) in red) for each input, corresponding to Table 8 (correlated case in left panel, non-correlated case in right panel). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

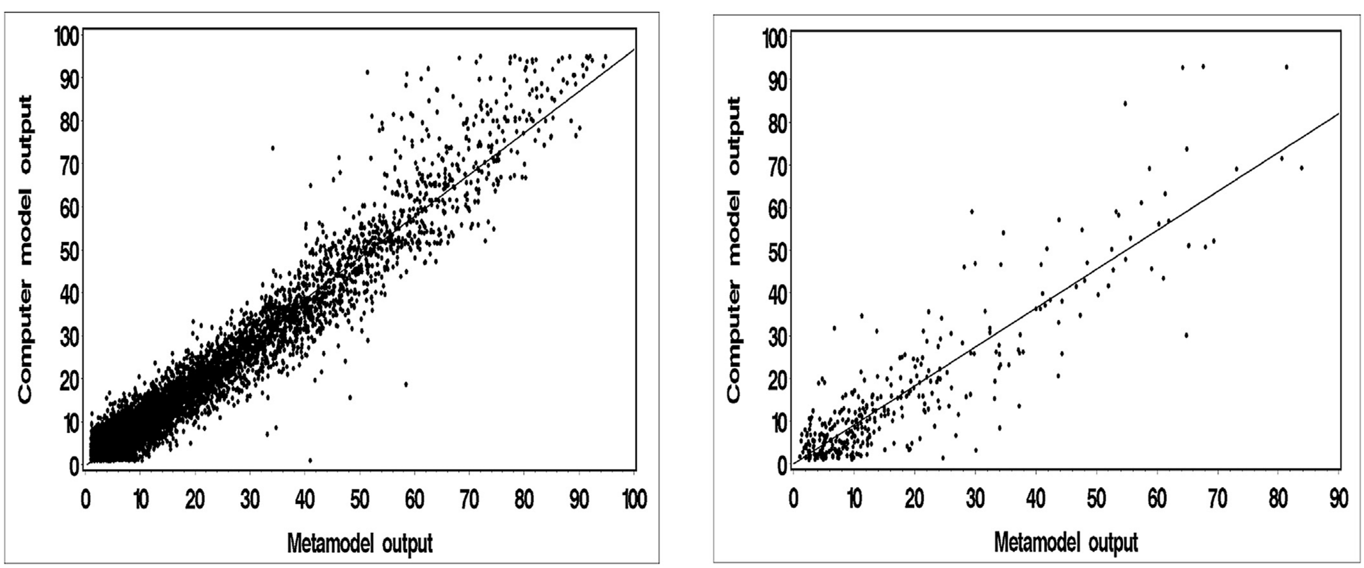

Fig. 10. CORRELATED CASE, M#7 metamodel. The left panel shows the observed-predicted scatter plot for the learning dataset (9500 runs), i.e., the 3D light interception computer model output vs. M#7 output ($R^2 = 0.960$ for the regression line). The right panel shows the observed-predicted scatter plot for the validation dataset (500 runs) ($R^2 = 0.789$ for the regression line).

because no correlation between the inputs was taken into account in their paper, on the one hand, and their goal was not to simultaneously obtain sensitivity indices and a metamodel, on the other.

In addition, the following two possibilities are worth highlighting to make it more compelling for computer model practitioners to use our method:

- PLSR can make it possible to perform a sequential run computing procedure with small $\mathbf{X}$ (or $\tilde{\mathbf{X}}$) design matrices of size n, eventually *lower* than P, the total number of monomials of the metamodel. This stepwise procedure can lead to a final number of runs that is less than that obtained by a non-sequential procedure. This procedure was successfully evaluated but it is not detailed here for reasons of space. It will be detailed in a future paper.
- We considered only the simple case with correlated continuous inputs, but the more difficult case where continuous inputs are also linked by some linear combinations of the general form $\alpha_{\min} \leq \alpha_1 X_1 + \ldots + \alpha_K X_K \leq \alpha_{\max}$, where $K \leq p$, and $\alpha_{\min}$, α_1, …, α_K, $\alpha_{\max}$ are real numbers, could also have been used.

Finally, a comparison of the results obtained with our method with results from other metamodeling methods should be fruitful and relevant, but no such rigorous comparison can be made today. Indeed, our method simultaneously proposes sensitivity indices and metamodeling in the presence of correlated inputs. It is true that some theoretical and sophisticated research studies (Chastaing et al., 2012) propose to deal with correlated inputs (and even dependent inputs), but the correlations can only be taken into account essentially via pairwise correlations between the inputs and not via all the correlations between all the inputs and, moreover, some specific probabilistic conditions are necessary. In addition, this latter approach is based on the complicated copula theory and therefore leads to considerable computations, even for $p \leq 4$. Other methods referred to in the Introduction section provide sensitivity indices but they are not comparable with ours, as explained in the Introduction.

The limits of the method are linked to the computer memory. We now give some details about this aspect. It depends on the following three factors: the number of monomials (that becomes very large if d is large; see Formula (3)), the input number, p, and the size, N, of the design matrices ($\mathbf{X}$ or $\tilde{\mathbf{X}}$). For instance, as a rule of thumb, the two cases:

- $d = 6$, $p = 15$, $N = 10000$, and a full metamodel (depending on P monomials),
- $d = 8$, $p = 15$, $N = 10000$, and a partial metamodel (depending on P' monomials),

seem to be the largest situations we could manage with a Pentium IV desk computer (with a clock speed of about 3 GHz) equipped with a 12-giga RAM.

7.2. Biophysical aspects

We now have metamodels that simultaneously provide good approximations (if $d \geq 5$) of the 3D light interception computer model and a clear aspect of the relative correlated input influences (their polynomial and total effects) via the new SI that we propose.

The ranking of the computer model inputs, obtained thanks to our new SI, is consistent with our knowledge about the functioning of light interception by plants. Firstly, plant height and width were shown to be the two most important variables for determining light interception by isolated plants (i.e., without neighboring, shading plants), regardless of other variables. These variables determine the volume in which the light-intercepting leaf area is distributed. Plant height is the most influential input and should also be the most influential when target plants are located inside canopies since many plants invest in vertical growth to outgrow their shading neighbors ("shade avoidance") (Brainard et al., 2005; Collins and Wein, 2000; Munier-Jolain et al., 2014). Plant width was the second most important factor since it determines the "efficient" light-intercepting leaf area exposed to incident sunlight when the sun is at the zenith. The total leaf area (LA) and the species extinction coefficient (k), which determine the potential absorbing leaf area, were shown to be more important than the distribution of leaf area inside the plant cylinder (driven by RH50 and b). When measuring and predicting plant variables, it is thus more important to focus on the former than the latter. However, this relative ranking could change for plants inside canopies.

The solar angle influences light absorption essentially via the latitude. The day effect was minor and mostly due to interactions, probably with latitude. Indeed, for latitudes close to the tropics (0°), the solar angle at noon varies between 67° and 90°, depending on the season. Outside the tropics, the noon solar angle is much lower and varies more. For instance, at the limit of the polar circle (latitude = 66° or −66°), it varies from 47° at the summer solstice, to 0° at the winter solstice.

In the metamodel, the grain of the 3D discretization in the FlorSys model (voxel size) was important. This was already demonstrated in a previous study when the light interaction model was evaluated with independent field observations (Munier-Jolain et al., 2013). Conversely, the dimensions of the simulated field (Xmax, Ymax) only presented a minor effect here, and almost all in interaction. Indeed, these dimensions would only affect light incidence onto the target plant if the latter's width exceeded field size.

Concerning computing times, five can be distinguished:

- The Computing Time for Building (CTB) one metamodel. The CTBs are given in the last columns of Tables 6 and 7
- The Computing Time for Running (CTR) one metamodel, i.e., to make one prediction with the metamodel.
- The Computing Time for Running the Computer Model (CTRCM), i.e., to make one prediction with the Computer Model (the 3D light interception computer model).
- The Computing Time for Running FlorSys (CTRF), i.e., to make one prediction of a future full crop with FlorSys.
- The Computing Time for Running FlorSys accelerated (CTRFa) thanks to the replacement of the Computer Model by a metamodel, for making one prediction of a future full crop.

At that time, we obtained CTR $\simeq 0.5 \times$ CTRCM, i.e., CTR $\simeq 0.5$s, which seems to be only a moderate decrease in computing time, whereas 10,000 plants will be simulated in a further step and a non-negligible total gain will therefore be obtained. The most crucial time we have to decrease is CTRF, which can take from several days to a few weeks depending, notably, on the voxel size used. With metamodels for all of the outputs, not only for one plant alone but for one plant in a cover with its neighborhood canopies, the first trials lead to CTRFa $\simeq 0.1 \times$ CTRF for a fixed one-centimeter voxel. In a future paper, very parsimonious metamodels (<30 monomials) - obtained by modern and efficient selection methods - will be presented. A better gain in CTRFa is expected.

8. Software/data availability

Two programs, referred to as "polychaosbasics" and "plspolychaos", were written in the R programming environment, R Core Team (2010), and are available as R packages on the CRAN website (https://cran.r-project.org/):

- https://cran.r-project.org/package=plspolychaos
- https://cran.r-project.org/package=polychaosbasis

They can be easily downloaded from this website. They are distributed under the GPL license.

- Objective of the "polychaosbasics" program: for independent uniform inputs, once the degree, d, has been chosen, the classical PC$_d$-PESI(OLS), PC$_d$-TSI(OLS) and the metamodel coefficients are computed from a provided dataset.
- Objective of the "plspolychaos" program: for correlated inputs, once the degree, d, and the maximum number, $h_{\max}$, of *PLS* components to be computed have been chosen, the new PC$_d$-PESI(PLS), PC$_d$-TSI(PLS), and the metamodel coefficients are computed from a provided dataset, according to two exclusive choices: full or partial metamodel.

For both programs:

- Developers:
  - Annie BOUVIER (main developer), contact address: INRA, Unité MaIAGE, Domaine de Vilvert, 78350 Jouy-en-Josas, France; telephone: +33 (0)1 34 65 22 16; fax: +33 (0)1 34 65 22 17; email: annie.bouvier@inra.fr.

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- Year first available: 2016.
- Hardware required: a standard desk or laptop computer; a Pentium IV desk computer equipped with 12-giga RAM was used for the computations in this paper.
- Free software.
- Program language: R language.
- Sizes: ”polychaosbasics” has 200 code lines and the size of its compressed tar-archive file is about 840 Kb; ”plspolychaos” has 600 code lines and the size of its compressed tar-archive file is about 2400 Kb.
- The ”FLORSYS1.txt” file (included in the R package) can be used as the input dataset (non-correlated inputs) for testing ”polychaosbasics”.
- The ”FLORSYS2.txt” file (included in the R package) was used as the input dataset (correlated inputs) for ”plspolychaos”, in this paper.

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Appendix. List of abbreviations (alphabetical order)

β	vector of the P metamodel coefficients to be estimated
β_k	k^{th} element of the β vector
$\widehat{\beta}^{[OLS]}$	ordinary least squares estimation (vector) of β
$\beta_k^{[OLS]}$	k^{th} element of the $\widehat{\beta}^{[OLS]}$ vector
$\widehat{\beta}_h^{[PLS]}$	Partial Least Squares estimation (vector) of β obtained with h PLS components
$\beta_{h,k}^{[PLS]}$	k^{th} element of the $\widehat{\beta}_h^{[PLS]}$ vector
$\widehat{\beta}_{h^*}^{[PLS]}$	Partial Least Squares estimation (vector) of β obtained with h^* (significant) PLS components
$\widehat{\beta}_{h^*,k}^{[PLS]}$	k^{th} element of the $\widehat{\beta}_{h^*}^{[PLS]}$ vector
CTB	Computing Time for Building a metamodel
CTR	Computing Time for Running one prediction, i.e., to make one prediction with a metamodel
CTRCM	Computing Time for Running the Computer Model, i.e., to make one prediction with the Computer Model (the 3D light interception computer model in this paper)
CTRF	Computing Time for Running FlorSys, i.e., to make one prediction of a future full crop with FlorSys
CTRFa	Computing Time for Running FlorSys accelerated thanks to the replacement of the Computer Model by a metamodel, for making one prediction of a future full crop
D	degree of the metamodel (the truncated PCE)
d^*	optimal degree of the metamodel
FOSSI	First-Order Sobol ’ Sensitivity Index defined by Sobol’ (1993)
GSA	Global Sensitivity Analysis
h	the current PLS component number
$h_{\max}$	the maximum number of PLS components chosen beforehand to be computed
h^*	the optimal value of h, i.e., the number of significant PLS components, corresponding to the maximum value of $Q^2_{cum}(h)$
IMSI_k	k^{th} Individual Monomial Sensitivity Index (see Eq. (11))
LHS	Latin Hypercube Sampling
M	computer model (in this case, the 3D light interception model)
M_d	deterministic polynomial approximation of M
$\widehat{\mathrm{M}}_d$	estimation of M_d
N	row number of a large size SFD
N	row number of a small size SFD
OLS	Ordinary Least Squares
OLSR	Ordinary Least Squares Regression
p	the number of inputs
P	the total number of monomials present in a full metamodel
P'	the total number of monomials present in a partial metamodel ($P' < P$)
PC_d-PESI(OLS)$_j$	Sensitivity Index of the X_j input that represent the Polynomial Effect, based on a truncated PCE of degree d estimated by OLSR
PC_d-TSI(OLS)$_j$	Sensitivity Index of the X_j input that represent the Total Effect, based on a truncated PCE of degree d estimated by OLSR
PC_d-PESI(PLS)$_j$	Sensitivity Index of the X_j input that represent the Polynomial Effect, based on a truncated PCE of degree d estimated by PLSR
PC_d-TSI(PLS)$_j$	Sensitivity Index of the X_j input that represent the Total Effect, based on a truncated PCE of degree d estimated by PLSR
PCE	Polynomial Chaos Expansion
PLS	Partial Least Squares
PLSR	Partial Least Squares Regression
$\Psi_k(\mathbf{X})$	a monomial of a multivariate orthogonal Legendre polynomial; it is also the notation for the corresponding vector (N or n elements)
$\Psi_k(\tilde{\mathbf{X}})$	a monomial of a multivariate orthogonal Legendre polynomial built from $\tilde{\mathbf{X}}$ (see definition below)
Q^2_h	fitting-prediction criterion computed for the h current step in the construction of a PLSR model (see Eq. (21))
$\mathrm{Q}^2_{cum}(h^*)$	cumulative fitting-prediction criterion computed for a PLSR model based on h^* components (see Eq. (24))
R^2	usual determination coefficient of the regression (OLSR or PLSR)
RMSEP	usual Root Mean Square Error of OLSR (see Eq. (26))
RMSEP_h	Root Mean Square Error of PLSR (see Eq. (25)) computed at the h current step
RMSEP_{h^*}	RMSEP_h computed at the h^* optimal step
SFD	(orthogonal) Space Filling Design
SI	Sensitivity Index (generic term)
SSI	Sobol’ Sensitivity Index
SU	Sensitivity Index proposed by Sudret (2008) that represents the Polynomial Effect, based on a truncated PCE of degree d, and estimated by OLSR. It is equivalent to our PC_d-PESI(OLS)

SUT Sensitivity Index proposed by Sudret (2008) that represents the Total Effect, based on a truncated PCE of degree d, and estimated by OLSR. It is equivalent to our PC_d-TSI(OLS)

t_h the PLS component of the h step

TH threshold for the $Q^2_{cum}(h)$ criterion to be chosen beforehand by the user

TSSI Total Sobol' Sensitivity Index defined by Sobol' (1993)

X_j the j^{th} input

$\mathbf{X}$ design matrix formed by the independent SFD, where the columns have been calibrated on the X_j ranges; the column-vectors of $\mathbf{X}$ are the vectors corresponding to the X_j inputs

$\tilde{\mathbf{X}}$ correlated design matrix formed by the Iman and Conover technique, from $\mathbf{X}$

Y output (or response) of the computer model (the PARa output in the case study of this paper)

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Annexe 2
Supplementary material of simplifying a complex model: sensitivity analysis and metamodelling of the complex mechanist model FLORSYS

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1 Short presentation of FLORSYS

1.1 The annual life-cycle

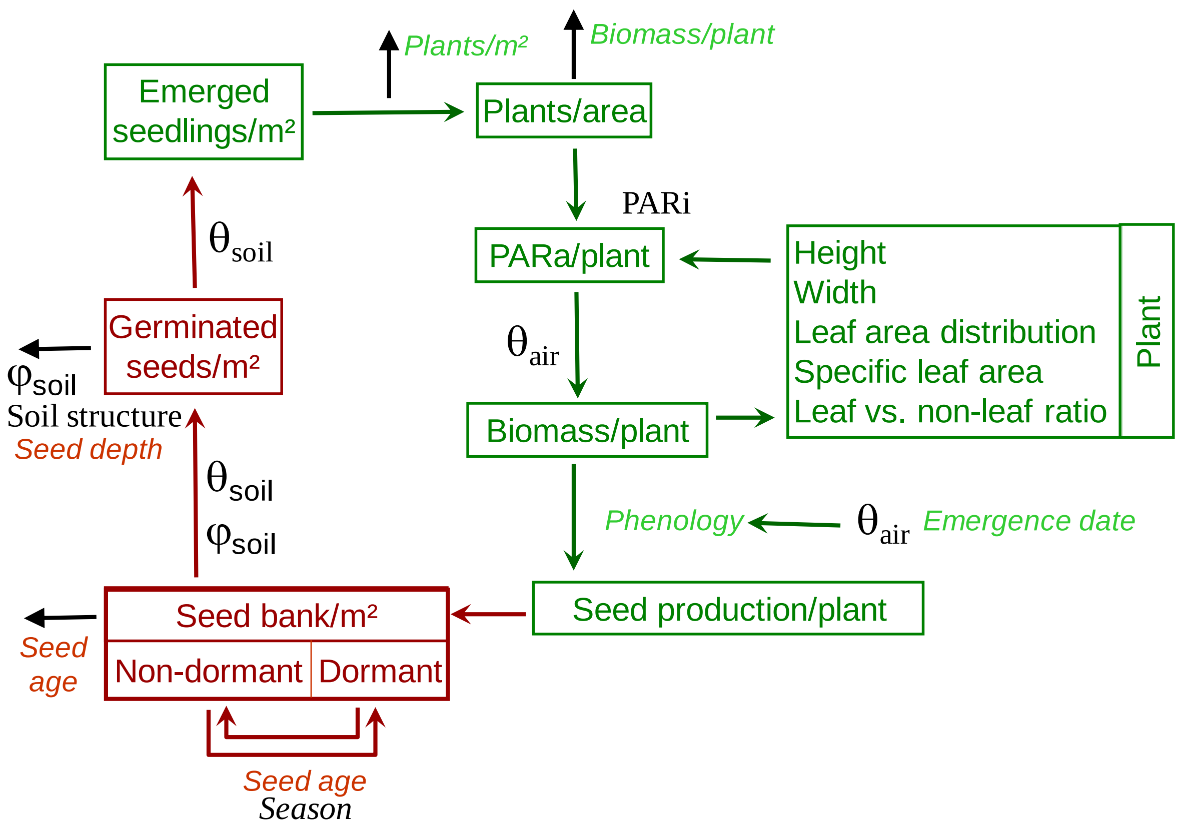

Figure S. I. 1 : Life-stages (plants/m²) of annual weeds simulated in FLORSYS (Colbach et al., 2014b; Gardarin et al., 2012; Munier-Jolain et al., 2014; Munier-Jolain et al., 2013) with the effects of weed state variables (e.g. *Plants/m²*, *Seed age*), soil conditions (e.g. θ_{soil}) and daily weather variables (e.g. PARi). All variables are calculated daily. Black arrows (→) indicate losses through mortality.

1.2 Species traits and parameters

FLORSYS parameters are currently available for 25 frequent weed species: *Abuthilon theophrasti* (EPPO code ABUTH), *Alopecurus myosuroides* (ALOMY), *Amaranthus retroflexus* (AMARE), *Ambrosia artemisiifolia* (AMBEL), *Avena fatua* (AVEFA), *Capsella bursa-pastoris* (CAPBP), *Chenopodium album* (CHEAL), *Datura stramonium* (DATST), *Digitaria sanguinalis* (DIGSA), *Echinochloa crus-galli* (ECHCG), *Galium aparine* (GALAP), *Geranium dissectum* (GERDI), *Matricaria perforata* (MATIN), *Mercurialis annua* (MERAN), *Panicum miliaceum* (PANMI), *Poa annua* (POAAN), *Polygonum aviculare* (POLAV), *Fallopia convolvulvus* (POLCO), *Polygonum maculosa* (previously *P. persicaria*, POLPE), *Senecio vulgaris* (SENVU), *Sonchus asper* (SONAS), *Solanum nigrum* (SOLNI), *Stellaria media* (STEME), *Veronica hederifolia* (VERHE), and *Veronica persica* (VERPE).

Table S. I. 1 : Major FLORSYS species traits and parameters and their range of variation

Trait/parameter	Unit	Mean	Min	Max
Relative growth rate	$cm^2\ °C^{-1}\ day^{-1}$	0.020	0.011	0.046
Initial leaf area (ILA)	cm^2	0.20	0.013	0.70
Variation coefficient of ILA	$cm^2\ cm^{-2}$	0.24	0.0061	1.27
Base temperature for growth and development	°C	4.4	0	12.0
Harvest index	$g\ g^{-1}$	0.29	0.010	0.86
Shape parameter for harvest index	No unit	1.01	0.77	1.40
Climbing	{yes, no}	12% Yes	No	Yes
Maximum plant height	cm	95	30	200
Maximum plant width	cm	106	20	200
Seed Weight	mg	3.07	0.14	18.50
Seed lipid content	$g\ g^{-1}$	0.16	0.030	0.47
Seed coat thickness	µm	65	10	231
Seed area	$mm^2\ mg^{-1}$	3.91	0.21	17.50
Seed shape index	$mm^2\ mm^{-2}$	0.21	0.050	0.47
Base temperature for germination	°C	4.3	0	11.5
Base soil water potential for germination	MPa	-1.12	-3.31	-0.45
Emergence season onset	Julian day	158	60	280
Emergence onset in spring	Julian day	85	20	140
End of emergence season	Julian day	177	70	310
Monocotyledonous species	{yes, no}	24% Yes	No	Yes
Specific leaf area (SLA)	$cm^2\ g^{-1}$	189	89	301
Sensitivity of SLA to shade	No unit	0.61	0.17	1.20
Leaf biomass vs. total biomass ratio (LBR)	$g\ g^{-1}$	0.70	0.55	0.84
Sensitivity of LBR to shade	No unit	0.051	-0.31	0.43
Specific plant height (SH)	$cm\ g^{-1}$	38	8	136
Shape parameter for SH	No unit	0.33	0.10	0.59
Sensitivity of SH to shade	No unit	0.58	-0.11	1.19
Specific plant width (SW)	$cm\ g^{-1}$	116	14	1531
Shape parameter for SW	No unit	0.41	0.20	0.91
Sensitivity of SW to shade	No unit	0.35	-0.040	0.84
Median leaf area height (MLAH)	$cm\ cm^{-1}$	0.49	0.37	0.67
Shape parameter for MLAH	No unit	2.71	1.64	4.14
Sensitivity of MLAH to shade	No unit	0.018	-0.54	0.62
Stimulating parasite germination	{yes, no}	40% Yes	No	Yes
Allowing parasite attachment	{yes, no}	36% Yes	No	Yes

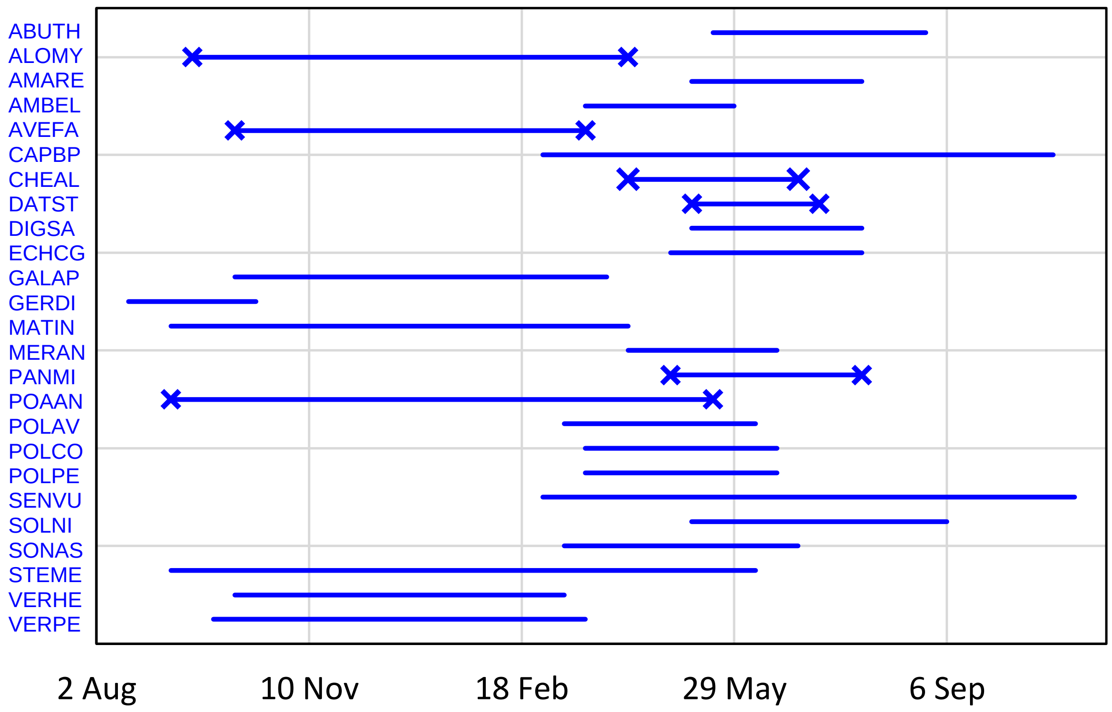

Figure S. I. 2 : Potential emergence seasons of the 25 weed species (indicated by their EPPO code) included in FLORSYS. Grass weeds are indicated by crosses. (Nathalie Colbach © 2016).

1.3 The effect of management practices

Table S. I. 2 : Effects of cropping system components on the weed life-cycle (density and timing of stages) as simulated by FLORSYS (Colbach et al., 2014a; Colbach et al., 2014b; Gardarin et al., 2012; Munier-Jolain et al., 2014; Munier-Jolain et al., 2013).

Cropping system component (crops and management techniques)	Intermediate effect	Effect on weeds
Tillage (including post-sowing mechanical weeding)	Soil structure Soil movements = f(soil structure)	Soil compaction increases mortality of germinated seeds Seed burial decreases germination and increases pre-emergent mortality due to insufficient seed reserve Seeds on soil surface germinate badly because of insufficient seed-soil contact Germinated seeds close to soil surface often die because the top soil dries faster Exposure of imbibed seeds to light if inverting tool Triggering of germination flush if the soil is tilled in moist conditions Destruction of germinated seeds, seedlings and plants; addition of newly produced seeds to seed bank if mature plants are killed
Crop species and variety (including undersown, associated and temporary crops)	Choice of cultivation techniques Sowing season Light availability in canopy	See effects of techniques Selects weed species that are non-dormant at sowing season Shading reduces photosynthesis and thus biomass accumulation and results in etiolation
Sowing date	Crop emergence date Date of last tillage	The earlier the weed seedlings emerge relative to the crop, the better they survive The later the last tillage, the more weed seeds have germinated already and are killed by the tillage
Sowing density	Reduces light availability in canopy	Shading reduces photosynthesis and thus biomass accumulation and results in etiolation
Sowing pattern	Variability in light availability in canopy	Irregular sowing leads to canopy gaps where weeds grow and reproduce better
Herbicides	Efficiency = f(active ingredient, technicity) Efficiency decreases with canopy density, seed depth (for root-entering herbicides) and weed stage	Foliar herbicides kill emerged plants, root-entering herbicides kill unemerged and emerged plants whose seeds are close to soil surface, pseudo-root herbicides kill emerging seedlings; root-entering and pseudo-root herbicides persist and act during several days. Addition of newly produced seeds to seed bank if mature plants are killed and germination flush if soil is moist
Mowing & harvesting operations		Cuts plants and reduces biomass; the older the plants at mowing and the less biomass remain, the more plants die; addition of newly produced seeds to seed bank if mature plants are killed and germination flush if soil is moist
Manure	Adds layer on soil surface	Improves germination of surface seeds, slightly decreases germination and emergence of buried seeds Adds seeds to soil seed bank
Irrigation	Increases soil moisture and water potential	Triggers weed seed germination if applied after drought Makes germination and emergence faster Interacts with techniques whose effects depends on soil moisture (tillage, mechanical weeding, soil compaction)
All (except irrigation)	Increase soil compaction via wheel traffic	Increases mortality of germinated seeds

The effect of other management techniques (e.g. nitrogen) is not yet implemented in FLORSYS

1.4 Weed-impact indicators

Table S. I. 3 : Synopsis of the indicators calculated from weed flora outputs predicted by the FLORSYS model. Indicators are calculated for each cropping season, i.e. from harvest of the previous crop to harvest of current crop (Colbach et al., submitted; Mézière et al., 2015).

A. Weed-related biodiversity indicators

Indicator	Description	Equation	Variables
Species richness	Number of weed species present during the cropping season ∈ [0, 25]		
Species equitability	Pielou's equitability (ratio of Shannon index of the community vs. Shannon maximum, i.e. if all the species of communities present the same abundance), varying between [0,1]	$E = H'/H_{max}$ with $H' = -\sum_{i=1}^{S} \frac{n_i}{N} \cdot \log_2(\frac{n_i}{N})$ and $H_{max} = \log_2 S$ E = 0 if N=0	n_i= daily number of plants of species i averaged over season (plants·m^{-2}) N= total daily number of weed plants averaged over season (plants·m^{-2})
Bird resource	Weed seeds important for farmland bird diet and present on soil surface between 1 October and 15 March	$B = \frac{1}{D}\sum_{d=1}^{D}(\log_{10}\left[\sum_{i=1}^{S}(s_{id} \cdot \gamma_i) + 0.0001\right] + 4)$	s_{id}=seed density on soil surface (seeds·m^{-2}) D = days γ_i=importance in the diet farmland birds (Wilson et al., 1999; Marshall et al., 2003); $\gamma \in \{1,2,3,4\}$.
Insect resource	Lipid-rich weed seeds for feeding granivore carabids, present on soil surface between 1 April and 1 October	$I = \frac{1}{D}\sum_{d=1}^{D}(\log_{10}\left[\sum_{i=1}^{S}(s_{id} \cdot \delta_i) + 0.0001\right] + 4)$	s_{id}=seed density of species i on soil surface on day d (seeds·m^{-2}) D = days δ_i=seed lipid content (%) of species i (Gardarin et al., 2011)
Pollinator resource	Weed flowers for feeding honey bees and open from 1 March and 1 November	$P = \frac{1}{D}\sum_{d=1}^{D}(\log_{10}\left[\sum_{i=1}^{S}(f_{id} \cdot \eta_i) + 0.0001\right] + 4)$	f_{id}=flowering plant density (plants·m^{-2}) D = days η_i=pollination value (Ricou et al., 2014); $\eta \in \{1, 2, ..., 7\}$.

B. Harmfulness indicators

Indicator	Description	Equation	Variables
Crop production			
Yield loss	Crop yield loss due to crop:weed competition for light (%)	$100 \cdot (Y_0 - Y)$	Y and Y_0=crop yield in weedy and weed-free simulations with the same cropping system ($g \cdot m^{-2}$)
Harvest pollution	Pollution of crop seed harvest by weed seeds and plant fragments (no unit), not calculated for grass crops, root crops and silage maize.	$\log_{10}\left[\frac{\sum_{i=1}^{S}(\alpha_{ic} \cdot S_i + \beta_{ic} \cdot B_i)}{Y} + 0.0001\right] + 4$	S_i, B_i =seed biomass and weed biomass produced by plants taller than harvester cutter bar ($g \cdot m^{-2}$) B_c=crop biomass at harvest ($g.m^{-2}$) Y=crop yield α_{ic}, β_{ic} = coefficients of harvest pollution by weed seeds or green biomass
Production activity			
Harvesting difficulty	Technical problems induced by weeds at harvest.	$\log_{10}\left[\frac{\sum_{i=1}^{S} B_i}{B_c} + 0.0001\right] + 4$	B_i, B_c =fresh weed biomass and crop biomass taller than harvester cutter bar at harvest ($g \cdot m^{-2}$)
Farmer's field perception			
Field infestation	Daily weed biomass in the field averaged sowing date to harvest date ($t.ha^{-1}.day^{-1}$)	$\frac{\sum_{d=1}^{D}\sum_{i=1}^{S} B_{id}}{D}$	B_{id}=fresh weed biomass of i on day d ($t \cdot ha^{-1}$) D=number of days
Pest increase due to weeds			
Disease risk	Additional crop yield loss due to increase in take-all disease in cereals caused by grass weeds (%)	$AD = YLD - YLD_0$	YLD and YLD_0 = crop yield loss due to disease in respectively weedy and weed-free simulations of the same cropping system. Output from TAKEALLSYS linked to FLORSYS with an interaction model (Mézière et al., 2013)
Parasite risk	Risk of crop infection by parasitic plant *Phelipanche ramosa* due to weeds	$-\alpha \cdot I_{seed\_bank\_decline}$ $+ \beta \cdot I_{increase\_crop\_infection}$ $+ \gamma \cdot I_{tot\_stim} \cdot I_{repro}$	$I_{seed\_bank\_decline}$ is the risk of total parasite germination stimulated by weeds and is estimated from above-ground biomass of weeds that belong to parasite-stimulating species and that have not yet flowered, averaged over cultural campaign $I_{increase\_crop\_infection}$ is the risk of parasite germination stimulated by weeds during host crops and is estimated from above-ground biomass of weed plants that belong to parasite-stimulating species and have not yet flowered, averaged over host crop season $I_{parasite\_reproduction}$ is the product of the risk of parasite germination stimulated by weeds, and the risk of parasite seed production of weeds, the latter being estimated from above-ground biomass of weeds that belong to parasite-susceptible species and reached maturity α, β and γ are positive parameters

Weed species i $\in$ {1,...S} with S the species richness. For indicators with log in the formula, 0.0001 was added to account for nil values.
A +4 constant was added to indicators using a $\log_{10}(y+0.0001)$ transformation to ensure that indicator values ≥ 0.

1.5 References

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Annexe 3
Supplementary material of simplifying a complex model: sensitivity analysis and metamodelling of the complex mechanist model FLORSYS

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1 Supplementary materials for metamodeling and sensitivity analysis

1.1 Variation Range test

Input ranges have been shown to influence in a sensitivity. To assess this influence on the inputs of the light interception submodel, we tested two inputs range size on sensitivity indices.

1.1.1 Materiel and Methods

For a sensitivity analysis it is essential to test the influence of the inputs' ranges. For a complete test of the influence it would be necessary to try different ranges for each inputs and intersect all the ranges for a full experimental design. Hence, a too high number of computation and a too large numeric space would be necessary. For an approximate but efficient way to have an idea of the influence of the ranges we tested only two different ranges small and large ones. We used a Plackett and Burman experimental design based on a Hadamard matrix to test the two levels of range (Plackett and Burman, 1946). This matrix allows us to test, for each input, large and small ranges and a combination of those ranges for the smallest possible number of simulations. To test the eleven inputs of the 3D light interception submodel, a H12 matrix was used, and only 12 combination of ranges, that is 12 experimental design, were produced. The two different ranges tested for the inputs were: (1) the large range covering all possible situations to be simulated by the model, *e.g.* every latitude between the polar circles, every day or every possible heights for the plants in the model, (2) the small range covering France latitudes, spring and summer days or the most frequent sizes of plants (Table 1).
For each of the 12 combination of ranges, a Latin Hypercube Sampling (McKay et al., 2000), LHS, was created for the 11 inputs and 29200 rows (this number was dependent of the number of day number and the number of different voxel values). Each row was computed with the 3D radiation interception submodel, to eliminate computation artefacts 10000 rows were selected removing extreme outputs results, i.e. at the limit of the range of the outputs, while keeping the orthogonality of the experimental design. Sobol sensitivity indices were estimated with Saltelli

(2002) method, i.e. total indices, accounting for interactions between the input and other inputs, and first order indices, accounting for the input's effects disregarding interactions with other inputs.
A linear regression on the sobol sensitivity indices of all the inputs for the 12 range combination was built to account for the effect of the range. The coefficients of the regression are obtained *via*:

Eq. 1 $$\boldsymbol{\beta_j = \frac{1}{N}\sum_{i=1}^{N} SI_i X_{ij}}$$

With p is the number of inputs, x_j is the input, ε is the residual of the model, N is the run/simulation number, SI_i is the sensitivity indices (first order or total), X_{ij} is the sign of the Hadamard matrix (Box et al., 1978).

1.1.2 Results

Table 1: Definition, range variation and unit for both inputs ranges for the 3D light interception submodel.

Name	Range of variation		Unit
	Min	Max	
Latitude	[42; 52]	[-66; +66]	angle degree
Day	[79; 264]	[1; 365]	
Xmax	[2; 3]	[1; 4]	m
Ymax	[2; 3]	[1; 4]	m
Voxel	[2; 8]	[1; 20]	cm
Height	[1; 84]	[1; 250]	cm
Width	[1; 68]	[1; 200]	cm
Cumulated leaf area	[1; 3334]	[1; 10000]	cm2
Extinction coefficient	[0.55; 0.83]	[0:01; 1:1]	no unit
RH50	[0.4; 0.7]	[0:01; 1]	$cm.cm^{-1}$
B	[2; 4]	[0:01; 6]	no unit

Table 2: Effects of the range of input variation on the 3D light interception submodel outputs for the sensitivity analysis to simplify FLOSYS. Coefficients from the additive regression based on Sobol sensitivity indices of the 12 simulations based on a Hadamard matrix.

		PARaP		**SID**		**PARi**		**PARi base**	
		small	*large*	*small*	*large*	*small*	*large*	*small*	*large*
1st ordre	Latitude	0.002	0.009	0.001	0.006	0.000	0.001	-0.033	0.001
	Day	0.007	-0.003	0.010	-0.001	0.001	0.000	0.057	-0.010
	Xmax	0.000	0.000	0.000	0.000	0.000	0.000	0.023	0.110
	Ymax	0.000	0.000	0.000	-0.001	0.000	0.000	-0.034	0.090
	Voxel	0.068	0.111	0.007	0.009	0.075	0.097	-0.052	0.001
	Height	0.373	0.366	0.009	0.002	0.824	0.717	0.071	0.003
	Width	0.288	0.182	0.590	0.238	0.006	0.003	1.512	0.299
	Cumulated leaf area	0.046	0.022	0.267	0.177	0.004	0.002	0.649	0.092
	Extinction coefficient	0.001	0.024	0.007	0.175	0.000	0.002	-0.150	0.071
	RH50	0.000	0.002	0.007	0.181	0.000	0.000	0.014	0.001
	b	-0.001	0.000	0.000	0.018	0.000	0.000	-0.001	0.002
total	Latitude	0.009	0.097	-0.004	0.029	0.077	0.084	-0.213	-0.001
	Day	0.035	0.070	0.016	0.014	0.078	0.082	-0.296	0.004
	Xmax	0.002	0.023	-0.011	-0.014	0.077	0.080	-0.213	0.180
	Ymax	0.002	0.025	-0.011	-0.012	0.077	0.080	-0.159	0.183
	Voxel	0.155	0.274	0.012	0.014	0.245	0.356	-0.187	-0.007
	Height	0.520	0.545	0.015	0.025	0.937	0.918	-0.305	-0.001
	Width	0.411	0.341	0.672	0.320	0.087	0.089	-0.741	0.536
	Cumulated leaf area	0.104	0.102	0.307	0.234	0.082	0.086	-0.084	0.201
	Extinction coefficient	0.003	0.086	-0.005	0.205	0.077	0.086	-0.071	0.206
	RH50	0.003	0.035	0.002	0.272	0.082	0.104	-0.260	-0.009
	b	0.003	0.035	-0.010	0.067	0.077	0.091	-0.246	-0.009

Table 3: Effects of the range of input variation on the 3D light interception submodel outputs for the sensitivity analysis to simplify FLOSYS. Coefficients from the additive regression based on Sobol sensitivity indices of the 12 simulations based on a Hadamard matrix.

Output	PARaP		SID		rPARi		$rPARi_{base}$	
indice type	1st order	Total	1st order	Total	1st order	Total	1st order	Total
regression coefficient β_0	*0.07*	*0.12*	*0.07*	*0.11*	*0.08*	*0.19*	*0.05*	*0.14*
Latitude	0.01	0.02	0	0.05	0.04	0.09	0.01	0.05
Day	0	0.02	0	0.06	0.05	0.09	0.02	0.05
Xmax	0	0	0	0	0	0.09	0.04	0.15
Ymax	0	0	0	0	0	0.09	0.09	0.15
Voxel	0.03	0.02	0.1	0.19	0.05	0.32	0.04	0.03
Height	0	0.03	0.76	0.47	0.07	0.92	0	0.08
Width	0.05	0.34	0	0.44	0.47	0.1	0.23	0.48
Cumulated leaf area	0	0.2	0	0.09	0.28	0.1	0.1	0.31
Extinction coefficient	0.01	0.07	0	0.04	0.1	0.09	0.08	0.11
RH50	0	0.1	0	0.01	0.14	0.1	0	0.08
B	0	0.01	0	0	0.03	0.09	0	0.06

1.2 Comparing methods to choose the best one for sensitivity indices estimation

Table 4: Sobol Sensitivity indices estimated via Saltelli 2002 method and Sensitivity indices estimated via regression PLS on polynomial chaos expansion.

		PARaP		**SID**		**rPARi**		**rPARi$_{base}$**	
		Saltelli	**PCE-OLS**	***Saltelli***	**PCE-OLS**	***Saltelli***	**PCE-OLS**	***Saltelli***	**PCE-OLS**
1er order	**Latitude**	0.01	0.01	0.01	0.01	0	0	0	0
	Jour	0	0	0	0	0	0	0	0
	Xmax	0	0	0	0	0	0	0.11	0.11
	Ymax	0	0	0	0	0	0	0.09	0.11
	Voxel	0.11	0.13	0.01	0.01	0.1	0.11	0	0
	Hauteur	0.37	0.42	0	0	0.72	0.75	0	0
	Largeur	0.18	0.22	0.24	0.26	0	0	0.3	0.32
	LA	0.02	0.03	0.18	0.2	0	0	0.09	0.1
	k	0.02	0.03	0.17	0.18	0	0	0.07	0.09
	RH50	0	0	0.18	0.2	0	0	0	0
	b	0	0	0.02	0.01	0	0	0	0
Total	**Latitude**	0.1	0.03	0.03	0.02	0.08	0	0	0
	Jour	0.07	0.01	0.01	0.01	0.08	0	0	0
	Xmax	0.02	0	0	0	0.08	0	0.18	0.19
	Ymax	0.02	0	0	0	0.08	0	0.18	0.18
	Voxel	0.27	0.22	0.01	0.02	0.36	0.23	0	0
	Hauteur	0.55	0.51	0.03	0.02	0.92	0.88	0	0.01
	Largeur	0.34	0.28	0.32	0.31	0.09	0	0.54	0.52
	LA	0.1	0.06	0.23	0.24	0.09	0	0.2	0.2
	k	0.09	0.05	0.2	0.21	0.09	0	0.21	0.19
	RH50	0.04	0.01	0.27	0.27	0.1	0	0	0
	b	0.03	0.01	0.07	0.05	0.09	0	0	0

1.3 Correlation test between inputs

Table 5: Target correlation matrix used to modify the initial experimental design with the addition of correlation between the 3D light interception submodel.

	Latitude	Day	Xmax	Ymax	Voxel	Height	Width	Cumulated leaf area	k	RH50	b
Latitude	1										
Day	0	1									
Xmax	0	0	1								
Ymax	0	0	0	1							
Voxel	0	0	0	0	1						
Height	0	0	0	0	0	1					
Width	0	0	0	0	0	0.6	1				
Cumulated leaf area	0	0	0	0	0	0.2	0.2	1			
Extinction coefficient	0	0	0	0	0	-0.2	0	0	1		
RH50	0	0	0	0	0	0.2	0.2	0	0.2	1	
b	0	0	0	0	0	0.3	0.3	0	-0.1	0.1	1

1.4 Sensitivity analysis results

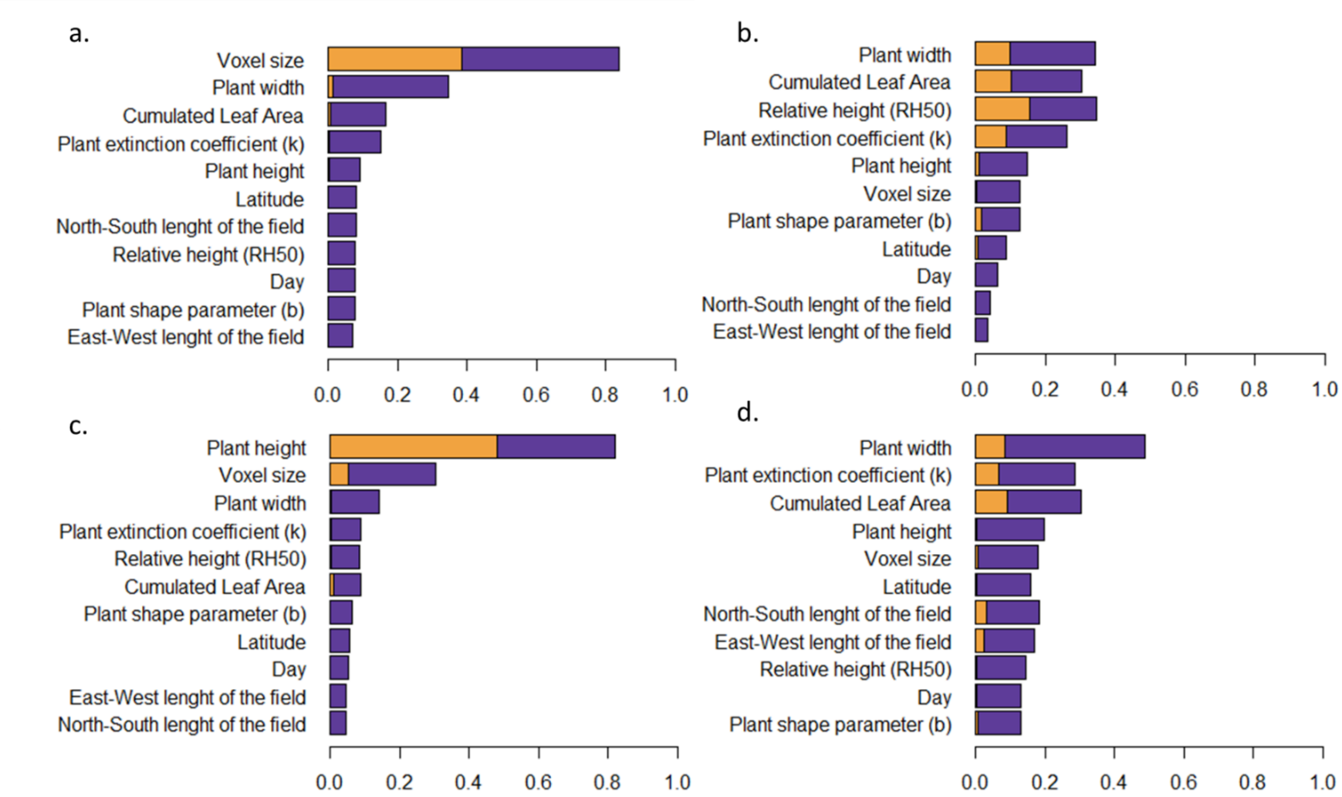

Figure 1: Sensitivity indices of inputs describing a single plant in a field for the light interception submodel of FlorSys. In light orange polynomial effects (i.e. with no interactions) in dark purple total effect of the inputs. a. absorbed PAR (PARa), b. Shading Index (SID), b. relative PAR intercepted by the plant (rPARi), c. relative PAR intercepted by the plant ($rPARi_{base}$).

For the shading index SID (impacting the morphology of plants) it it differents plants varaibles that come first as the relative height; the width, the cumulaterd leaf area and the extinction coefficient. For the rPARi at the base; it is the width, the cumulated leaf area and the extinction coefficient that are the most important inputs. And for rPARi, it is the height and the voxel. It seems that when the height is important, the voxel also is important.

1.5 Distribution of an output depending on the input

1.5.1 Single plant

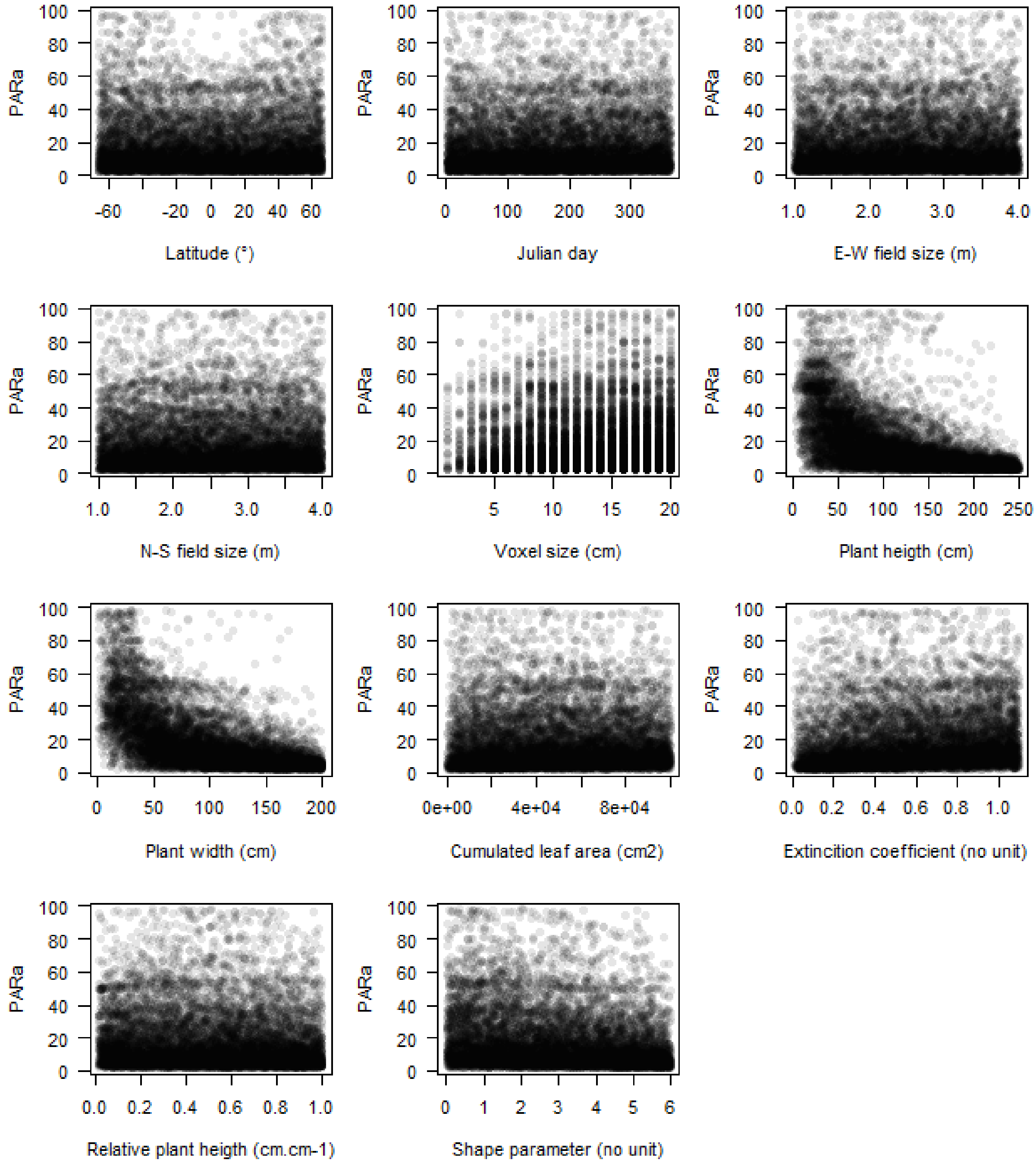

Figure 2: Scatterplot of the photosynthetically active radiation absorbed by a plant (PARaP) simulated by the process-based version of FLORSYS as a function of the 11 inputs for a single plant in the virtual field. Each point represents one run on the space filling LHS design. From the 29200 initial LHS rows, only 10000 were kept to eliminate computation artefacts.

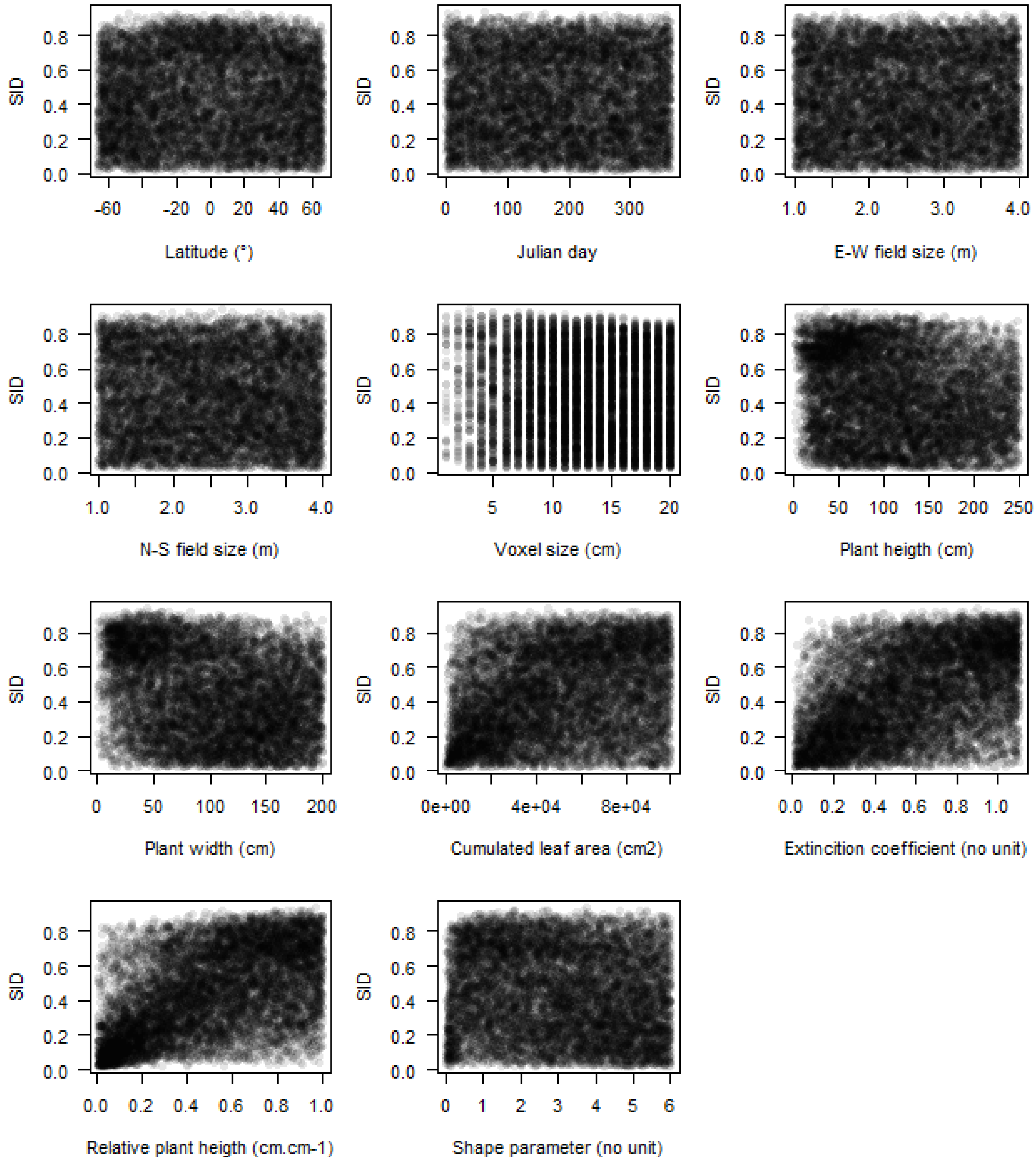

Figure 3: Scatterplot of the light interception submodel daily shading intensity (SID) simulated by the process-based version of FLORSYS as a function of the 11 inputs for a single plant in the virtual field. Each point represents one run on the space filling LHS design. From the 29200 initial LHS rows, only 10000 were kept to eliminate computation artefacts.

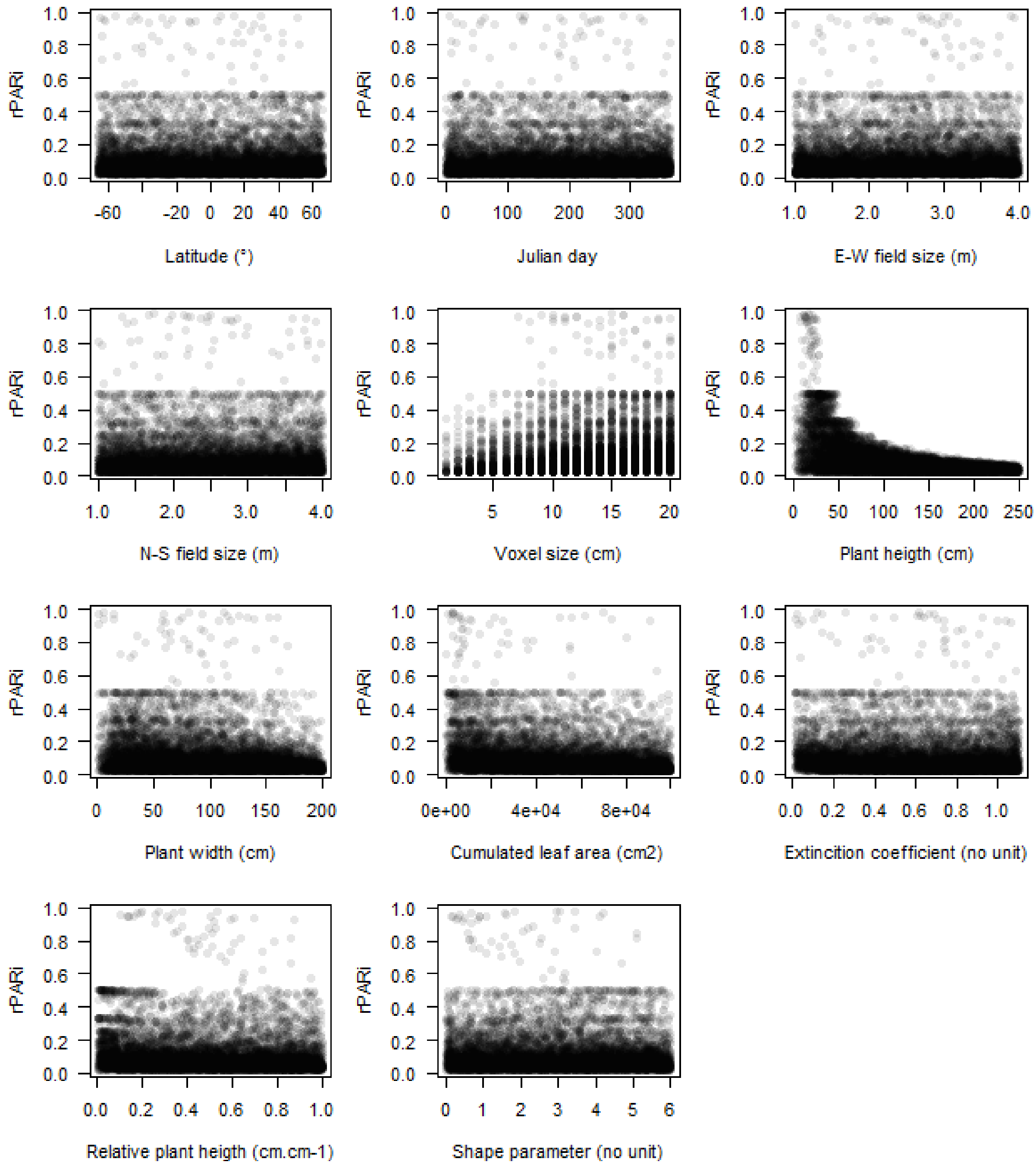

Figure 4: Scatterplot of the light interception submodel relative photosynthetically active radiation intercepted (rPARi) simulated by the process-based version of FLORSYS as a function of the 11 inputs for a single plant in the virtual field. Each point represents one run on the space filling LHS design. From the 29200 initial LHS rows, only 10000 were kept to eliminate computation artefacts.

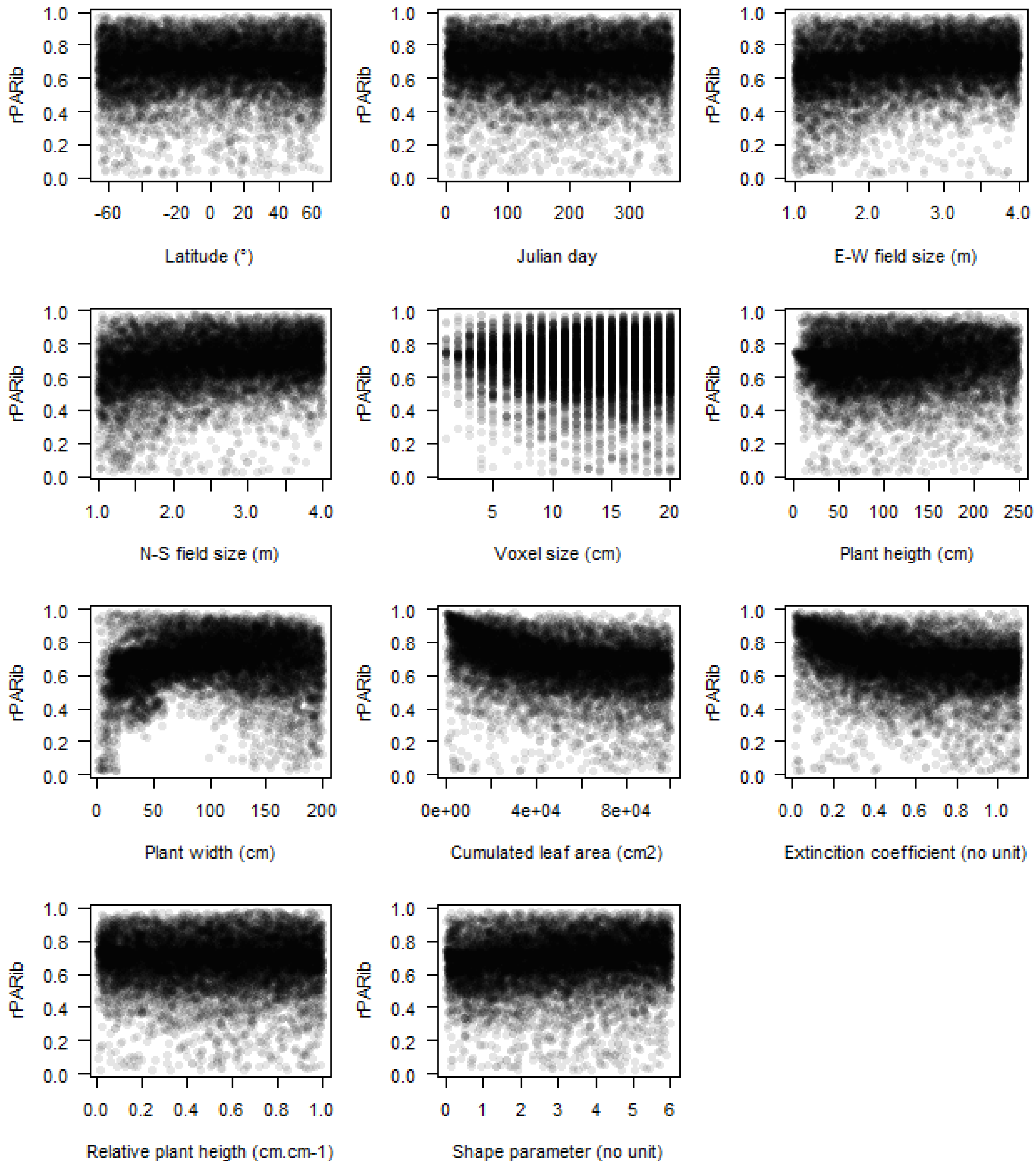

Figure 5: Scatterplot of the light interception submodel relative photosynthetically active radiation intercepted at the base of the plant ($rPARi_{base}$) simulated by the process-based version of FLORSYS as a function of the 11 inputs for a single plant in the virtual field. Each point represents one run on the space filling LHS design. From the 29200 initial LHS rows, only 10000 were kept to eliminate computation artefacts.

1.5.2 Plant in canopy

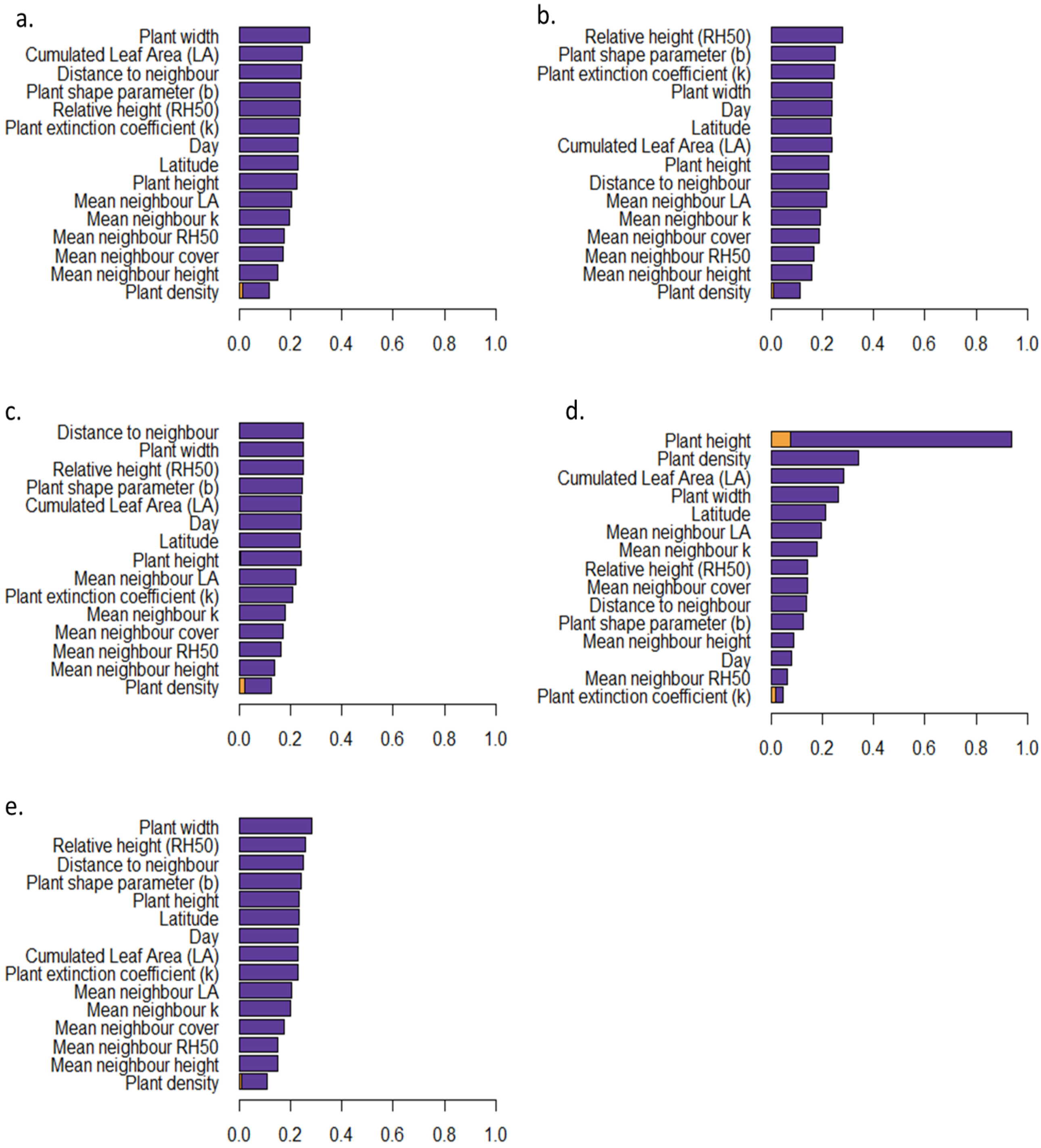

Figure 6: Sensitivity indices, in dark purple polynomial effects (i.e. with no interactions) in light orange total effect of the inputs. a. the Photosynthetically active radiation (PAR) absorbed by the plant, b. shading index (SID), c. relative PAR intercepted at the top of the plant ($rPARi_{top}$), d. relative PAR intercepted by the plant (rPARi), e. relative PAR intercepted at the base of the plant ($rPARi_{base}$).

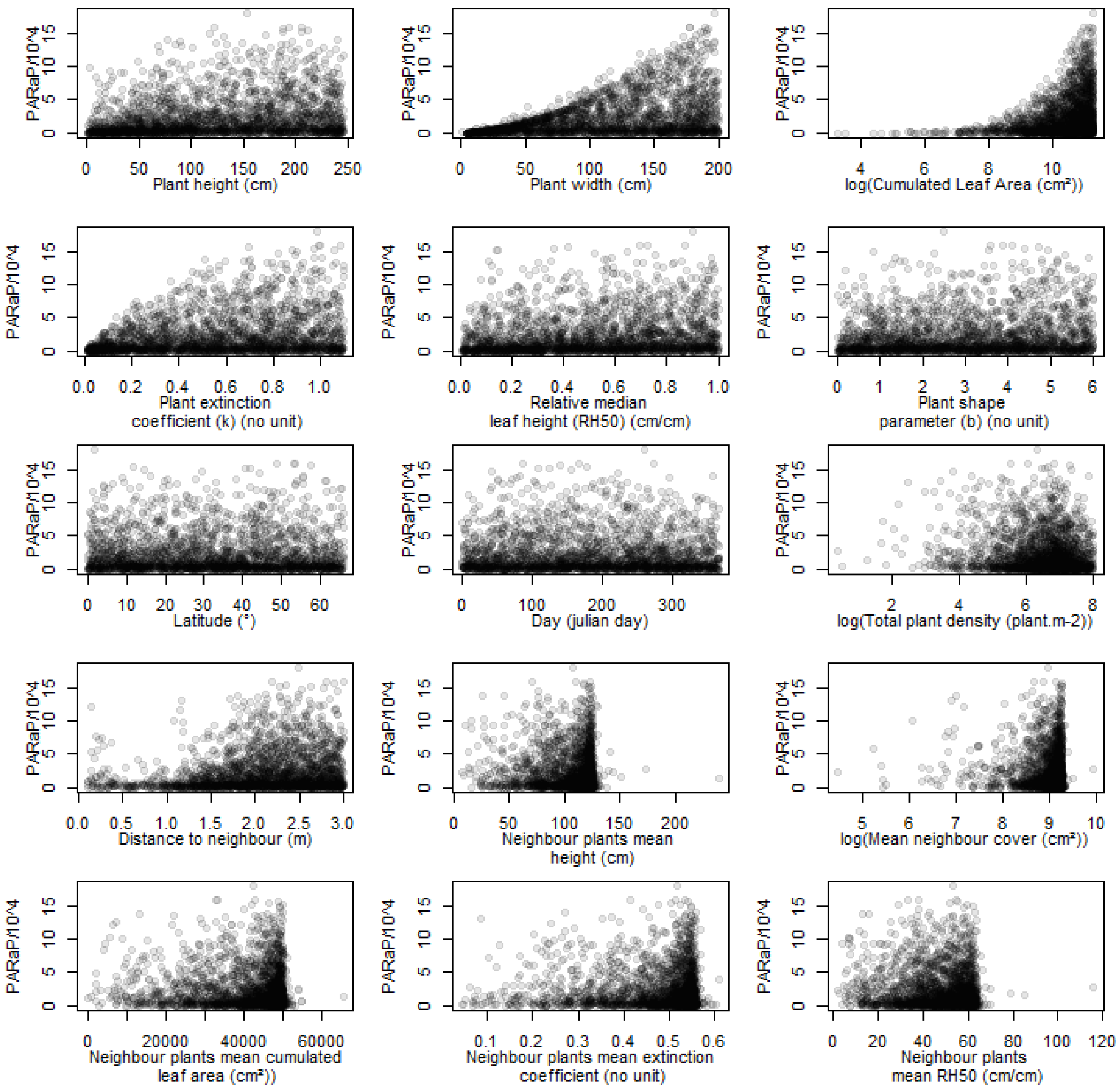

Figure 7: Scatterplot of the light interception submodel photosynthetically active radiation absorbed by the plant (PARaP in MJ cm^{-2} MJ^{-1} cm² $plant^{-1}$ / 10^4) in function of the 15 inputs of a target plant surrounded by neighbour plants in the virtual field. Each point represents a run on the space filling LHS design. From the 20440 initial LHS rows 2536 were kept to eliminate computation artefacts.

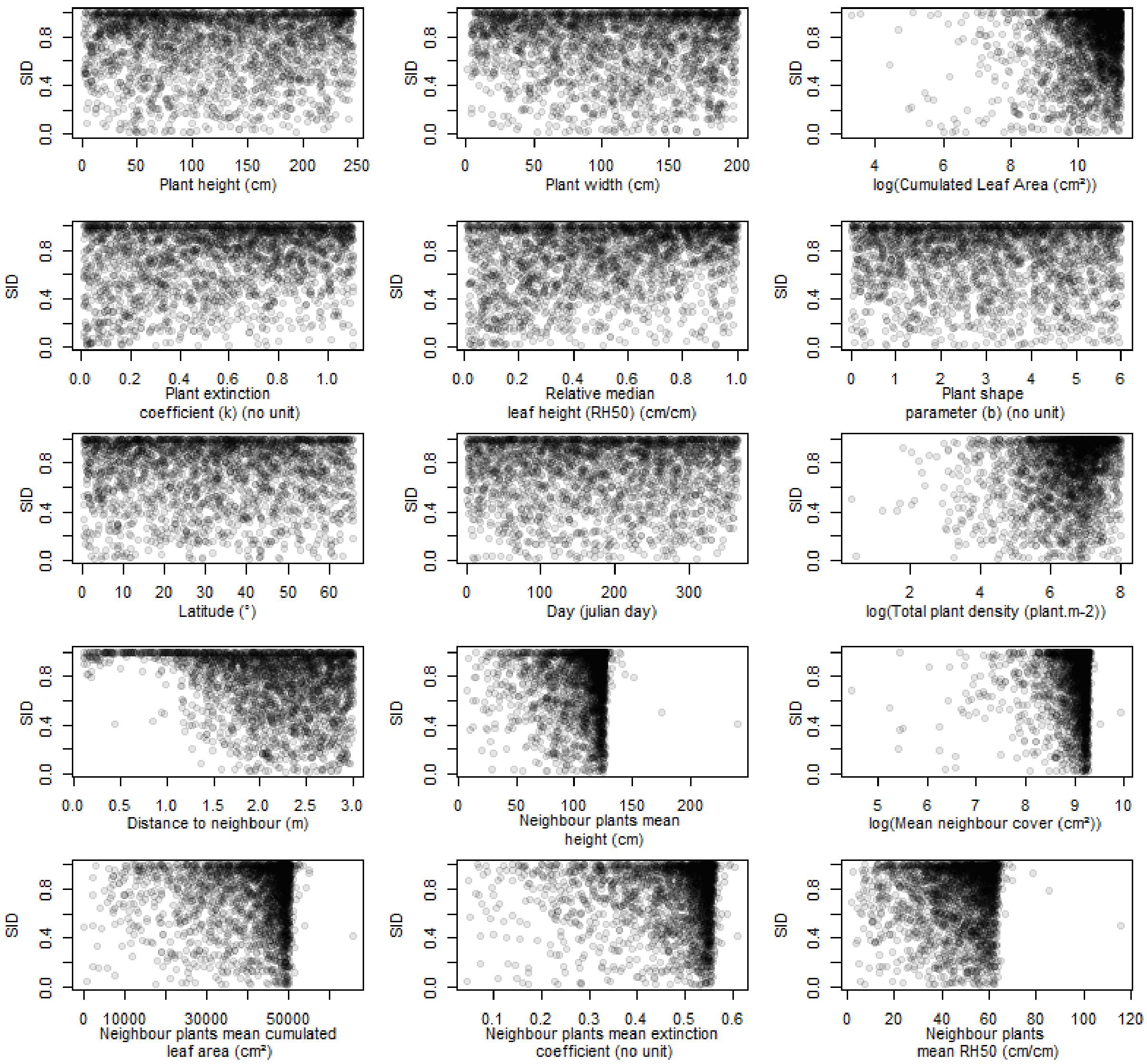

Figure 8: Scatterplot of the light interception submodel daily shading intensity (SID in MJ MJ^{-1}) in function of the 15 inputs of a target plant surrounded by neighbour plants in the virtual field. Each point represents a run on the space filling LHS design. From the 20440 initial LHS rows 2536 were kept to eliminate computation artefacts.

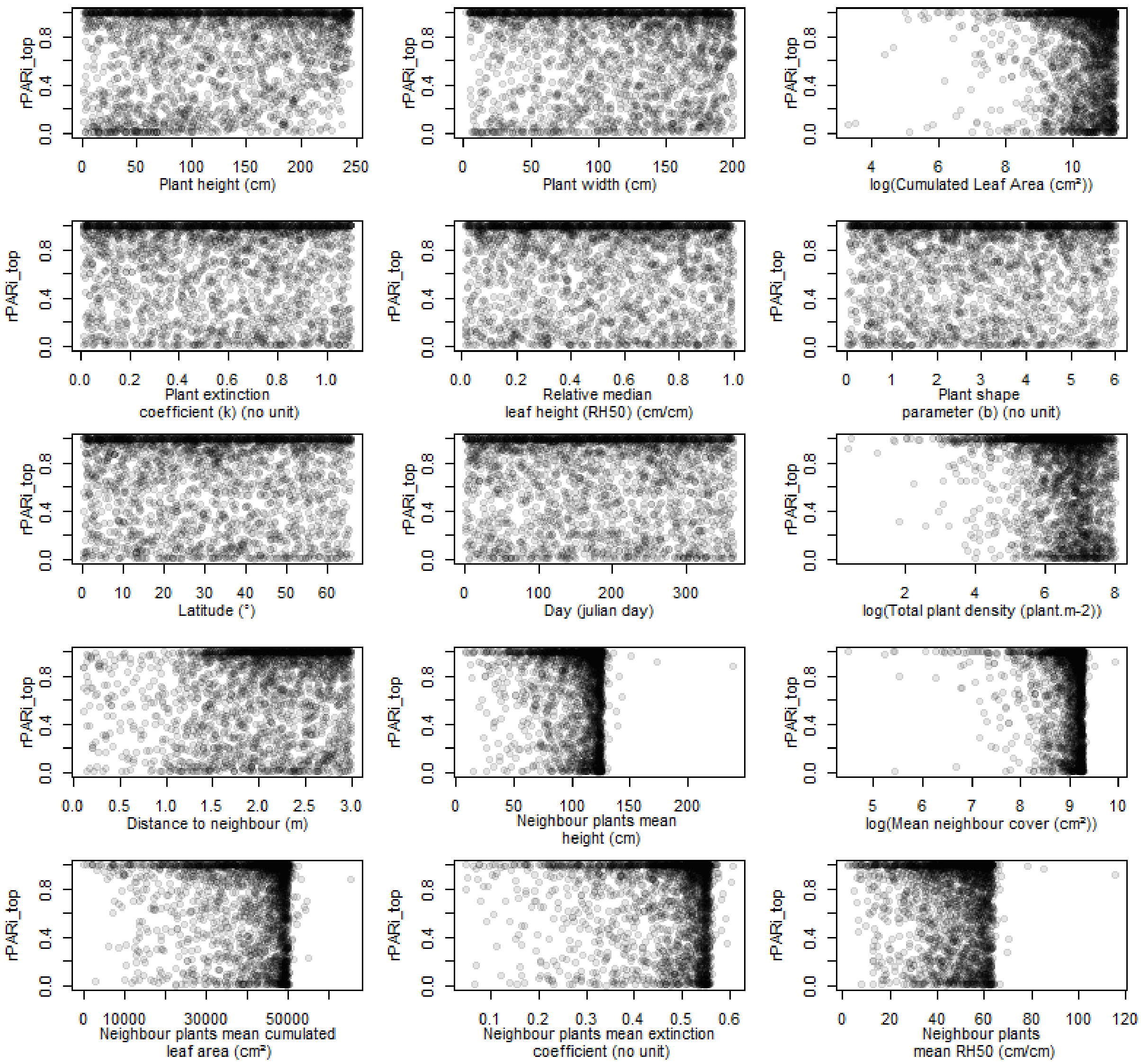

Figure 9: Scatterplot of the light interception submodel relative photosynthetically active radiation intercepted at the summit of the plant ($rPARi_{top}$ in $MJ.cm^{-2}$ MJ^{-1} cm^2) in function of the 15 inputs of a target plant surrounded by neighbour plants in the virtual field. Each point represents a run on the space filling LHS design. From the 20440 initial LHS rows 2536 were kept to eliminate computation artefacts.

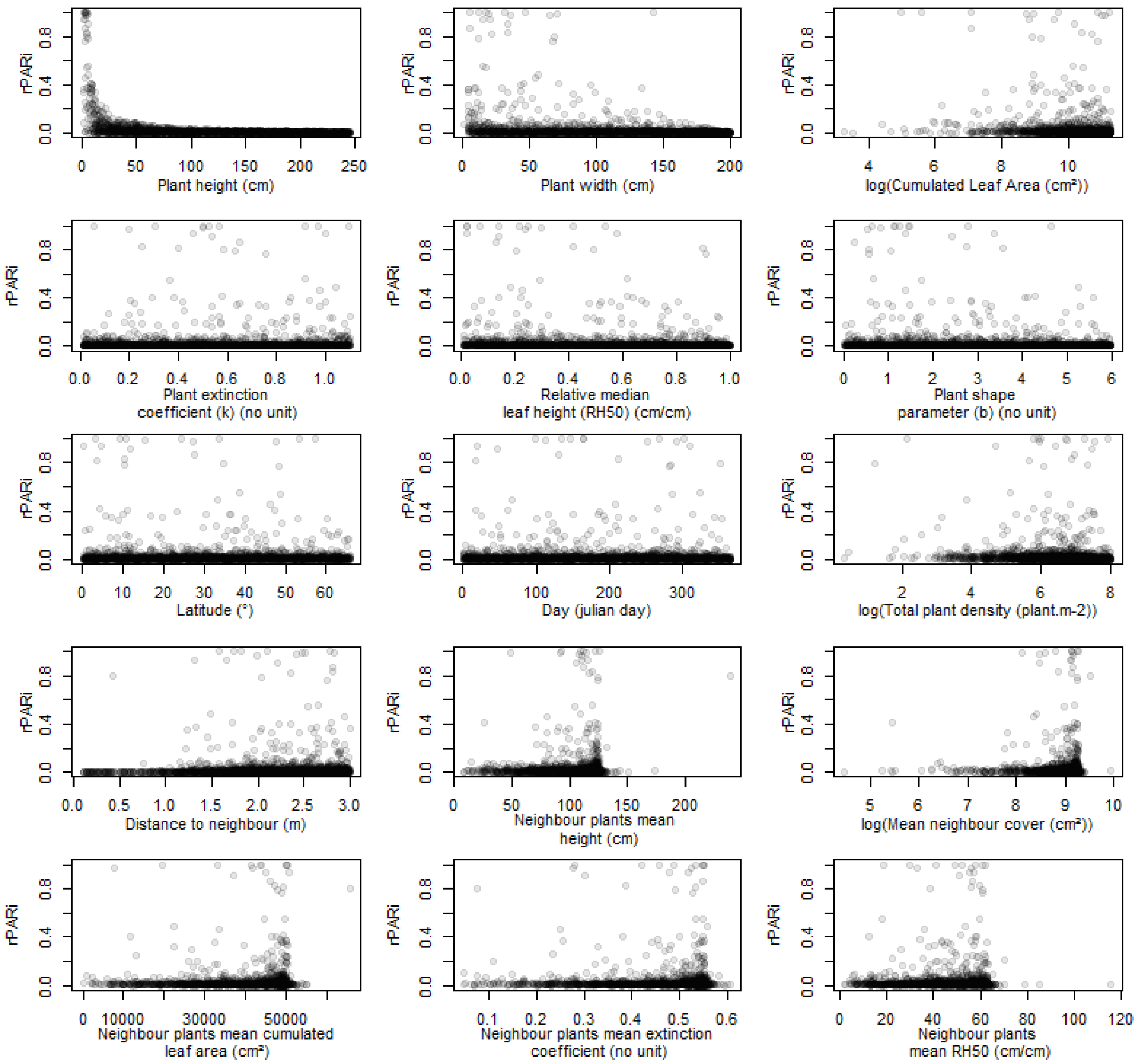

Figure 10: Scatterplot of the light interception submodel relative photosynthetically active radiation intercepted by the plant (rPARi in MJ.cm^{-2} MJ^{-1} cm²) in function of the 15 inputs of a target plant surrounded by neighbour plants in the virtual field. Each point represents a run on the space filling LHS design. From the 20440 initial LHS rows 2536 were kept to eliminate computation artefacts.

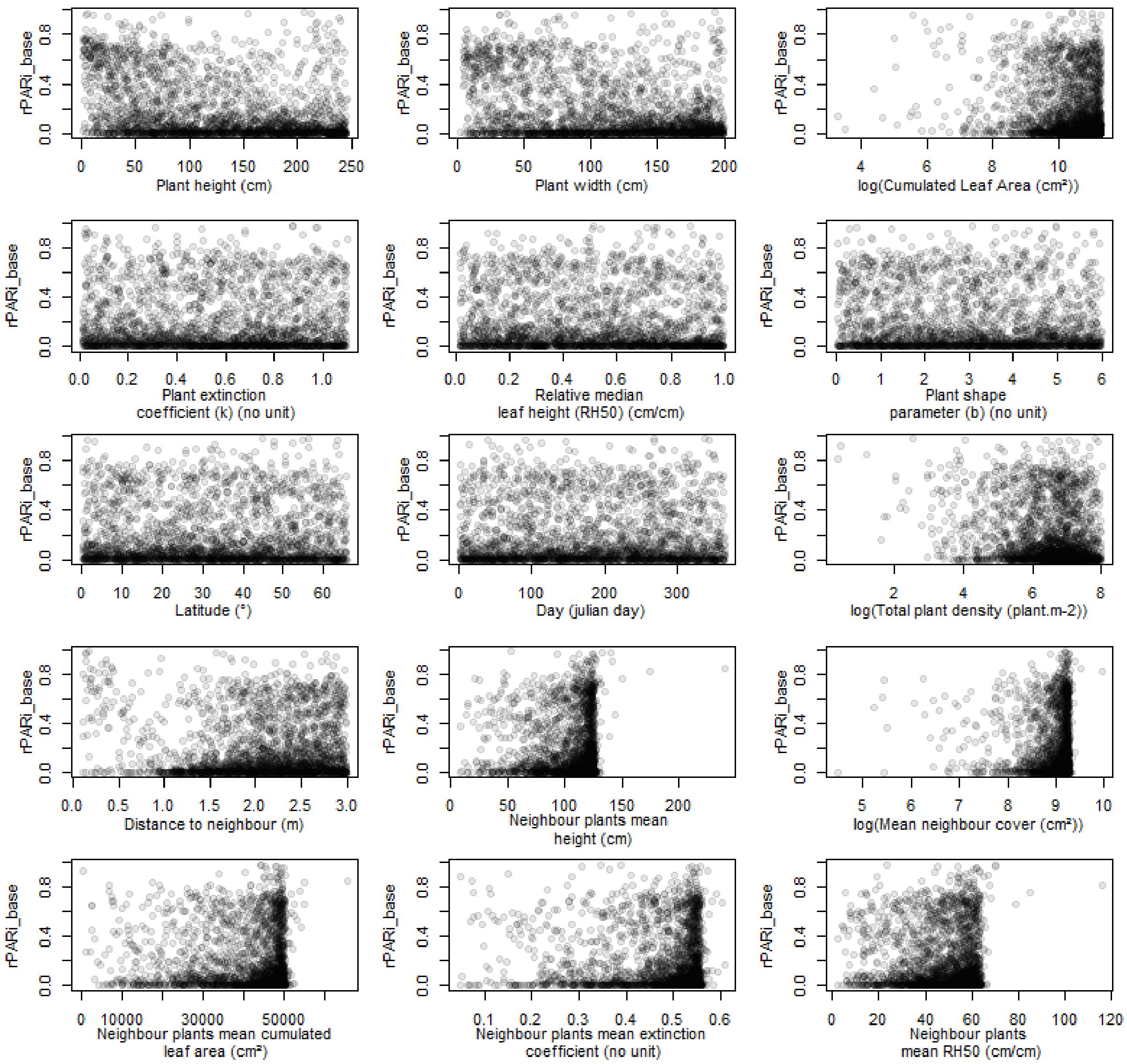

Figure 11: Scatterplot of the light interception submodel relative photosynthetically active radiation intercepted at the base of the plant ($rPARi_{base}$ in MJ.cm^{-2} MJ^{-1} cm²) in function of the 15 inputs of a target plant surrounded by neighbour plants in the virtual field. Each point represents a run on the space filling LHS design. From the 20440 initial LHS rows 2536 were kept to eliminate computation artefacts.

1.6 Effect of voxel edge size on simulation time

When developing the process-based light interception model in FLORSYS, Munier-Jolain et al. (2013) chose 7 cm as the best compromise to reconcile prediction quality and simulation time. This conclusion was based on oilseed rape whose plants have large leaves. A voxel of 7 cm might not be adapted for species with smaller leaves.

Our sensitivity analysis showed that the voxel size can be important for some inputs. The smaller the voxel is, the more precise the location and the morphology of the simulated plants are. But this precision has a cost in computation time (Figure 12). A voxel of 4 cm is a good precision and computation time: increasing the voxel further does not notably decrease simulation time anymore.

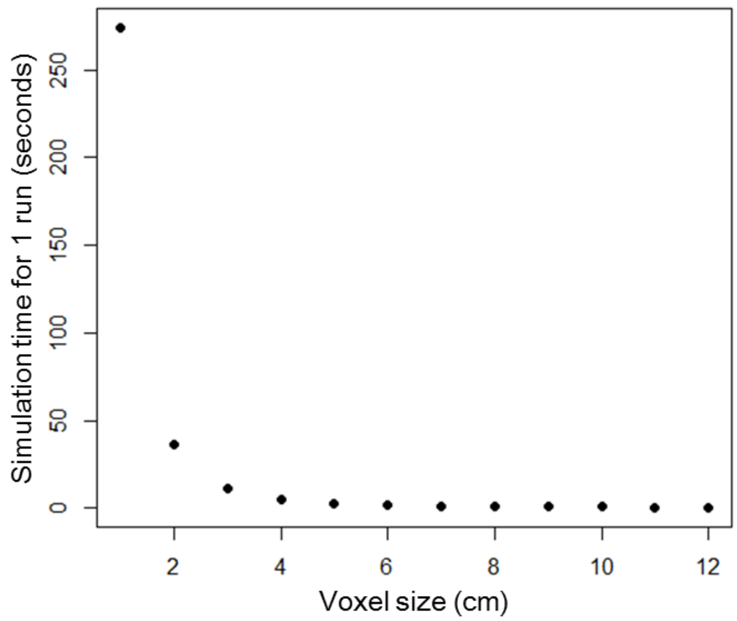

Figure 12: Simulation time of a test of diverse plants in a field of 8 x 8m² and a density of 300 plants.m-2 run for different voxel sizes.

1.7 References

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Annexe 4
Supplementary material of simplifying a complex model: sensitivity analysis and metamodelling of the complex mechanist model FLORSYS

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1 Supplementary materials for canopy construction

1.1 Correlation to build the diverse canopies

Table 1: Correlations between the variables used to build diverse canopies to metamodel the light interception submodel of FLORSYS. To have the full names of the variables see main article. Cdens, Wdens, rdisc, empty, nbholes, gap, rhole, pltype, Cpostype, Wpostype, orirank, ranksize, ppara, perp, dispW, nbpatch have a 0 correlation with all variables. Target plant inputs (Latitude, Day, Height, Width, LA, k, RH50, b) have the same correlations as (S2 Table 5) and a 0 correlation with all other variables.

	Wmeanht	Wmeanwd	WmeanLA	Wmeank	WmeanRH	Wmeanb	Cmeanht	Cmeanwd	CmeanLA	Cmeank	CmeanRH	Cmeanb	Wvcht	Wvcwd	WvcLA	Wvck	WvcRH	Wvcb	Cvcht	Cvwd	CvcLA	Cvck	CvcRH	Cvcb
Wmeanht	1	0.6	0.2	-0.2	0.2	0.3	0	0	0	0	0	0	0	-0.3	0	0.4	0	0	0.35	0.25	0	0	0	0
Wmeanwd	0.6	1	0.2	0	0.2	0.3	0	0	0	0	0	0	0	-0.3	0	0	0	0	0	0	0	0	0	0
WmeanLA	0.2	0.2	1	0	0	0.3	0	0	0	0	0	0	0	0	0.4	0	0	0	0	0	0	0	0	0
Wmeank	-0.2	0	0	1	0.2	-0.1	0	0	0	0	0	0	0	0	0	-0.6	-0.2	0	0	0	0	0	0	0
WmeanRH	0.2	0.2	0	0.2	1	0.1	0	0	0	0.3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Wmeanb	0.3	0.3	0.3	-0.1	0.1	1	0	0	0	0	0	0	0	0	0	0	0	0.5	0	0	0	0	-0.3	0
Cmeanht	0	0	0	0	0	0	1	0.6	0.2	-0.2	0.2	0.3	0	0	0	0	0	0.2	0	0	-0.25	0	0	0
Cmeanwd	0	0	0	0	0	0	0.6	1	0.2	0	0.2	0.3	0	0	0	0	-0.3	0	0	-0.2	0	0	0	0
CmeanLA	0	0	0	0	0	0	0.2	0.2	1	0	0.3	0	0	0	0	0	0	0	0	0	0	0	0	0
Cmeank	0	0	0	0	0.3	0	-0.2	0	0	1	0.2	-0.1	0	0	0	0.4	0.5	0.2	0	0	0	0	0	0
CmeanRH	0	0	0	0	0	0	0.2	0.2	0.3	0.2	1	0.1	-0.3	-0.2	0	0	-0.3	0	0	0	-0.2	0	0	0
Cmeanb	0	0	0	0	0	0	0.3	0.3	0	-0.1	0.1	1	0	0	0	0.3	0.2	0	0	0	0.35	0	0.8	0.4
Wvcht	0	0	0	0	0	0	0	0	0	0	-0.3	0	1	0.6	0.4	0	0	0	0	0	0	0	0	0
Wvcwd	-0.3	-0.3	0	0	0	0	0	0	0	0	-0.2	0	0.6	1	0.4	0	0	0	0	0	0	0	0	0
WvcLA	0	0	0.4	0	0	0	0	0	0	0	0	0	0.4	0.4	1	0.3	0	0	-0.2	0	0	0	0.2	0.3
Wvck	0.4	0	0	-0.6	0	0	0	0	0	0.4	0	0.3	0	0	0.3	1	0.6	0.3	0	0	0	0	0.4	0
WvcRH	0	0	0	-0.2	0	0	0	-0.3	0	0.5	-0.3	0.2	0	0	0	0.6	1	0.4	0	0	0	0	0.4	0
Wvcb	0	0	0	0	0	0.5	0.2	0	0	0.2	0	0	0	0	0	0.3	0.4	1	0	0	0	0	0	0
Cvcht	0.35	0	0	0	0	0	0	0	0	0	0	0	0	0	-0.2	0	0	0	1	0.8	0.5	0	0	0
Cvwd	0.25	0	0	0	0	0	0	-0.2	0	0	0	0	0	0	0	0	0	0	0.8	1	0.5	0	0	0
CvcLA	0	0	0	0	0	0	-0.25	0	0	0	-0.2	0.35	0	0	0	0	0	0	0.5	0.5	1	0	0.5	0.4
Cvck	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
CvcRH	0	0	0	0	0	-0.3	0	0	0	0	0	0.8	0	0	0.2	0.4	0.4	0	0	0	0.5	0	1	0.6
Cvcb	0	0	0	0	0	0	0	0	0	0	0	0.4	0	0	0.3	0	0	0	0	0	0.4	0	0.6	1

To obtain the correlations coefficients, the same method as for the single plant was used.
We randomly sampled plants occurring in 12 diverse cropping systems of past simulations run with 13 crop species and 25 weed species (Colbach et al., 2016). For each one, we sampled at least 100 plants a month, correlation coefficients between the 11 inputs values were computed for these plants. These correlations and expert knowledge were used to construct the target correlation matrix for the 11 inputs. The Voxel input and the four inputs, Latitude and Day (which determine solar angle), Xmax and Ymax (which determine field sample size), were considered to be independent and uncorrelated.

1.2 Distribution of aggregated inputs:

The aggregation of the inputs created non-uniform distribution.

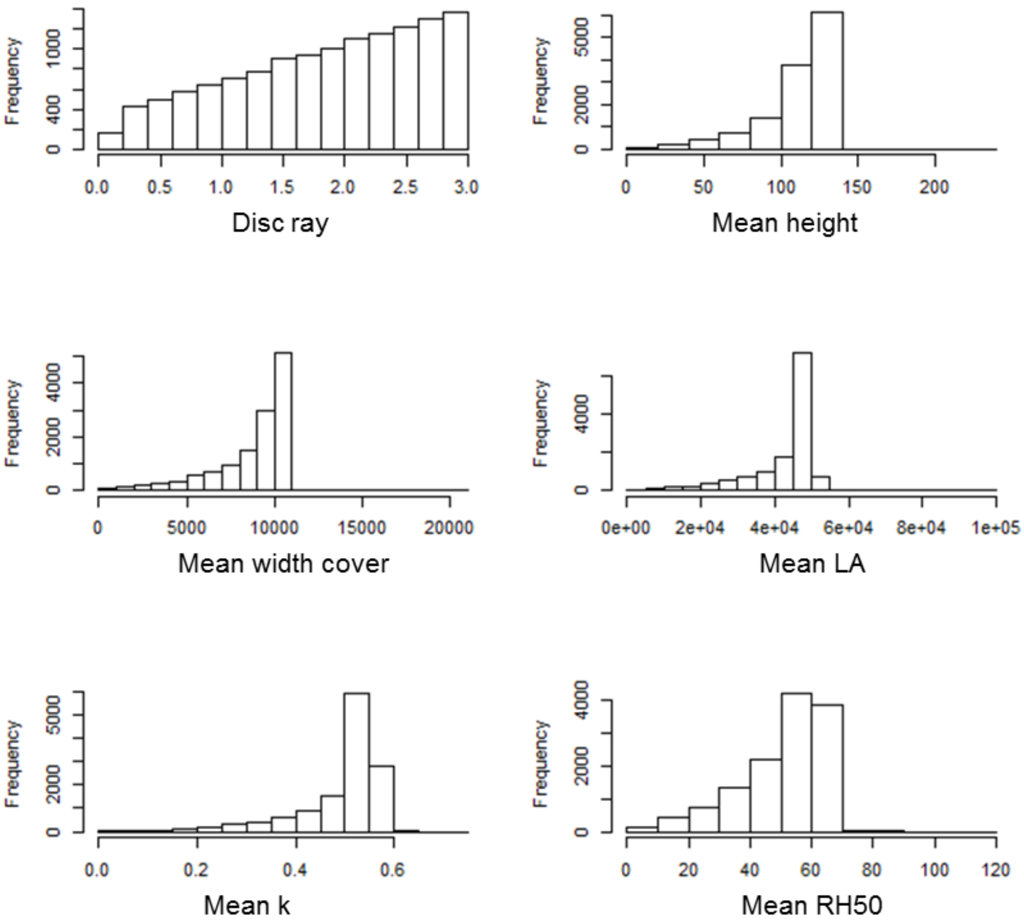

Figure 1: Distribution of the occurrences of the aggregated inputs. The crop:weed canopies were built via random uniform inputs (e.g. mean weeds height, variation coefficient of weed height).

1.3 Canopy structure

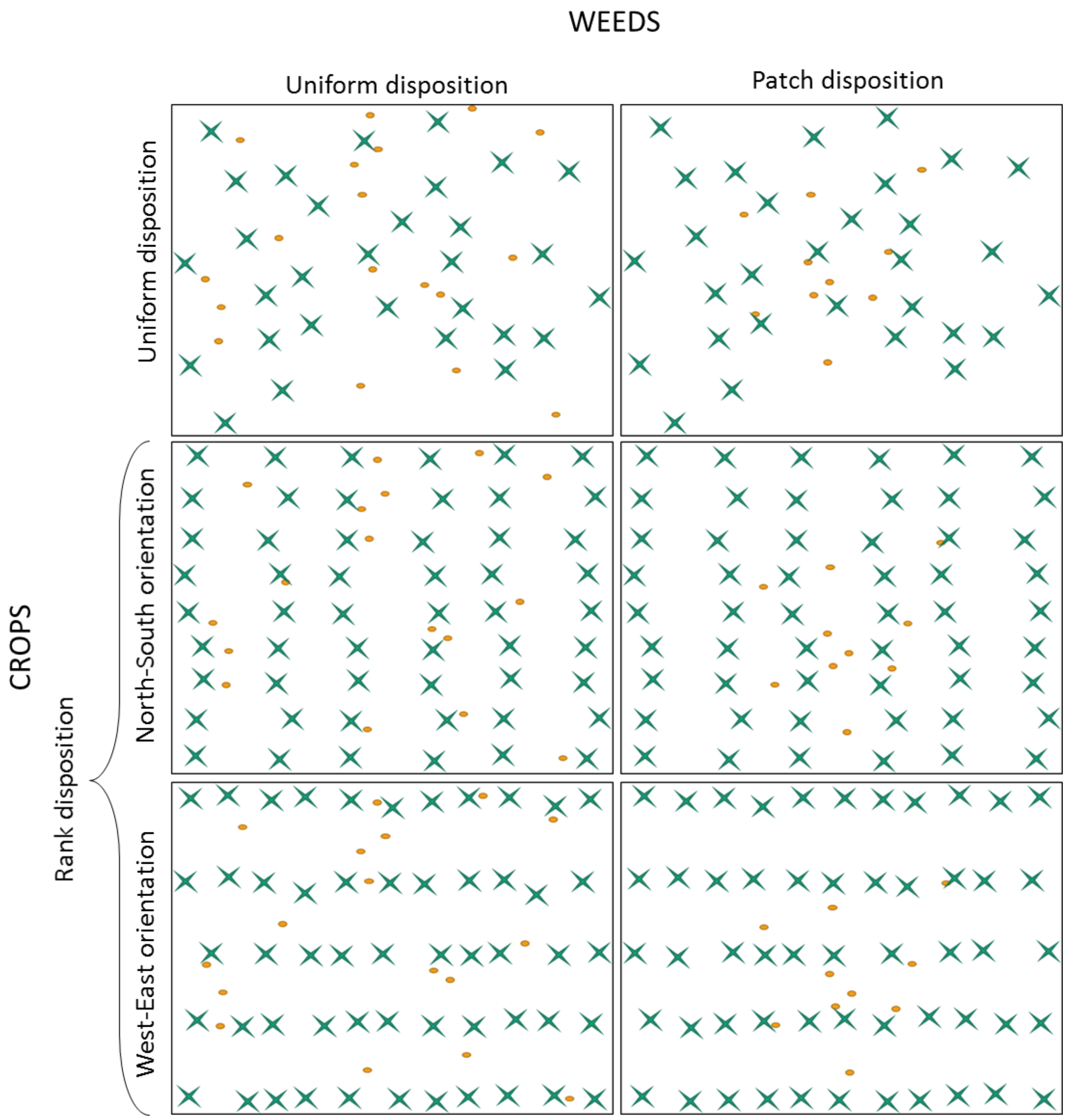

Figure 2: Schematic examples of all possible combinations of plants disposition in FLORSYS, green crosses are crops and orange dots are weeds.

1.4 Equations of aggregated values

Eq. 1

$$mean\ height = \frac{\sum_{i=1}^{n}(\frac{1}{d_i + 1} * height_i)}{\sum_{i=1}^{n}(\frac{1}{d_i + 1})}$$

Eq. 2

$$mean\ neighbour\ cover = \frac{\sum_{i=1}^{n}(\frac{1}{d_i + 1} * \pi \left(\frac{mean\ width_i}{2}\right)^2)}{\sum_{i=1}^{n}(\frac{1}{d_i + 1})}$$

Eq. 3

$$mean\ LA = \frac{\sum_{i=1}^{n}\left(\frac{1}{d_i + 1} * LA_i\right)}{\sum_{i=1}^{n}(\frac{1}{d_i + 1})}$$

Eq. 4

$$mean\ k = \frac{\sum_{i=1}^{n}\left(\frac{1}{d_i + 1} * k_i\right)}{\sum_{i=1}^{n}(\frac{1}{d_i + 1})}$$

Eq. 5

$$mean\ RH50 = \frac{\sum_{i=1}^{n}\left(\frac{1}{d_i + 1} * height_i * RH50_i\right)}{\sum_{i=1}^{n}(\frac{1}{d_i + 1})}$$

With: d the distance of the target plant to the neighbour plant i (+1 to account for a zero distance when the neighbour is located in the same voxel as the target), n the number of neighbour plants, $mean\ width_i$ is the width of neighbor plant i with the mean width transformed into an area to get the projected plant area, LA_i is the leaf area cumulated by the plant the neighbor plant i, k_i is the extinction coefficient of the neighbor plant i, $height_i$ is the height of neighbour i and $RH50_i$ is the relative median leaf height below which is located half of the leaf area.

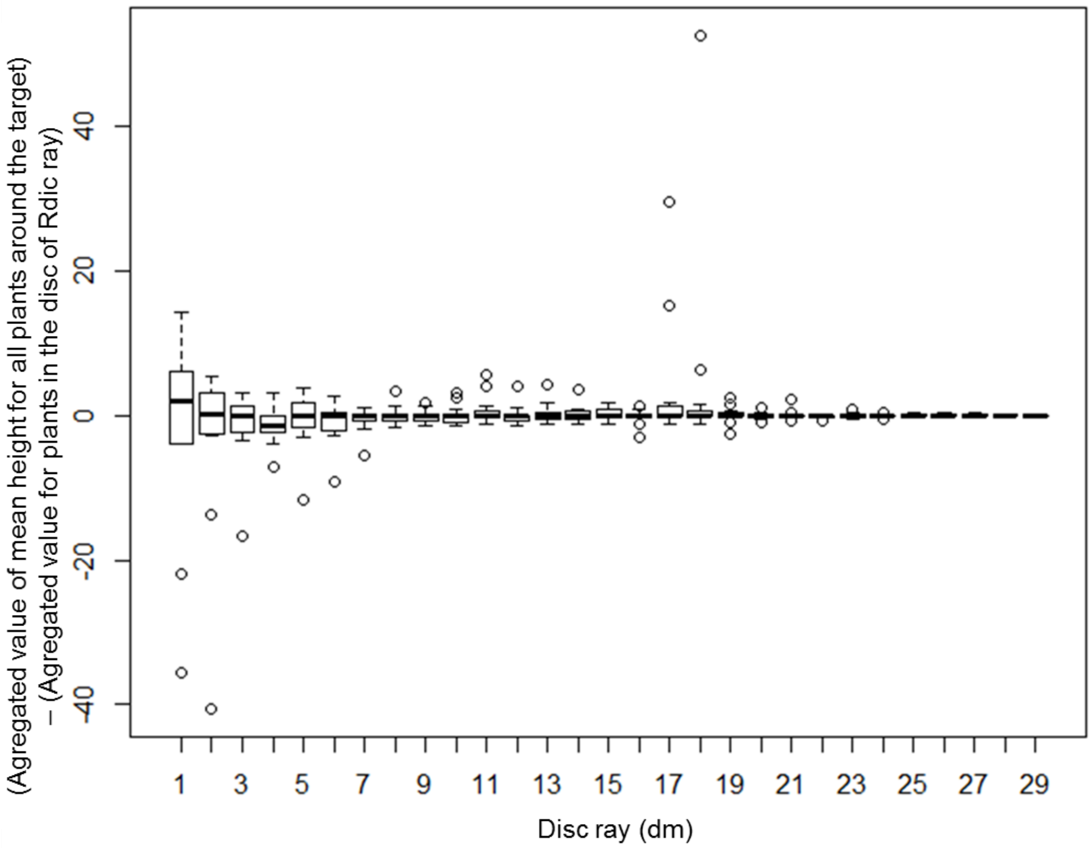

Figure 3: Influence of the disc ray size to the plants into account in the aggregated mean height value calculation for the metamodel of the light interception submodel of FLORSYS.

1.5 Height overtaking percentage

Proxy to estimate the canopy structure around the target plant, if the target plant is below the mean neighbour plants the height overtaking percentage is below 0, the plant is the same size as its neighbours the height overtaking percentage is equal to 0, the target plant is higher than the canopy, the height overtaking percentage is over 0.

Eq. 6: $$\textbf{Height overtaking percentage} = \frac{\textbf{Target plant height} - \textbf{Mean neighbour plant height}}{\textbf{Mean neighbour plant height}} \times \mathbf{100}$$

1.6 Variables importance

Table 2: CART variable importance of the inputs, only inputs that have an importance > 1 are presented.

Variable name	Score of variable importance
Distance to nearest neighbour (gap ray) × Distance to nearest neighbour (gap ray)	18
Distance to nearest neighbour (gap ray)	18
1 / Distance to nearest neighbour (gap ray) × Distance to nearest neighbour (gap ray)	18
Distance to nearest neighbour (gap ray) × Summer and Fall Julian days	12
Extinction coefficient / (1 + Distance to nearest neighbour (gap ray))	12
Distance to nearest neighbour (gap ray) /(1 + Plant density)	12
Distance to nearest neighbour (gap ray) × Mean neighbour height	1
Distance to nearest neighbour (gap ray) × Target plant overtaking percentage on neighbour plant	1
Target plant overtaking percentage on neighbour plant	1
Target plant overtaking percentage on neighbour plant / (1 + Distance to nearest neighbour (gap ray))	1
Target plant overtaking percentage on neighbour plant / (1 +Plant density)	1
Mean neighbours width cover	1
Target plant width / (1 + Distance to nearest neighbour (gap ray))	1

Determining if plant is single, *i.e.* on bare soil without any interference from neighbour plants, depends on the size of the target plant, the size of the largest plant in the field, and the distance to the nearest neighbour. In that case, the chaos metamodel for single plants is used, predicting light interception and absorption only from target-plant characteristics (*e.g.* height, leaf area…) and physical inputs. If the target plant is very small, the chaos metamodel for small plants is used. If the plant is surrounded by neighbour plants, the density and average characteristics (*e.g.* height, leaf area…) of these neighbour plants are calculated. Light interception and absorption is predicted from target-plant characteristics, average neighbour characteristics and physical inputs. Implementing the polynomial chaos metamodel in FLORSYS generated monstrous plants, as FLORSYS is a dynamic model, every small imprecision was exceedingly increased every day.

1.7 References

Colbach, N., Bertrand, M., Busset, H., Colas, F., Dugué, F., Farcy, P., Fried, G., Granger, S., Meunier, D., Munier-Jolain, N.M., Noilhan, C., Strbik, F., Gardarin, A., 2016. Uncertainty analysis and evaluation of a complex, multi-specific weed dynamics model with diverse and incomplete data sets. Environmental Modelling & Software 86, 184-203.

Annexe 5
Supplementary material of simplifying a complex model: sensitivity analysis and metamodelling of the complex mechanist model FLORSYS

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1 Supplementary materials for metamodel implementation in FlorSys

1.1 Detailed algorithm for including metamodels in FLORSYS

1.1.1 Principle

Each day, for each target plant (crop or weed), we determine:

- Whether the plant can be considered as single, i.e. on bare soil without any interference from neighbour plants. This depends on the size of the target plant, the size of the largest plant in the field, and the distance to the nearest neighbour. In that case, the chaos metamodel for single plants is used, predicting light interception and absorption only from target-plant characteristics (e.g. height, leaf area etc) and physical inputs. If the target plant is very small, the chaos metamodel for small plants is used.
- If the plant is surrounded by neighbour plants, the density and average characteristics (e.g. height, leaf area etc) of these neighbour plants are calculated. The nearer the neighbours are to the target, the more their characteristics contribute to the average canopy characteristics. Light interception and absorption is predicted from target-plant characteristics, average neighbour characteristics and physical inputs.

If the inputs are outside the ranges accepted by the metamodels, additional equations predict light interception and absorption from ecophysiological knowledge, or from likely constants (principle in section 1.4.1). If the neighbour plants are still too small to answer to the cover metamodel requirements, predictions are a linear combinations of predictions for single plants and for plants inside a canopy.
The search for neighbour plants can be time-consuming when plant densities are high. As a consequence, alternative algorithms were tested (section 1.2).

1.1.2 Description

The following sections explain the different steps executed each day (d) to calculated light interception output variables from the metamodel functions. The detailed equations are listed in Table 1, the variables in Table 2. The numbers between [] cited below refer to the equations in Table 1. A target plant (p) is any crop or weed plant for which light-interception outputs are predicted. It belongs to a species (s) and an emergence cohort (c), i.e. all plants of species s that have emerged on the same day.

1.1.2.1 What has happened before the light-interception submodel in FLORSYS?

In FLORSYS, the following events occur daily before the light-interception submodel:

- Updating soil temperature, moisture and soil water potential,
- Soil seed bank mortality,
- Effects of tillage, herbicide, mechanical weeding, nitrogen fertilization, manure (if any) on weed plants and seeds,
- Crop sowing (if any)
- Seed germination, plant emergence, perennial regrowth of weeds and crops, if any,
- Effect of frost (if any) on plants.

The following events occur daily after the light-interception model:

- Plant growth,
- Calculating daily weed impact to integrate into indicators,
- Effect of mowing and harvesting operations (if any) on crops and weeds,
- Effect of weeds on take-all disease,
- Seed migration between fields,
- Gamete mutation during reproduction,
- Seed rain (if any) to soil seed bank, including seed interception by canopy if this option is activated in FLORSYS. This option is at present deactivated and has not yet been published.
- Phenology, i.e. increase thermal time since sowing and change stages if necessary.

1.1.2.2 Environmental and canopy variables valid for whole field

The largest plant in the field is determined, as the maximum plant height or plant radius of all crop and weed plants [1]. This will later be used to determine at which distance from the target plant neighbour plants must be considered (section 1.1.2.3.2).
The total density of crop and weed plants is updated, if any plants have emerged or died since the previous day [2]. Plant death can be due to cultural operations, frost or plant age.
The incident photosynthetically active radiation (PAR) above the canopy is the incident radiation (usually an input from a weather station) that can actually be used by plant photosynthesis and that is not reflected by the canopy [3] (Varlet-Grancher *et al.*, 1989).
The Julian day d (in number of days since Jan. 1) is transformed into number of days to or since summer solstice to account for the position of the sun relative to the zenith [4]. Another environmental input that influence the sun's position is the latitude where the simulated field is located.

1.1.2.3 Local neighbourhood of target plant

1.1.2.3.1 Initialization of neighbourhood variables

For each target plant is determined the maximum distance at which neighbouring plants must be considered (Figure 1, [5]).

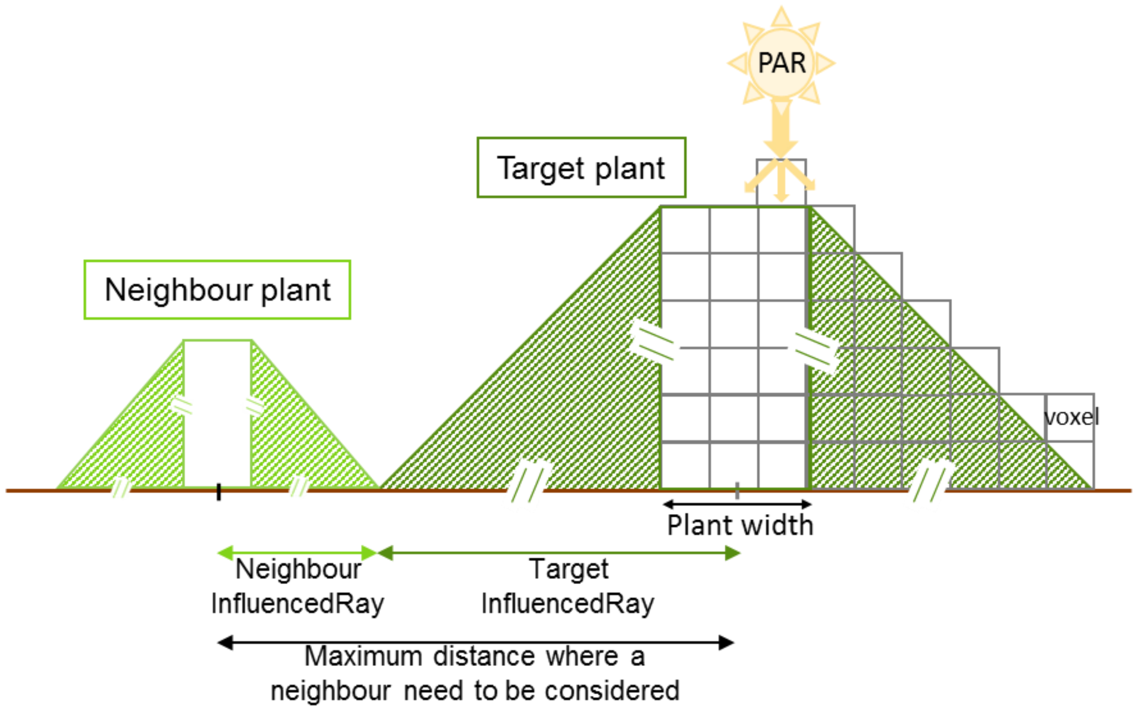


Figure 1: Schema of the influenced area (in striped colour) that can be influenced by other plants in the light interception submodel of FlorSys. With InfluencedRay, the ray of the area were the plant can be influenced for the target plant or that can influence the target for neighbour plants. Target InfluencedRay: Target plant disc ray possibly influenced by other plants. Neighbour InfluencedRay: Neighbour plant disc ray influencing target plant. The sizes depends on the way the light is tickling down and is estimated in the submodel (Munier-Jolain et al., 2013).

Before starting the search for the nearest neighbour plant and calculating average canopy characteristics, the neighbourhood variables must be initialized at zero, except for the distance to the nearest neighbour which is initialized at its maximum possible value [5]. This is the smallest dimension of the field sample which is equivalent to the distance of the target plant to its replicate, when the field sample is replicated indefinitely (Figure 2).

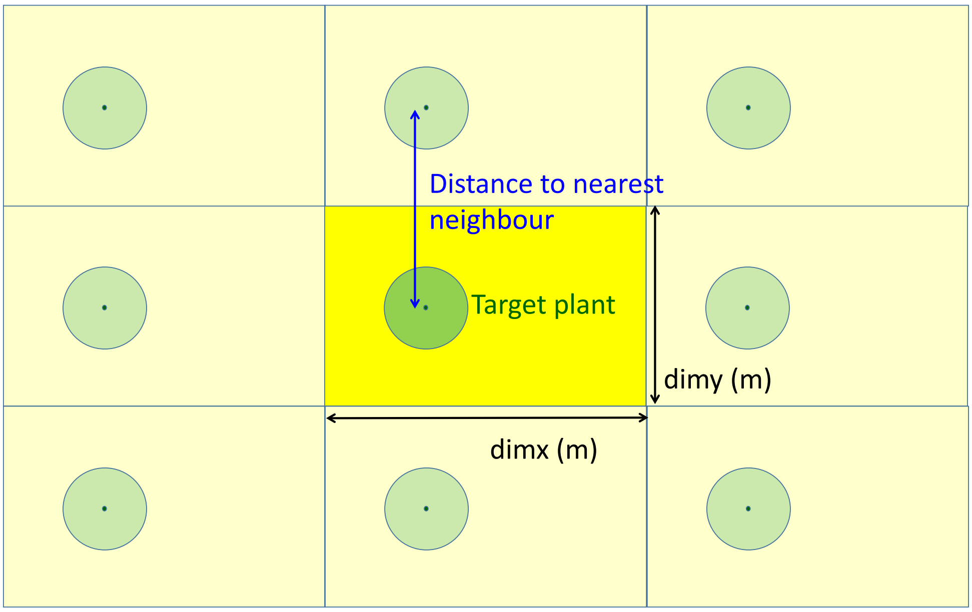


Figure 2. Replication of the field sample (center) to reconstitute a realistic field in FLORSYS

1.1.2.3.2 Searching for neighbours

The search loop is only run if there is more than one plant in the field [7][8]. It starts at the voxel (x_p,y_p) where the target plant is located, and then spirals clockwise through the voxels (Figure 3). The loop stops once the distance to the analyzed voxel exceeds the influence distance. A round beyond the strict influence zone ($DTP_{pxy} \leq ID_p + vs \cdot \cos(\Pi/4)$ in [7][8]) is necessary to avoid cutting off the voxel loop when being at a corner voxel and thus missing edge voxels that are still inside the influence zone.

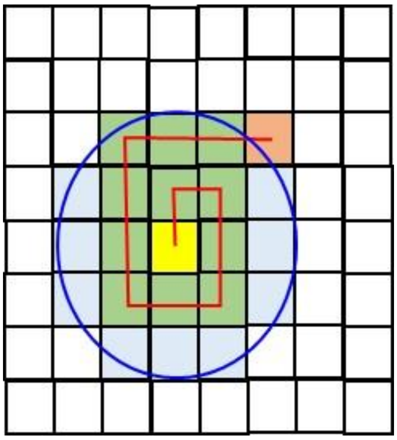


Figure 3. Schematic representation of loop searching for neighbours. The center of the target plant is in the central yellow voxel, the red line shows the clockwise loop searching through voxel, the green voxels have already been searched, the blue voxels must still be searched because their centers are inside the influence zone shown by the blue circle. If the algorithm would not run a search round beyond the influence zone, the search loop would stop in the red voxel (whose center is outside the influence zone), even though the blue voxels have not yet been searched.

To make the simulations faster, the search loop only runs as long as the whole plant base area and two complete rounds beyond the closest neighbour have not yet been searched ($DTP_{pxy} \leq W_p/2$ or $DTP_{pxy} \leq DNN_p + 2 \cdot vs \cdot \cos(\Pi/4)$). Once these two conditions are fulfilled, the search stops, even if the whole influence zone has not yet been analysed. This stopping condition is acceptable as the weight of the neighbour plants decreases with the distance to the target plant.

With each newly searched voxel, the area of the searched zoned is updated, and the distance to the target plant is calculated [7]. If there are any plants (other than the target plant) in the search voxel, the distance from the target plant to the neighbour is updated, the neighbour plant characterics (weighted by the distance to the target plant plus one to account for nil distances) are added to the canopy variables, and the number of neighbours is updated (again weighted by the distance to target) [8]. The canopy (cover) density counts neighbours without weighting them.

1.1.2.3.3 Finalizing calculations

If no neighbours were found in the search loop (i.e. if the distance to the nearest neighbour exceeds the influence distance), canopy variables are nil, canopy density is one plant in the field sample, and distance to nearest neighbour is the minimum of the two field dimensions [9], i.e. the same values as during the initialization (section 1.1.2.3.1). This reinitialization is necessary as the nearest neighbour identified during the search loop can be further than the influence distance (section 1.1.2.3.2).

If the distance to the nearest neighbour is less than the influence distance, the summed canopy variables are transformed into average canopy variables [10]. The cover density is the sum of the number of neighbours in the searched area, and the target plant relative to the whole field sample.

A further variable assesses how tall or small the target plant is relative to its neighbourhood, by calculating the height difference between the target plant and its neighbourhood, relative to the canopy height [11]. If there are no neighbours, a large default value is chosen

1.1.2.4 Predicting light-interception outputs, considering all plants as "single"

A plant is considered as "single" if there are no close neighbours, and the light-interception outputs are calculated solely from physical and target-plant inputs, disregarding canopy characteristics. Two metamodels are used, depending on the size of the target plants, and additional conditions were determined to produce predictions if inputs are outside the input range accepted by the metamodels.

1.1.2.4.1 Principles for managing out-of-bounds conditions

Even though very large ranges of variation of X_i were chosen to generate the input sets via LHS, the number of data points close to the bounds were few. Moreover, some of these were eliminated because they resulted, in combination with other X_i values, in conditions impossible to include in the chaos polynomial. Consequently, the range of accepted inputs for the *single plant* and *cover* metamodels (Table 4 in section 1.3.2) did not cover all the X_i values possible in FLORSYS simulations. To remedy to this deficiency, several strategies were used:

- A third data set for small single plant was generated and a third metamodel was build for these very small plants (Table 4 in section 1.3.2);
- For single target plants that were still too small to answer the *small single plant* metamodel, constants based on the analysis of the extreme conditions of the data sets were used (all except PARa), or ecophysiological rules were applied (PARa);
- If either the target plant or the average canopy plant was too small, particularly their leaf area was too small, a linear combination of predictions for single plants (either small or large) and plants in canopy were used. This was particularly true for canopy leaf area whose lower bound was extremely high (Table 4 in section 1.3.2);
- If average canopy variables exceeded the upper bound for the *cover* metamodel, constants were used. These constants were based on the analysis of the data sets, focusing on those inputs with the strongest polynomial effect in the sensitivity analysis, with rules listed from the most to the least important input in the sensitivity analysis.

Details can be found in section 1.4.

A particular case consists of mature target plants or canopies that have already lost their leaves. If this occurs, the lower bound values of the cover metamodel were used as inputs [30][31]. As the average stage of the canopy is unknown, the canopy plant height was used (which must be > 0, [31]) to discriminate mature leaf-less canopies from bare soil conditions.

1.1.2.4.2 Metamodel inputs

The metamodel inputs depend on the metamodels (Table 4 in section 1.3.2). The *small single plant* metamodel uses two physical inputs (latitude, day), and six target-plant characteristics (height, width, leaf area, extinction coefficient, median leaf area height, shape parameter for leaf-area distribution) [13]. The *large single plant* metamodel uses five physical inputs (latitude, day, field sample dimensions, voxel edge size), and six target-plant characteristics (height, width, leaf area, extinction coefficient, median leaf area height, shape parameter for leaf-area distribution) [14]. The *cover* metamodel uses two physical inputs (latitude, day), six target-plant characteristics (height, width, leaf area, extinction coefficient, median leaf area height, shape parameter for leaf-area distribution), and seven neighbourhood inputs (plant density, cover radius, average plant height, area, leaf area, median leaf area height, extinction coefficient of canopy surrounding target plant) [15]. Cover radius is the distance beyond which no more neighbour plants are found. This variable was used to constitute the canopy for the sensitivity analysis. Here, it is fixed at upper input bound to maximise the effect of the other inputs and emulate the usual situation where plants are located everywhere in the field.

1.1.2.4.3 Absorbed photosynthetically active radiation (PARa)

The photosynthetically active radiation absorbed by the plant (PARa) will determine how much biomass the plant will accumulate today. If the leaf area of the target plant is lower than the minimum accepted inputs for the *small single plant* metamodel, then PARa is the product of the plant leaf area and its extinction coefficient [16], to reflect the basic ecophysiological principle of light absorption (Monsi and

Saeki, 1953, 2005). It is further divided by plant volume to get the PARa per cm³. This conversion is necessary as the metamodels predict a PARa per voxel, with a voxel size varying with the metamodels (4 cm, vs and 4 cm for *small single plant*, *large single plant* and *cover* metamodels, respectively).
If the leaf area is larger but either the plant height or width are lower than the minimum accepted inputs for the *small single plant* metamodel, then PARa is 1 (for absorbing all the light in the voxel) divided by plant volume [17]. The inputs for this metamodel are two physical
If plant leaf area, height and width are larger but the leaf is lower than the minimum accepted input for the *large single plant* metamodel, then PARa is predicted by the *small single plant* metamodel [18]. The metamodel prediction is in MJ MJ^{-1} per voxel, with a y voxel edge size of 4 cm. The metamodel output is thus divided by 4^3 to obtain PARa per cm^3.
Finally, if the plant area exceeds the minimum accepted input for the *large single plant* metamodel, then PARa is predicted by the *large single plant* metamodel [19]. The metamodel prediction is for a voxel edge size of vs, i.e. the voxel edge size chosen by the FLORSYS user. The metamodel output is thus divided by vs^3 to obtain PARa per cm^3.

1.1.2.4.4 Daily shading intensity (SID)

The daily shading intensity SID will determine how much the plant will etiolate in future. It also triggers the switch from RGR-based growth (leaf area increase only depends on thermal time) to LIGHT-COMPETITION growth (plant biomass accumulation increases with absorbed PARa) (Colbach et al., 2014), and is thus very important for small plants.
If the leaf area of the target plant is lower than the minimum accepted input for the *large single plant* metamodel and plant width is lower than the maximum accepted input for the *small single plant* metamodel, then the SID is predicted from the *small single plant metamodel* [20]. Otherwise, the *large single plant* metamodel is used [21].

1.1.2.4.5 Light intercepted by the whole plant (PARi)

The proportion of light intercepted by a whole plant (PARi) is only needed if a herbicide is applied tomorrow. PARi is a proxy for the proportion of herbicide intercepted by plant, and influences the efficacy of non-systemic herbicides (Colbach et al., 2017).
If the leaf area of the target plant is lower than the minimum accepted input for the *large single plant* metamodel and plant height is lower than 1.5 times the maximum accepted input for the *small single plant* metamodel, then PARi is predicted from the *small single plant metamodel [22]*[20]. Otherwise, the *large single plant* metamodel is used [23].

1.1.2.4.6 Light intercepted by the plant summit (PARis)

The proportion of light intercepted by the top of the plant (PARis) is only needed if a herbicide is applied tomorrow. PARis is a proxy for the probability whether the plant receives any herbicide, and influences the efficacy of systemic herbicides (Colbach et al., 2017).
PARis is 1 in single plants [24], as there are no neighbours to hinder light transmission, and self-shading does not impact the top of the plant.

1.1.2.4.7 Light arriving below plant base, on soil surface (PARib)

The proportion of light arriving on soil surface, below plant base (PARib) is a proxy for seed rain proportion arriving on soil surface below plant base. Dense persistent canopies (e.g. in grassland) can severely limit seed bank replenishment (Doisy et al., 2014).
If the leaf area of the target plant is lower than the minimum accepted input for the *large single plant* metamodel and plant width is smaller than half the maximum accepted input for the *small single plant* metamodel, then PARib is predicted from the *small single plant metamodel* [25][20]. Otherwise, the *large single plant* metamodel is used [26].

1.1.2.5 Determine whether the target plant is single

Usually, more than one plant grows in a field. Even if there are more than one plant in the field, plants without close neighbours can be considered as single [27]. This happens when no plants were found in the search loop (section 1.1.2.3), the distance to the nearest neighbour exceeds the influence distance, or the local canopy density is less than the minimum input value accepted the *cover* metamodel. These conditions were based on logical assumptions.

Another series of conditions for considering a target plant as single are based on an analysis of the data set used for the sensitivity analysis (see article Figure 5). This analysis resulted in four further situations for considering a plant as single [28]:

- if the nearest neighbour is further than 1.6 m, and the target plant is taller than the neighbouring canopy, e.g. twice as tall when the nearest neighbour is 1 m away ($OH_{pd} \geq 100/1$), or three times as tall when the nearest neighbour is 0.5 m away ($OH_{pd} \geq 100/0.5 = 200$ cm cm^{-1}); the further the nearest neighbour, the smaller the target plant can be and still be considered single;
- if the nearest neighbour is further than 1.6 m, and the day is close to summer solstice (and thus the sun close to the zenith); e.g. less than 138 days if the nearest neighbour is 0.5 m away ($NDS_d < 92\ (1+0.5) = 138$ days) ; the further the nearest neighbour, the further from summer solstice the day can be;
- if the nearest neighbour is further than 1.6 m, and latitude is close to the equator (and thus the sun close to the zenith); less than 16° if the nearest neighbour is 1 m away ($|\text{latitude}| < 8\ (1+1)$); the further the nearest neighbour, the further from equator the field can be;
- if the nearest neighbour is between 1.2 and 1.6 m, and the target plant is narrow; e.g. less than 64 cm if the nearest neighbour is 1 m away ($W_{pd} < 32\ (1+1) = 64$ cm); the further the nearest neighbour, the larger the target plant can be.

In all other situations, the plant cannot be considered as single [29].

1.1.2.6 Predicting light-interception outputs, depending on target-plant status

In the following sections, the light-interception outputs will be calculated, depending on whether target plants can be considered as single or not. There are also many conditions and transformations to account for inputs that are outside the ranges accepted by the different metamodel. Further transformations and variables are calculated to make the outputs compatible for the subsequent FLORSYS submodels.

1.1.2.6.1 Absorbed photosynthetically active radiation (PARa)

If the target plant can be considered as single, then the absorbed photosynthetically active radiation (PARa) per cm³ is the one calculated for single plants in section 1.1.2.4.3 [32].

If the plant is inside a canopy, but its leaf area or the average leaf area of this canopy are below the minimum accepted input values for the *cover* metamodel, then the PARa is a linear combination of the prediction by the *cover* metamodel (divided by 4^3 to convert into MJ MJ^{-1} cm^{-3}), and the prediction for single plants of section 1.1.2.4.3, weighted respectively by $CLA_{pd} / (CLA_{pd} + 1)$ and $1 / (CLA_{pd} + 1)$, to make the weight of the *cover* metamodel prediction increase with the average canopy leaf area [33].

The following five equations [34]-[38] fix the PARa at a constant, depending on whether canopy leaf area, canopy extinction coefficient, canopy median leaf-area plant height, canopy plant area, or canopy plant height weighted by the inverse of the distance to the nearest neighbour (plus 1, to account for neighbours in the same voxel as the target plant) exceed the 0.99 percentile of input values used to build the *cover* metamodel. The constants are the average PARa (e.g. 0.419 MJ MJ^{-1} voxel^{-1}) in the dataset used to build the *cover* metamodel for the 0.01 largest X_i input values (e.g. $CLA / (DNN_p + 1) >$ 49119.8953 cm² m^{-1}). All constants are divided by 4^3 to convert into MJ MJ^{-1} cm^{-3}.

The next equation [39] the PARa at a constant if the canopy (cover) density exceeds the maximum accepted input value for the *cover* metamodel. The constant is divided by 4^3 to convert into MJ MJ^{-1} cm^{-3}.

Only if none of the previous eight conditions [32]-[39] is true, the *cover* metamodel is used to predict the PARa, again after dividing by 4^3 to convert into MJ MJ^{-1} cm^{-3} [40].

Biologically, the PARa per cm³ cannot exceed $K_{pd} \cdot LA_{pd} / V_{pd}$ [41], which correspond to a plant without any overlapping leaves, intercepting 100% of incident PAR_d, with the extinction coefficient K_{pd}

determining the proportion that is actually absorbed, and the plant volume V_{pd} determining how much of this occurs per cm³ plant. Moreover, the PARa per cm³ must be in [0,1] MJ MJ^{-1} cm^{-3} [42], which is not always respected by the metamodels.
The PARa per cm³ is then multiplied by today's incident PAR_d and the plant volume to obtain the total photosynthetically active radiation absorbed by plant [43], which will be transformed later by FLORSYS into new biomass (Colbach et al., 2014).
To ensure that the whole plant community in the field does not absorb more than the available incident PAR_d, the ratio of the PARa summed all plants and the incident PAR is calculated [44]. If this ratio exceeds 1, the PARa of each plant is readjust [45].

1.1.2.6.2 Daily shading intensity (SID)

The principle for calculating the daily shading intensity (SID) depending on plant-status and on input values relative to input ranges accepted by the metamodels is the same as for PARa [46]-[54]. The differences concern the order of treating out-of-bound inputs (e.g. in contrast to PARa, canopy plant width CW_{pd} is considered earlier [50] than canopy median leaf-area plant height $CH50_{pd}$ [51]). The constants are, of course, different, and no division by voxel volume is necessary.
A further equation ensures that SID is in [0,1] MJ MJ^{-1} [55]. The daily shading intensity SID is then transformed into the cumulated shading intensity since plant emergence SI (Munier-Jolain et al., 2014). On the day the plant emerges, SI_{dp} is nil [56]. Otherwise, cumulated shading intensity is the average daily shading intensity since emergence weighted the number of days since emergence [57].

1.1.2.6.3 Light interception by the whole plant (PARi), by the plant summit (PARis), below plant base (PARib)

The principle for calculating the relative proportion of light intercepted by the whole plant (PARi) [58]-[68], by the plant summit (PARis) [70]-[73], and below the plant base (PARib) [75]-[79] depending on plant-status and on input values relative to input ranges accepted by the metamodels is the same as for PARa and SID. Except for ensuring that the outputs are in [0,1] MJ MJ^{-1} [69][74][80], no further transformation is needed. The only exception is PARi which can be readjusted if its sum over all crop and weed plants exceeds 1 (section 1.1.2.7.2).

1.1.2.7 Aggregated outputs (for calculating weed-impact indicators)

1.1.2.7.1 Crop and weed cover

Crop and weed cover are the relative light intercept by crop and weed plants, respectively. They are proxies for rain interception by crop and weed plants, and are used to calculate weed contribution to reducing soil erosion etc.
Crop cover is the relative light intercepted by plants, weighted by plant base area, summed over all plants of all crop species and emergence cohorts, and divided by the field sample area [81]. The multiplication of field dimensions by 100 is needed to convert them from m to cm, to be consisted with plant width which is in cm.
The same principle is used for weed cover [82].

1.1.2.7.2 Light arriving on soil surface in field (PARib_field)

The proportion of incident light arriving on soil surface in the field (PARib_field) is 1 minus the crop and weed cover [83]. As the metamodel predicts the light intercepted by each plant individually (section 1.1.2.6.3) instead of simultaneously as in the process-based light-interception submodel (Munier-Jolain et al., 2013), the variables summing PARi values can exceed the biologically correct bounds, i.e. PARib_field can be negative. In that case, crop and weed cover [84] as well as light interception per plant [85] must be readjusted, whereas light incidence on soil surface must be put to 0 [86].

1.1.3 Equations for detailed algorithm

1.1.3.1 Daily steps

Table 1. Detailed steps of daily algorithm for predicting light-interception variables from metamodels.

Distances refer to the centres of plants or voxels.
d Julian day
∀p means for all plants p of all emergence cohort c of all species s
Target-plant variables are in blue
Canopy (cover) variables are in green
Tables and functions relative to metamodel are in red
Light-interception output variables are in black bold

	When	Equation	Meaning of variables
	Global canopy variables		
[1]	∀d	$LP_d = 0$ $\forall p\ LP_d = \max(LP_d, H_{pd}, W_{pd}/2)$	LP_d (cm) largest plant in field H_{pd} (cm) and W_{pd} (cm) are plant height and width, respectively
[2]	∀d If plants have emerged or died today	$NP_d = \sum_p 1/(dimx \cdot dimy)$	NP_d total number of plants (crops and weeds) per m² dimx (m) and dimy (m) are the dimensions of the field area sample
	Environmental conditions		
[3]	∀d	$PAR_d = (1 - albedo) \cdot ppa \cdot radiation_d$	PAR_d incident photosynthetically active radiation (MJ cm^{-2}) above canopy $Radiation_d$ incident radiation above canopy (MJ/cm²) albedo = 0.05 MJ MJ^{-1}, radiation loss due to reflection ppa = 0.48 MJ MJ^{-1}, proportion of photosynthetically active incident radiation
[4]	∀d	If d < 172 Then NDS_d =355 - d Else if d > 355 then d = 710-d;	NDS_d days until or since summer solstice
	Determine local neighbourhood of target plant		
[5]	∀d,p	$ID_{pd} = \min(70,\ LP_d + W_{pd}/2)$	ID_{pd} (cm) is the maximum influence distance from the plant center
[6]	∀d,p	$DNN_{pd} = 100 \cdot \min(dimx,dimy)$ $EA_{pd} = 0$ $CH_{pd} = CA_{pd} = CLA_{pd} = CH50_{pd} = CK_{pd} = CD_{pd} = 0$ $NN_{pd} = 0$	DNN_{pd} (cm) distance to nearest neighbour EA_{pd} (cm²) explored area CH_{pd}, CA_{pd}, CLA_{pd}, $CH50_{pd}$, CK_{pd}, CD_{pd} average plant height, area, leaf area, median leaf area height, extinction coefficient and density of canopy surrounding plant p

			NN_{pd} number of neighbour plants in EA_{pd}
[7]	$\forall d,p$ If $NP_d > 1/(dimx \cdot dimy)$ $\forall x,y/\ DTP_{pxy} \leq ID_p + vs \cdot \cos(\Pi/4)$ and $((DTP_{pxy} \leq W_p/2$ or $DTP_{pxy} \leq DNN_p + 2 \cdot vs \cdot \cos(\Pi/4))$	$EA_{pd} = EA_{pd} + vs^2$ $DTP_{pxy} = vs \cdot \sqrt{(x_p^2 - x^2) + (y_p^2 - y^2)}$	vs (cm) voxel edge size Plant p is located in voxel (x_p, y_p) DTP_{pxy} (cm) distance from voxel (x,y) to target plant p
[8]		$\forall p' \neq p/(x_{p'}, y_{p'}) = (x,y)$ $DNN_p = \min(DNN_{pd}, DTP_{pxy})$ $CH_{pd} = CH_{pd} + H_{p'd}/(1+ DTP_{pxy})$ $CA_{pd} = CA_{pd} + \Pi\ (W_{p'd}/2)^2 / (1+ DTP_{pxy})$ $CLA_{pd} = CLA_{pd} + LA_{p'd}/(1+ DTP_{pxy})$ $CH50_{pd} = CH50_{pd} + H_{p'd}\ RH50_{p'd} /(1+ DTP_{pxy})$ $CK_{pd} = CK_{pd} + K_{p'd}/(1+ DTP_{pxy})$ $CD_{pd} = CD_{pd} + 1$ $NN_{pd} = NN_{pd} + 1/(1+ DTP_{pxy})$	$LA_{p'd}$ (cm^2) total plant leaf area $K_{p'd}$ species extinction coefficient $RH50_{p'd}$ (cm cm^{-1})relative plant height below which half of its leaf area is located
[9]	$\forall d,p$ If $DNN_{pd} > ID_{pd}$	$CH_{pd} = CA_{pd} = CLA_{pd} = CH50_{pd} = CK_{pd} = 0$ $CD_{pd} = 1/(dimx \cdot dimy)$ $DNN_{pd} = 100 \cdot \min(dimx, dimy)$	
[10]	$\forall d,p$ If $DNN_{pd} \leq ID_{pd}$	$CH_{pd} = CH_{pd} / NN_{pd}$ $CA_{pd} = CH_{pd} / NN_{pd}$ $CLA_{pd} = CLA_{pd} / NN_{pd}$ $CH50_{pd} = CH50_{pd} / NN_{pd}$ $CK_{pd} = CK_{pd} / NN_{pd}$ $CD_{pd} = CD_{pd}/EA_{pd} + 1/(dimx \cdot dimy)$	
[11]	$\forall d,p$	If $CH_{pd} > 0$ Then $OH_{pd} = 100\ (H_{pd} - CH_{pd})/\ CH_{pd}$ Else $OH_{pd} = 100$	OH_{pd} over heading, i.e. relative difference between target plant height and canopy height
	Predictions with the different metamodels		
[12]	$\forall d,p$	$V_{pd} = \Pi \cdot H_{pd} \cdot W_{pd}/2$	V_{pd} (cm^3) plant volume
[13]	$\forall d,p$	Small single plants X_i = {latitude, d, H_{pd}, W_{pd}, LA_{pd}, K_{pd}, $RH50_{pd}$, b_{pd}}	X_i inputs for metamodels CR_{pd} (m) no neighbour plants beyond this distance, fixed at upperBoundsover[CR] upperBoundsover[X_i] maximum input value accepted for input X_i in the *cover* metamodel
[14]		Large single plants X_i = {latitude, d, dimx, dimy, vs, H_{pd}, W_{pd}, LA_{pd}, K_{pd}, $RH50_{pd}$, b_{pd}}	
[15]		Plants inside canopy (cover) X_i = {latitude, d, H_{pd}, W_{pd}, LA_{pd}, K_{pd}, $RH50_{pd}$, b_{pd}, CD_{pd}, CR_{pd}, CH_{pd}, CA_{pd}, CLA_{pd}, CK_{pd},, $CH50_{pd}$}	
	Predictions for single plants		
[16]	$\forall d,p$	If LA_{pd} < lowerBoundsSmallSingle[LA] Then $PARa\_s\_cm^3_{pd} = K_{pd} \cdot\ LA_{pd} / V_{pd}$	lowerBoundsSmallSingle [X_i] is the minimum input value accepted for input X_i in the *small single plant* metamodel
[17]		Else if H_{pd} < lowerBoundsSmallSingle[H]	

		Or W_{pd} < lowerBoundsSmallSingle[W] Then **PARa_s_cm³$_{pd}$** = 1/ V_{pd}	**PARa_s_cm³$_{pd}$** relative photosynthetically active radiation ($MJ \cdot MJ^{-1} \cdot cm^{-3}$) absorbed by plant if single lowerBoundsSingle [X_i] is the minimum input value accepted for input X_i in the *single plant* metamodel smallSingleMetamodel(Y, X_i) predicts output Y from X_i inputs for small single plants, considering a voxel edge size of 4 cm singleMetamodel(Y, X_i) predicts output Y from X_i inputs for large single plants, using vs as voxel edge size
[18]		Else if LA_{pd} < lowerBoundsSingle[LA] Then **PARa_s_cm³$_{pd}$** = smallSingleMetamodel (PARa, X_i)/4^3	
[19]		Else **PARa_s_cm³$_{pd}$** = singleMetamodel (PARa, X_i)/vs^3	
[20]	∀d,p	if LA_{pd} < lowerBoundsSingle[LA] and W_{pd} < upperBoundsSmallSingle[W] then **SID_s$_{pd}$** = smallSingleMetamodel (SID, X_i)	upperBoundsSmallSingle [X_i] is the maximum input value accepted for input X_i in the *small single plant* metamodel **SID_s$_{pd}$** daily shading intensity (MJ/MJ) of plant if single
[21]		else **SID_s$_{pd}$** = SingleMetamodel (SID, X_i)	
[22]	∀d,p If a herbicide is applied tomorrow	If LA_{pd} < lowerBoundsSingle[LA] And H_{pd} < 1.5 upperBoundsSmallSingle[H] then **PARi_s$_{pd}$** = smallSingleMetamodel (PARi, X_i)	**PARi_ s$_{pd}$** relative light (MJ/MJ) intercepted by plant if single; proxy for rate of herbicide intercepted by plant
[23]		else **PARi _s$_{pd}$** = SingleMetamodel (PARi, X_i)	
[24]	∀d,p If a herbicide is applied tomorrow	**PARix _s$_{pd}$** = 1	**PARis_ s$_{pd}$** relative light (MJ/MJ) intercepted by plant summit if single, proxy for probability of plant receiving any herbicide
[25]	∀d,p	If LA_{pd} < lowerBoundsSingle[LA] And W_{pd} < upperBoundsSmallSingle[W]/2 then **PARib_s$_{pd}$** = smallSingleMetamodel (PARib, X_i)	**PARib_ s$_{pd}$** relative light (MJ/MJ) arriving below plant base if single; , proxy for seed rain proportion arriving on soil surface below plant base
[26]		else **PARib _s$_{pd}$** = SingleMetamodel (PARib, X_i)	
	Determine whether target plant can be considered as single		
[27]	∀d,p	If NN_{pd} = 0 Or DNN_p > ID_{pd} Or CD_{pd} < lowerBoundsCover[CD] Then singlePlant = true	lowerBoundsCover[X_i] is the minimum input value accepted for input X_i in the *cover* metamodel NN_{pd} now in m
[28]		Else if NN_{pd} > 1.6 m and NN_{pd} $OH_{pd} \geq 100$ Or NN_{pd} > 1.6 m and NDS_d /(1+NN_{pd}) < 92 Or NN_{pd} > 1.6 m and |latitude| /(1+NN_{pd}) < 8 Or $NN_{pd} \in$]1.2, 1.6 m] and W_{pd} /(1+NN_{pd}) < 32 cm Then singlePlant = true	
[29]		Else singlePlant = false	
	Particular case of mature leaf-less target plants or canopies		
[30]	∀d,p	If LA_{pd} = 0 and $STAGE_{pd}$ >= FLOWER Then LA_{pd} = lowerBoundsCover[LA]	$STAGE_{pd}$ is the growth stage of the target plant
[31]		If CLA_{pd} = 0 and CH_{pd} > 0 Then CLA_{pd} = lowerBoundsCover[CLA]	

	Predictions, depending on whether plants are single or in a canopy		
[32]	∀d,p	If singlePlant = true Then $\mathbf{PARa\_cm^3_{pd}} = \mathbf{PARa\_s\_cm^3_{pd}}$	$\mathbf{PARa\_cm^3_{pd}}$ relative photosynthetically active radiation (MJ MJ^{-1} cm^{-3}) absorbed by plant, taking account of whether it is single or in a canopy coverMetamodel (Y, X_i) predict output Y from X_i inputs for plants inside a canopy, with a 4-cm voxel edge size upper99percentile [X_i] is 99% percentile of X_i input values used to build the *cover* metamodel
[33]		Else if LA_{pd} < lowerBoundsCover[LA] Or CLA_{pd} < lowerBoundsCover[CLA] Then $\mathbf{PARa\_cm^3_{pd}}$ = (CLA_{pd} · coverMetamodel (PARa, X_i) / 4^3 + 1 · $\mathbf{PARa\_s\_cm^3_{pd}}$) / ($CLA_{pd}$ + 1)	
[34]		Else if CLA_{pd} / (DNN_p + 1) > upper99percentile[CLA] Then $\mathbf{PARa\_cm^3_{pd}}$ = 0.419 / 4^3	
[35]		Else if CK_{pd} / (DNN_p + 1) > upper99percentile[CK] Then $\mathbf{PARa\_cm^3_{pd}}$ = 0.386/ 4^3	
[36]		Else if $CH50_{pd}$ / (DNN_p + 1) > upper99percentile[CH50] Then $\mathbf{PARa\_cm^3_{pd}}$ = 0.310/ 4^3	
[37]		Else if CA_{pd} / (DNN_p + 1) > upper99percentile[CA] Then $\mathbf{PARa\_cm^3_{pd}}$ = 0.414/ 4^3	
[38]		Else if CH_{pd} / (DNN_p + 1) > upper99percentile[CH] Then $\mathbf{PARa\_cm^3_{pd}}$ = 0.174/ 4^3	
[39]		Else if CD_{pd} > upperBoundsCover[CD] Then $\mathbf{PARa\_cm^3_{pd}}$ = 0.0113/ 4^3	
[40]		Else $\mathbf{PARa\_cm^3_{pd}}$ = coverMetamodel (PARa, X_i) / 4^3	
[41]	∀d,p	$\mathbf{PARa\_cm^3_{pd}}$ = min($\mathbf{PARa\_cm^3_{pd}}$, = K_{pd}· LA_{pd} / V_{pd})	
[42]		$\mathbf{PARa\_cm^3_{pd}}$ = min($\mathbf{PARa\_cm^3_{pd}}$, 1) $\mathbf{PARa\_cm^3_{pd}}$ = max($\mathbf{PARa\_cm^3_{pd}}$, 0)	
[43]	∀d,p	$\mathbf{PARa_{pd}} = \mathbf{PARa\_cm^3_{pd}}\ PAR_d\ V_{pd}$	$\mathbf{PARa_{pd}}$ photosynthetically active radiation (MJ $plant^{-1}$) absorbed by plant
[44]	∀d	$\mathbf{TPARa_d} = \sum_p \mathbf{PARa_{pd}}$ $Ratio_d$ = $\mathbf{TPARa_d}$ / (PAR_d dimx dimy 100 100)	$\mathbf{TPARa_d}$ total photosynthetically active radiation (MJ) absorbed by all plants $Ratio_d$ ratio (MJ/MJ) of predicted absorbed photosynthetically active radiation vs incident photosynthetically active radiation in field
[45]	∀d,p If $Ratio_d$ > 1	$\mathbf{PARa_{pd}} = \mathbf{PARa_{pd}} / Ratio_d$	
[46]	∀d,p	If singlePlant = true Then $\mathbf{SID_{pd}} = \mathbf{SID\ \_s_{pd}}$	$\mathbf{SID_{pd}}$ daily shading intensity (MJ/MJ) of plant, taking account of whether it is single or in a canopy
[47]		Else if LA_{pd} < lowerBoundsCover[LA] Or CLA_{pd} < lowerBoundsCover[CLA] Then $\mathbf{SID}\ _{pd}$ = (CLA_{pd} · coverMetamodel (SID, X_i) + 1 · $\mathbf{SID\ \_s_{pd}}$) / (CLA_{pd} + 1)	
[48]		Else if CLA_{pd} / (DNN_p + 1) > upper99percentile[CLA] Then $\mathbf{SID}\ _{pd}$ = 0.960	

[49]		Else if CK_{pd} / (DNN_p + 1) > upper99percentile[CK] Then **SID** $_{pd}$ = 0.960	
[50]		Else if CW_{pd} / (DNN_p + 1) > upper99percentile[CW] Then **SID** $_{pd}$ = 0.953	
[51]		Else if $CH50_{pd}$ / (DNN_p + 1) > upper99percentile[CH50] Then **SID** $_{pd}$ = 0.944	
[52]		Else if CH_{pd} / (DNN_p + 1) > upper99percentile[CH] Then **SID** $_{pd}$ = 0.949	
[53]		Else if CD_{pd} / (DNN_p + 1) > upperBoundsCover [CD] Then **SID** $_{pd}$ = 1	
[54]		Else **SID** $_{pd}$ = coverMetamodel (SID, X_i)	
[55]	∀d,p	**SID** $_{pd}$ = min(**SID** $_{pd}$, 1) **SID** $_{pd}$ = max(**SID** $_{pd}$, 0)	
[56]	∀d,p	If NDE_{dp} = 0 Then $\mathbf{SI}_{pd}$ = 0	NDE_{dp} number of days since plant emerged $\mathbf{SI}_{pd}$ cumulated shading intensity since plant emergence (MJ days MJ^{-1} day^{-1})
[57]		Else $\mathbf{SI}_{pd} = \frac{\sum_{d'=0}^{d}\left(d' \cdot SID_{pd'}\right)}{\sum_{d'=0}^{d} d'}$	
[58]	∀d,p If a herbicide is applied today	If singlePlant = true Then $\mathbf{PARi}_{pd}$ = $\mathbf{PARi\_s}_{pd}$	$\mathbf{PARi}_{pd}$ relative light (MJ/MJ) intercepted by plant, taking account of whether it is single or in a canopy
[59]		Else if LA_{pd} < lowerBoundsCover[LA] Or CLA_{pd} < lowerBoundsCover[CLA] Then $\mathbf{PARi}_{pd}$ = (CLA_{pd} · coverMetamodel (PARi, X_i) + 1 · $\mathbf{PARi\_s}_{pd}$) / (CLA_{pd} + 1)	
[60]		Else if H_{pd} > upperBoundsCover [H] Then $\mathbf{PARi}_{pd}$ = 0.006498	
[61]		Else if CD_{pd} > upperBoundsCover [CD] Then $\mathbf{PARi}_{pd}$ = 0.000009	
[62]		Else if H_{pd} > upperBoundsCover [W] Then $\mathbf{PARi}_{pd}$ = 0.00409	
[63]		Else if CLA_{pd} / (DNN_p + 1) > upper99percentile[CLA] Then $\mathbf{PARi}_{pd}$ = 0.00124	
[64]		Else if CK_{pd} / (DNN_p + 1) > upper99percentile[CK] Then $\mathbf{PARi}_{pd}$ = 0.00148	
[65]		Else if CA_{pd} / (DNN_p + 1) > upper99percentile[CA]	

		Then $\mathbf{PARi_{pd}} = 0.00165$	
[66]		Else if CH_{pd} / (DNN_p + 1) > upper99percentile[CH] Then $\mathbf{PARi_{pd}} = 0.00133$	
[67]		Else if $CH50_{pd}$ / (DNN_p + 1) > upper99percentile[CH50] Then $\mathbf{PARi_{pd}} = 0.00480$	
[68]		Else $\mathbf{PARi_{pd}}$ = coverMetamodel (PARi, X_i)	
[69]	∀d,p	$\mathbf{PARi_{pd}} = \min(\mathbf{PARi_{pd}}, 1)$ $\mathbf{PARi_{pd}} = \max(\mathbf{PARi_{pd}}, 0)$	
[70]	∀d,p If a herbicide is applied today	If singlePlant = true Then $\mathbf{PARis_{pd}} = \mathbf{PARis\_s_{pd}}$	$\mathbf{PARis_{pd}}$ relative light (MJ/MJ) intercepted by plant at summit, taking account of whether it is single or in a canopy
[71]		Else if LA_{pd} < lowerBoundsCover[LA] Or CLA_{pd} < lowerBoundsCover[CLA] Then $\mathbf{PARis_{pd}}$ = (CLA_{pd} · coverMetamodel (PARis, X_i) + 1 · $\mathbf{PARis\_s_{pd}}$) / (CLA_{pd} + 1)	
[72]		Else if CD_{pd} > upperBoundsCover [CD] Then $\mathbf{PARis_{pd}} = 0.0333$	
[73]		Else $\mathbf{PARis_{pd}}$ = coverMetamodel (PARis, X_i)	
[74]	∀d,p	$\mathbf{PARis_{pd}} = \min(\mathbf{PARis_{pd}}, 1)$ $\mathbf{PARis_{pd}} = \max(\mathbf{PARis_{pd}}, 0)$	
[75]	∀d,p	If singlePlant = true Then $\mathbf{PARib_{pd}} = \mathbf{PARib\_s_{pd}}$	$\mathbf{PARib_{pd}}$ relative light (MJ/MJ) arriving on soil surface, below plant base, taking account of whether it is single or in a canopy
[76]		Else if LA_{pd} < lowerBoundsCover[LA] Or CLA_{pd} < lowerBoundsCover[CLA] Then $\mathbf{PARib_{pd}}$ = (CLA_{pd} · coverMetamodel (PARib, X_i) + 1 · $\mathbf{PARib\_s_{pd}}$) / (CLA_{pd} + 1)	
[77]		Else if $CH50_{pd}$ / (DNN_p + 1) > upper99percentile[CH50] Then $\mathbf{PARib_{pd}} = 0.00179$	
[78]		Else if CD_{pd} > upperBoundsCover [CD] Then $\mathbf{PARib_{pd}} = 0.\ 00501$	
[79]		Else $\mathbf{PARibs_{pd}}$ = coverMetamodel (PARib, X_i)	
[80]	∀d,p	$\mathbf{PARib_{pd}} = \min(\mathbf{PARib_{pd}}, 1)$ $\mathbf{PARib_{pd}} = \max(\mathbf{PARib_{pd}}, 0)$	
	Field-scale light interception variables		
[81]	∀d	$\mathbf{cropCover_d} = \cdot \sum_{p/s\in crop} \left(PARi_p \cdot \Pi \cdot \left(\frac{W_{pd}}{2}\right)^2 \right)$ / (dimx 100 dimy 100)	$\mathbf{cropCover_d}$ relative light (MJ cm² MJ^{-1} cm^{-2}) intercepted by crop cover, proxy for rain interception by crop cover

[82]		**weedCover**$_{\mathbf{d}}$ = $\cdot \sum_{p/s \in weed} \left(PARi_p \cdot \Pi \cdot \left(\frac{W_{pd}}{2} \right)^2 \right)$ / (dimx 100 dimy 100)	**weedCover**$_{\mathbf{d}}$ relative light (MJ cm² MJ^{-1} cm^{-2}) intercepted by crop cover, proxy for rain interception by weed cover
[83]	∀d	**PARib_field**$_{\mathbf{d}}$ = 1 - cropCover$_d$ - weedCover$_d$	**PARib_field**$_{\mathbf{d}}$ relative light (MJ/MJ) arriving on soil surface in average in field, proxy for seed rain proportion arriving on soil surface
[84]	∀d If **PARIb_field**$_{\mathbf{d}}$ < 0	**cropCover**$_{\mathbf{d}}$ = **cropCover**$_{\mathbf{d}}$ / (1 - **PARIb_field**$_{\mathbf{d}}$) **weedCover**$_{\mathbf{d}}$ = **weedCover**$_{\mathbf{d}}$ / (1 - **PARIb_field**$_{\mathbf{d}}$)	
[85]		∀p **PARi**$_{\mathbf{pd}}$ = **PARi**$_{\mathbf{pd}}$ / (1 - **PARIb_field**$_{\mathbf{d}}$)	
[86]		**PARib_field**$_{\mathbf{d}}$ = 0	

1.1.3.2 List of variables

Table 2. List of variables. Indices d and p indicate that variables refer to day and plant p, respectively

Variable	Unit	Meaning
(x_p, y_p)		Plant p is located in voxel (x_p, y_p)
albedo	MJ MJ^{-1}	Radiation loss due to reflection (0.05 MJ MJ^{-1})
b_{pd}		Shape parameter for leaf area distribution along plant height
CA_{pd}	cm^2	Average plant area (i.e. Π··width/2) of canopy surrounding plant p
CD_{pd}	Plants m^{-2}	Local plant density (including target plant) of canopy where plant p is located
$CH50_{pd}$	cm	Average plant median leaf height (height below which half of the leaf area is located) of canopy surrounding plant p
CH_{pd}	cm	Average plant height of canopy surrounding plant p
CK_{pd}		Average plant extinction coefficient of canopy surrounding plant p
CLA_{pd}	cm^2	Average plant leaf area of canopy surrounding plant p
coverMetamodel (Y, X_i)		Metamodel function which predicts output Y from X_i inputs for plants inside a canopy, with a 4-cm voxel edge size
$cropCover_d$	MJ cm^2 MJ^{-1} cm^{-2}	Relative light intercepted by crop cover, proxy for rain interception by crop cover
CR_{pd}	m	No neighbour plants beyond this distance, fixed at upperBoundsover[CR]
d	Julian day	day
dimx and dimy	m	Dimensions of the simulated field area sample, input chosen by user
DNN_{pd}	cm	Distance to nearest neighbour plant
DTP_{pxy}	cm	Distance from voxel (x,y) to target plant p
EA_{pd}	cm^2	Area explored during search for neighbour plants
H_{pd}	cm	Plant height
ID_{pd}	cm	Neighbour plants located further than this distance from target-plant center do not influence target plant
K_{pd}		Extinction coefficient of plant species
LA_{pd}	cm^2	Total leaf area of plant
latitude	°	Latitude of simulated field
lowerBoundsCover$[X_i]$		Minimum input value accepted for input X_i in the *cover* metamodel
lowerBoundsSingle $[X_i]$		Minimum input value accepted for input X_i in the *single plant* metamodel
lowerBoundsSmallSingle$[X_i]$		Minimum input value accepted for input X_i in the *small single plant* metamodel
LP_d	cm	Largest plant in field
NDE_{dp}	days	Number of days since plant emerged
NDS_d	days	Days until or since summer solstice
NN_{pd}	plants	Number of neighbour plants in EA_{pd}
NP_d	Plants m^{-2}	Total number of plants (crops and weeds) per m^2
OH_{pd}	cm cm^{-1}	Over heading, i.e. relative difference between target plant height and canopy height
p		Target plant, of emergence cohort c of species s
$PARa\_cm^3_{pd}$	MJ MJ^{-1} cm^{-3}	Relative photosynthetically active radiation (absorbed by plant, taking account of whether it is single or in a canopy
$PARa\_s\_cm^3_{pd}$	MJ·MJ^{-1}·cm^{-3}	Relative photosynthetically active radiation absorbed by plant if single
$PARa_{pd}$	MJ $plant^{-1}$	Photosynthetically active radiation absorbed by plant
PAR_d	MJ cm^{-2}	Incident photosynthetically active radiation above canopy
$PARi\_s_{pd}$	MJ MJ^{-1}	Relative light intercepted by plant if single
$PARib\_s_{pd}$	MJ MJ^{-1}	Relative light arriving below plant base if single, proxy for seed rain proportion arriving on soil surface below plant base
$PARib\_field_d$	MJ MJ^{-1}	Relative light arriving on soil surface in average in field, proxy for seed rain proportion arriving on soil surface in field

$PARib_{pd}$	MJ MJ^{-1}	Relative light arriving on soil surface, below plant base, taking account of whether it is single or in a canopy; proxy for seed rain proportion arriving on soil surface below plant base
$PARi_{pd}$	MJ MJ^{-1}	Relative light intercepted by plant, taking account of whether it is single or in a canopy, proxy for rate of herbicide intercepted by plant
$PARis\_s_{pd}$	MJ MJ^{-1}	Relative light intercepted by plant summit if single, proxy for probability of plant receiving any herbicide
$PARis_{pd}$	MJ MJ^{-1}	Relative light intercepted by plant at summit, taking account of whether it is single or in a canopy, proxy for probability of plant receiving any herbicide
ppa	MJ MJ^{-1}	Proportion of photosynthetically active incident radiation (0.48 MJ MJ^{-1})
$Radiation_d$	MJ cm^{-2}	Incident radiation above canopy, input from weather station
$Ratio_d$	MJ MJ^{-1}	Ratio of predicted absorbed photosynthetically active radiation vs incident photosynthetically active radiation in field
$RH50_{pd}$	cm cm^{-1}	Relative plant height below which half of its leaf area is located
SID_s_{pd}	MJ MJ^{-1}	Daily shading intensity of plant if single
SID_{pd}	MJ MJ^{-1}	Daily shading intensity of plant, taking account of whether it is single or in a canopy
singleMetamodel(Y, X_i)		Metamodel function which predicts output Y from X_i inputs for large single plants, using vs as voxel edge size
SI_{pd}	MJ days MJ^{-1} day^{-1}	Cumulated shading intensity since plant emergence
smallSingleMetamodel(Y,X_i)		Metamodel function which predicts output Y from X_i inputs for small single plants, considering a voxel edge size of 4 cm
$STAGE_{pd}$		Growth stage of the target plant {COTYLEDON, SEEDLING, VEGETATIVE, FLOWER, MATURE, DEAD}
$TPARa_d$	MJ MJ^{-1}	Total photosynthetically active radiation absorbed by all plants
upper99percentile [X_i]		99% percentile of X_i input values used to build the *cover* metamodel
upperBoundsCover [X_i]		Maximum input value accepted for input X_i in the *cover* metamodel
upperBoundsSmallSingle[X_i]		Maximum input value accepted for input X_i in the *small single plant* metamodel
V_{pd}	cm^3	Plant volume
vs	cm	Voxel edge size (input chosen by user)
$weedCover_d$	MJ cm^2 MJ^{-1} cm^{-2}	Relative light intercepted by crop cover, proxy for rain interception by weed cover
W_{pd}	cm	Plant width
X_i		Inputs for metamodels For *small single metamodel*: latitude, d, H_{pd}, W_{pd}, LA_{pd}, K_{pd}, $RH50_{pd}$, b_{pd} For *large single metamodel*: latitude, d, dimx, dimy, vs, H_{pd}, W_{pd}, LA_{pd}, K_{pd}, $RH50_{pd}$, b_{pd} For *cover metamodel*: latitude, d, H_{pd}, W_{pd}, LA_{pd}, K_{pd}, $RH50_{pd}$, b_{pd}, CD_{pd}, CR_{pd}, CH_{pd}, CA_{pd}, CLA_{pd}, CK_{pd},, $CH50_{pd}$
Y		Metamodel outputs per plant: PARa (MJ MJ^{-1} $voxel^{-1}$) relative photosynthetically active radiation absorbed by plant, with voxel edge size = 4 cm, vs, 4 cm for small single, single and cover metamodels, respectively SID (MJ MJ^{-1}) daily shading intensity PARi (MJ MJ^{-1}) relative light intercepted by plant PARis (MJ MJ^{-1}) relative light intercepted by plant summit PARib (MJ MJ^{-1}) relative light arriving below plant base

1.2 Modifications to increase simulation speed

1.2.1 The nominal version: always using local canopy variables

See section 1.1

1.2.2 Using canopy variables averaged over whole field at high plant densities

1.2.2.1 Principle

To increase simulation speed, the algorithm presented in section 1.1 was modified when plant densities in the field exceed 500 plants/m². Instead of calculating canopy variables of each target plants from its closest neighbours, canopy variables are calculated once a day from the whole field population. The distance to the nearest neighbour is only calculated if plants have emerged or died since the previous day. If the distance to the nearest neighbours exceeds the influence distance, the plant is considered to be single; otherwise the average canopy variables are used for the metamodels.

1.2.2.2 Details

1.2.2.2.1 Average canopy variables

The average canopy plant height, area, leaf area, median leaf area height and extinction coefficient are calculated once a day, from all crop and weed plants presented that day [87].

1.2.2.2.2 Distance to nearest neighbour considering the maximum possible influence zone

If plants have emerged or died since the previous day, the distance to the nearest neighbour (considering the maximum possible influence zone) is recalculated. First, the distance is initialized at the maximum possible distance [88] (see section 1.1.2.3.1 for explanation). Then, voxels are searched clockwise, starting from the target plant, as long as the distance from the searched voxel to the target-plant center is less than the influence zone plus one round (Figure 3), and the distance is less than the distance to the nearest neighbour plus one round [89]. As for the influence zone, the additional round is to ensure that the search loop does not stop in a corner voxel while there are plants in closer voxels (Figure 3). If there are plants (other than the target plant) in the searched voxel, the distance to the nearest neighbour is updated [89].
In contrast to the fully local loop of section 1.1.2.3, no local canopy variables are calculated, and the search loops stops once the nearest neighbour was found.
After the loop, the newly calculated distance to the nearest neighbour is compared to the maximum influence distance. If it is indeed smaller than the influence distance, it is stored for future use; otherwise the initial value is reinstated [90]. This step is necessary because of the additional round outside the influence zone (Figure 3) which can sometimes retain a neighbour outside the influence zone.

1.2.2.2.3 Adapting canopy variables to target plant

If plants have emerged or died since the previous day, today's potential distance to the nearest neighbour (considering the maximum influence zone) has been recalculated (section 1.2.2.2.2) and is now used for today. Otherwise, the distance calculated in the past is used [91].
Each day, the influence distance is updated, to take account of today's target-plant width and today's size of the largest plant in the field [92]. This distance changes every day, and is then used to update the distance to the nearest neighbour and the local canopy variables, considering today's plant dimensions. If the potential distance to the nearest neighbour exceeds today's influence distance, then today's canopy variables are put to nil, today's canopy density is 1 for the whole field, and the actual distance to the nearest neighbour is put to its maximum possible value [93]. Otherwise, the global canopy variables are used for the target plant, the canopy density is the total field density, and the distance to the nearest neighbour remains unchanged [94].

1.2.2.2.4 Other steps

The rest of the equations of Table 1 remain unchanged.

1.2.3 Only using average canopy variables

The fastest version uses average canopy variables throughout the simulation, applying the principles of section 1.2.2 regardless of plant densities.

1.3 Details on the metamodels

1.3.1 Features common to all chaos-based metamodels

1.3.1.1 The outputs

Y	unit	Meaning
PARa	MJ MJ voxel^{-1}	photosynthetically active radiation per voxel absorbed by plant
SID	MJ MJ^{-1}	daily shading intensity of plant
PARi	MJ MJ^{-1}	relative light intercepted by plant
PARix	MJ MJ^{-1}	relative light intercepted by plant summit
PARib	MJ MJ^{-1}	Relative incident light below plant base

Caution: the voxel edge size varies with the metamodel type (section 1.3.2).

1.3.1.2 Calibrating inputs

Whatever the chaos-based metamodel, inputs are calibrated to fit into [-1,1], using the minimum and maximum accepted input values for each X_i lowerBounds [X_i] and upperBounds [X_i], respectively:

Calibrated X_i = X_i = -1 + 2 (X_i - lowerBounds [X_i]) / (upperBounds [X_i] - lowerBounds [X_i]))

1.3.1.3 Equations

Table 3. Modifications in the algorithm in case of total plant density exceeding 500 plants/m²

	When	Equation	Meaning of variables
[87]	∀d	$CH_d = \sum_p H_{pd} / \sum_p 1$ $CA_d = \Pi \sum_p \left(\frac{W_{pd}}{2}\right)^2 / \sum_p 1$ $CLA_d = \sum_p LA_{pd} / \sum_p 1$ $CH50_d = \sum_p \left(H_{pd} \cdot RH50_{pd}\right) / \sum_p 1$ $CK_d = \sum_p K_{pd} / \sum_p 1$	CH_d, CA_d, CLA_d, $CH50_d$, CK_d, average plant height, area, leaf area, median leaf area height, extinction coefficient
[88]	∀d,p If plants have emerged or died since the previous day	ID = 70 $DNN_{pd} = 100 \cdot \min(dimx,dimy)$	ID (cm) is the maximum influence distance from the plant center DNN_{pd} (cm) distance from center of target plant p to nearest neighbour inside influence zone of day d
[89]	∀d,p If plants have emerged or died since the previous day $\forall x,y / DTP_{pxy} \leq ID_p + vs \cdot \cos(\Pi/4)$ and $DTP_{pxy} \leq DNN_{pd} + vs \cdot \cos(\Pi/4)$	$DTP_{pxy} = vs \cdot \sqrt{\left(x_p^2 - x^2\right) + \left(y_p^2 - y^2\right)}$ $\forall p' \neq p / (x_{p'}, y_{p'}) = (x,y)$ $DNN_{pd} = \min(DNN_{pd}, DTP_{pxy})$	
[90]	∀d,p If plants have emerged or died since the previous day	If $DNN_{pd} < ID$ Then $DNN_p = DNN_{pd}$ else $DNN_p = 100 \min(dimx, dimy)$	DNN_p (cm) distance from center of target plant p to nearest neighbour if closer than 70 cm (valid until next time plants have emerged or died)
[91]	∀d,p If no plants have emerged or died since the previous day	$DNN_{pd} = DNN_p$	
[92]	∀d,p	$ID_{pd} = \min(70\ \ LP_d + W_{pd}/2)$	ID_{pd} (cm) is the maximum influence distance from the plant center today (varies with plant width and thus changes every day)
[93]	∀d,p If $DNN_{pd} > ID_{pd}$	$CH_{pd} = CA_{pd} = CLA_{pd} = CH50_{pd} = CK_{pd} = 0$ $CD_{pd} = 1/(dimx \cdot dimy)$ $DNN_{pd} = 100 \cdot \min(dimx,dimy)$	CH_{pd}, CA_{pd}, CLA_{pd}, $CH50_{pd}$, CK_{pd}, CD_{pd} average plant height, area, leaf area, median leaf area height, extinction coefficient and density of canopy surrounding plant p
[94]	∀d,p If $DNN_{pd} \leq ID_{pd}$	$CH_{pd} = CH_d$ $CA_{pd} = CA_d$ $CLA_{pd} = CLA_d$ $CH50_{pd} = CH50_d$ $CK_{pd} = CK_d$ $CD_{pd} = NP_d$	

1.3.2 The different chaos-based metamodels

See Table 2 for meaning of variables.

Table 4. Summary of chaos-based metamodels

	Small single plants	Large single plants	Plants in canopy
Function	smallSingleMetamodel(Y,X_i)	singleMetamodel(Y,X_i)	canopyMetamodel(Y,X_i)
Inputs	latitude, d, H_{pd}, W_{pd}, LA_{pd}, K_{pd}, $RH50_{pd}$, b_{pd}	latitude, d, dimx, dimy, vs, H_{pd}, W_{pd}, LA_{pd}, K_{pd}, $RH50_{pd}$, b_{pd}	latitude, d, H_{pd}, W_{pd}, LA_{pd}, K_{pd}, $RH50_{pd}$, b_{pd}, CD_{pd}, CR_{pd}, CH_{pd}, CA_{pd}, CLA_{pd}, CK_{pd},, $CH50_{pd}$
Accepted range			
Latitude (°)	0 66	-66 66	0 65.93
d	1 365	1 365	1 365
dimx (m)	constant	1.000261 4	constant
dimy (m)	constant	1.000226 3.999	constant
vs (cm)	Constant (4 cm)	1 20	Constant (cm)
H_{pd} (cm)	0.5 8	1.567 249.986	1.03 245.81
W_{pd} (cm)	0.5 7.998	1.071 200	1.21 199.99
LA_{pd} (cm²)	1 18.5	18.268 99996.49	26.69 79936.00
K_{pd}	0.0100 1.1	0.0101 1.099	0.010 1.10
$RH50_{pd}$ (cm cm^{-1})	0.01 1	0.01 1	0.011 1.00
b_{pd}	0.01 6	0.0101 5.999	0.011 6.00
CD_{pd} (plants/m²)	nil	nil	1.43 157332.66
CR_{pd} (m)	nil	nil	0.10 3.00
CH_{pd} (cm)	nil	nil	8.15 239.54
CA_{pd} (cm²)	nil	nil	87.35 20759.90
CLA_{pd} (cm²)	nil	nil	894.35 65581.83
CK_{pd}	nil	nil	0.047 0.61
$CH50_{pd}$ (cm)	nil	nil	1.98 115.83

1.4 Analysing and managing out-of-bound inputs

1.4.1 Principle

- Analyse relationship between input and output for out-of-bound area, using the data from the sensitivity analysis and focusing on those inputs with the strongest polynomial effect in the sensitivity analysis
- Fix output either to a minimum or maximum value, or link if to the out-of-bound input with a simple regression,
- If several rules for different inputs, start with the most important input based on sensitivity analysis
- If possible, use ecophysiological knowledge to determine rules

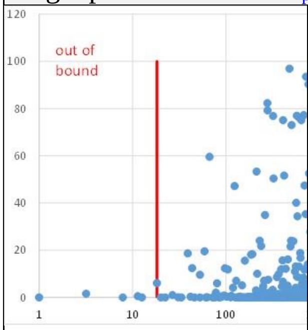
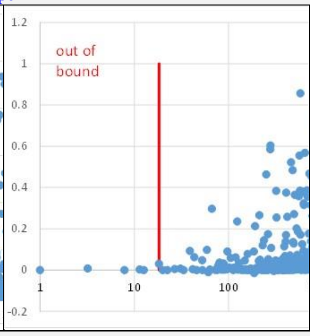
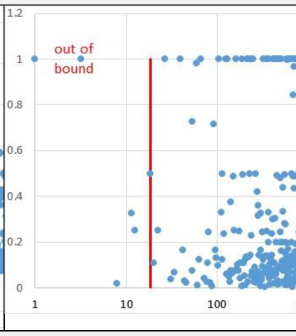
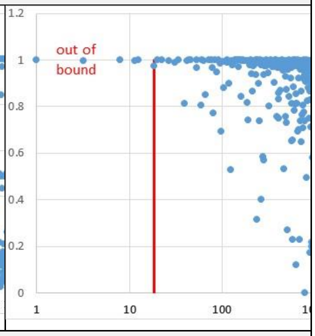
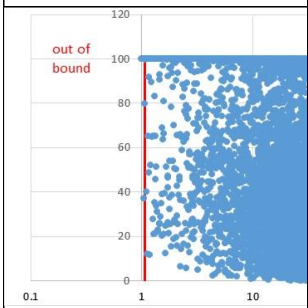
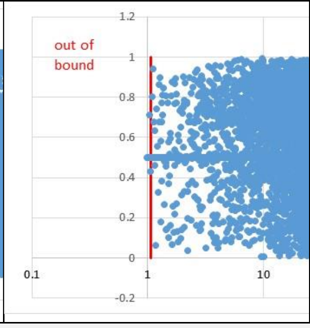
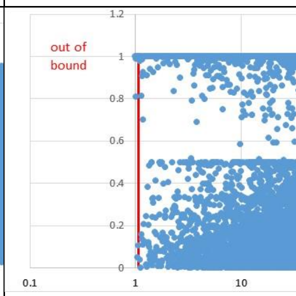
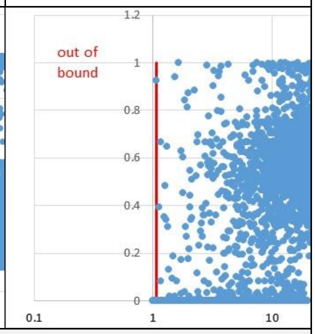
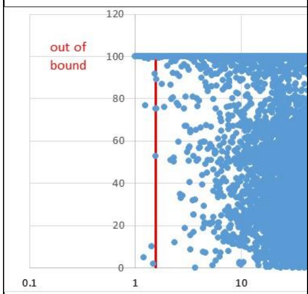
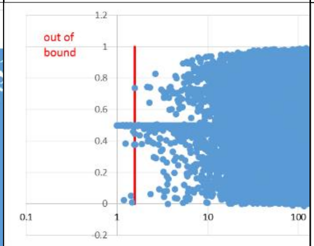
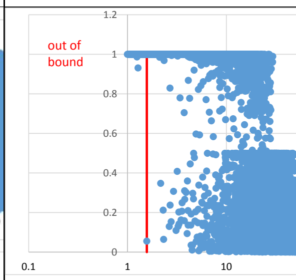
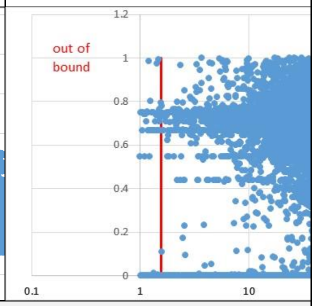
1.4.2 Equations

Detailed equations can be found in section 1.1.3.1.

1.4.3 Analysis of out-of-bound situations

1.4.3.1 Data set for large single plants

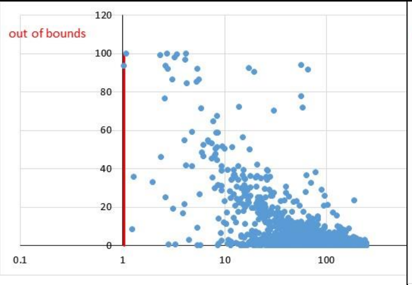
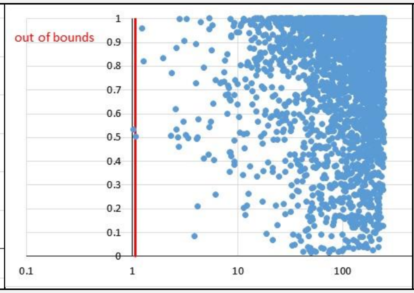
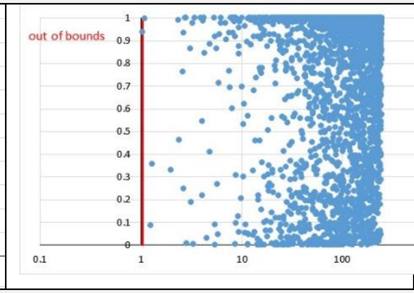
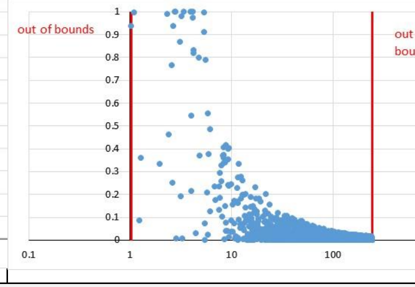
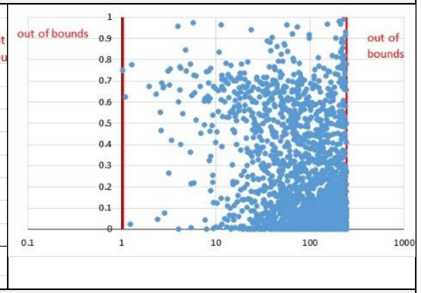
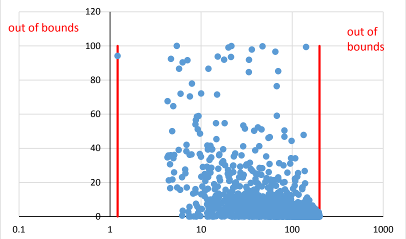
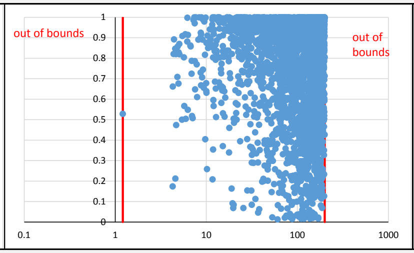
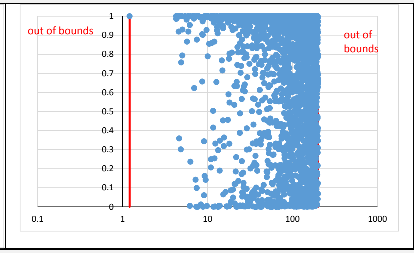
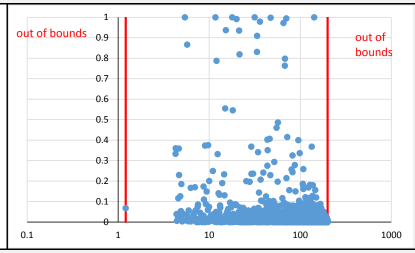
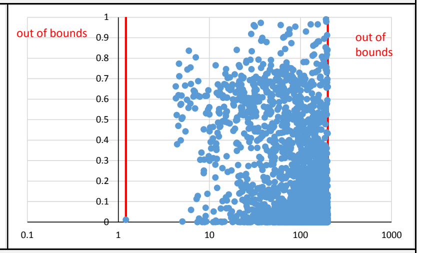
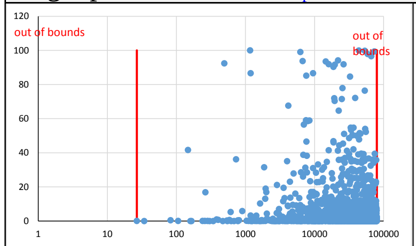
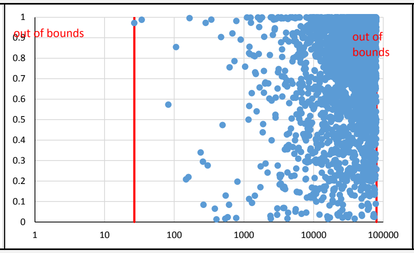
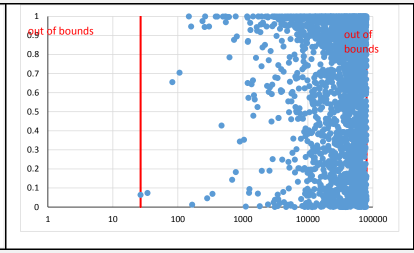
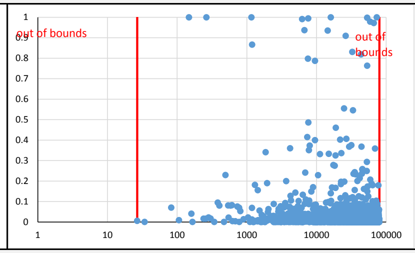
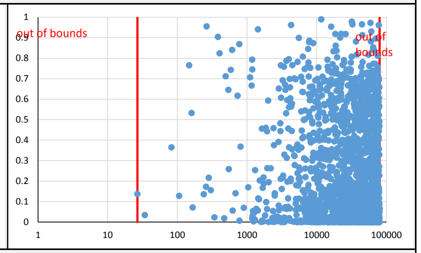
Table 5. Graphs of metamodel outputs (Y) vs. inputs (X_i) from the complete data set (before cleaning for metamodel construction), with a particular focus on out-of-bound conditions. Numbers are the average Y values simulated by FLORSYS for X_i < lower bound

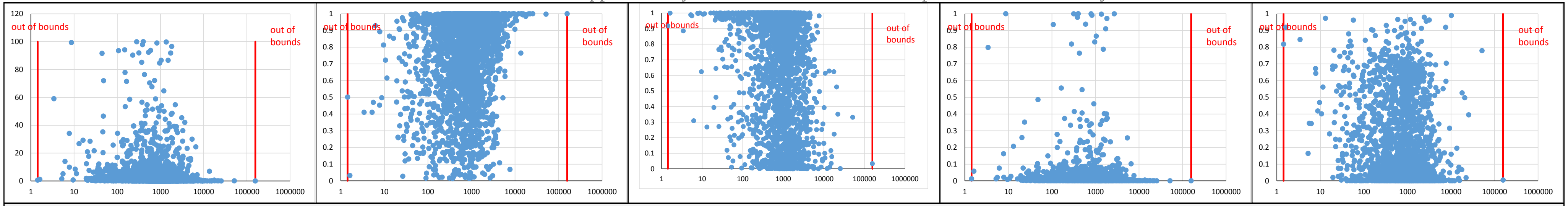
PARa per voxel (100 MJ MJ^{-1} $voxel^{-1}$)	SID (MJ MJ^{-1})	PARi plant (MJ MJ^{-1})	PARi base (MJ MJ^{-1})
Target plant leaf area LA_{pd}			
			
Target plant width W_{pd}			
93.09961733	0.511639583	0.828985083	0.07720375
			
Target plant height H_{pd}			
94.19534227		0.984662806	
			
Comments			
	The 0.5 shading for small plants is caused by an artefact in the voxelized canopy description, i.e. when plants are smaller than the voxel		

PARis was not analysed as it is always 1 for single plants.

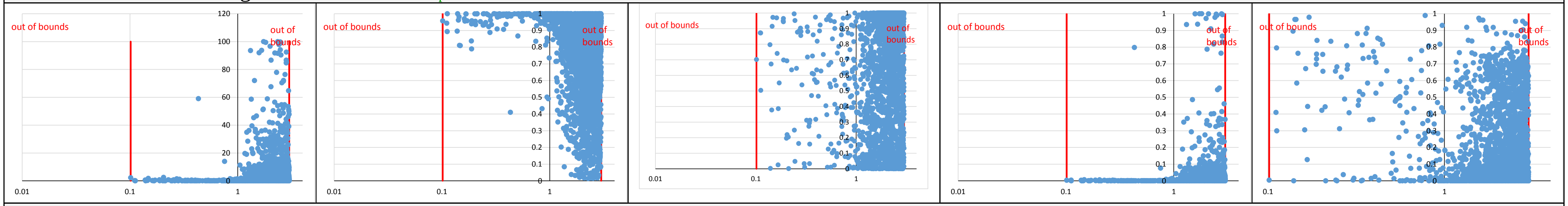
1.4.3.2 Data set for target plant in canopy

Table 6. Graphs of metamodel outputs (Y) vs. inputs (X_i) from the complete data set (before cleaning for metamodel construction), with a particular focus on out-of-bound conditions.

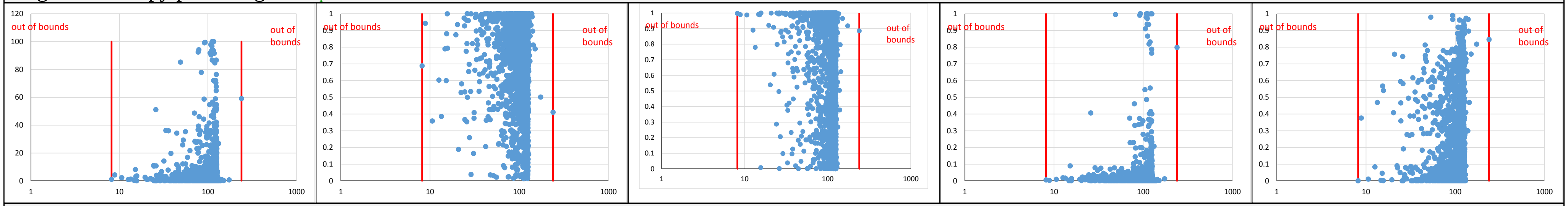
PARa per voxel (100 MJ MJ^{-1} voxel^{-1})	SID (MJ MJ^{-1})	PARi summit (MJ MJ^{-1})	PARi plant (MJ MJ^{-1})	PARi base (MJ MJ^{-1})
Target plant height H_{pd}				
				
Target plant width W_{pd}				
				
Target plant leaf area LA_{pd}				
				
Cover density CD_{pd}				



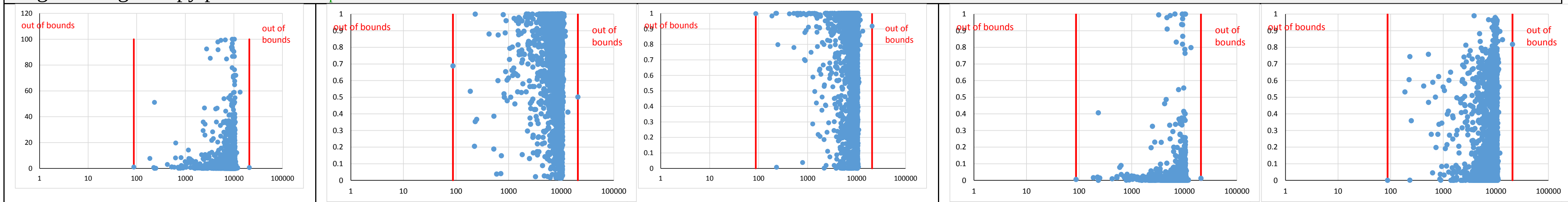
Max distance at which neighbours are found CR_{pd}



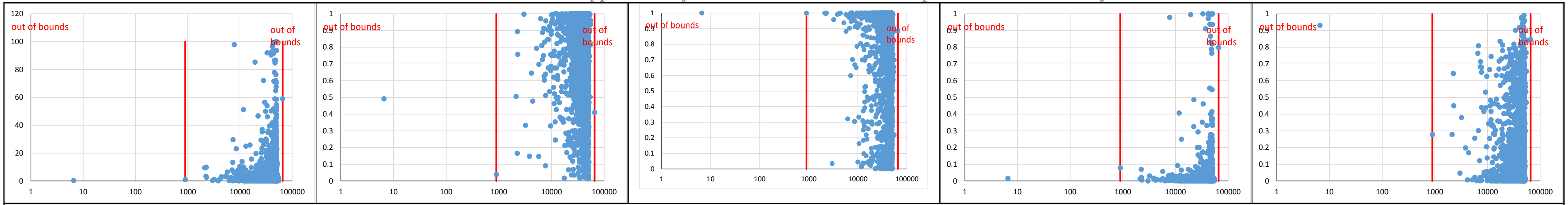
Neighbour canopy plant height CH_{pd}



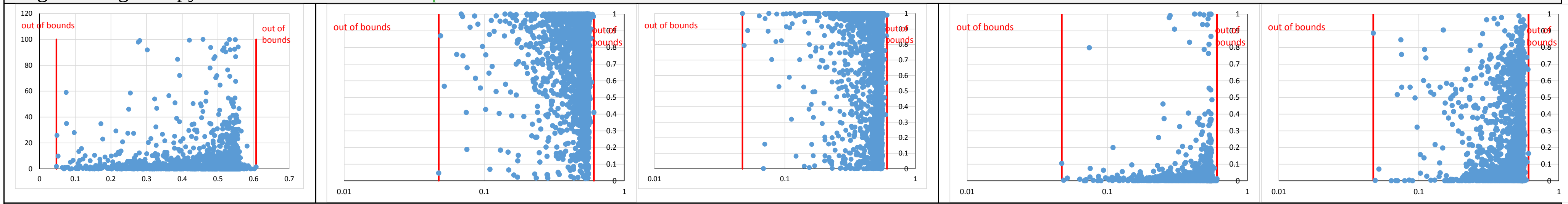
Neighbouring canopy plant area CA_{pd}



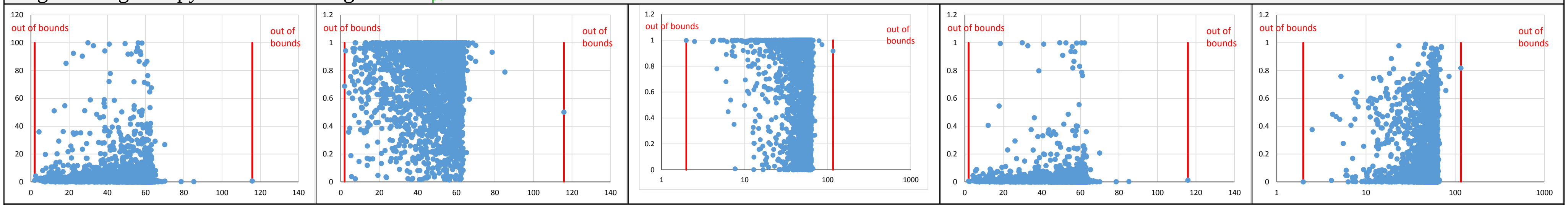
Neighbouring canopy plant leaf area CLA_{pd}



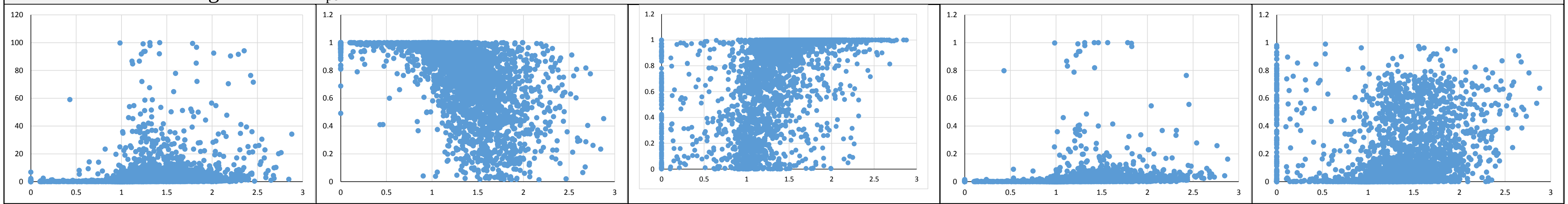
Neighbouring canopy extinction coefficient CK_{pd}



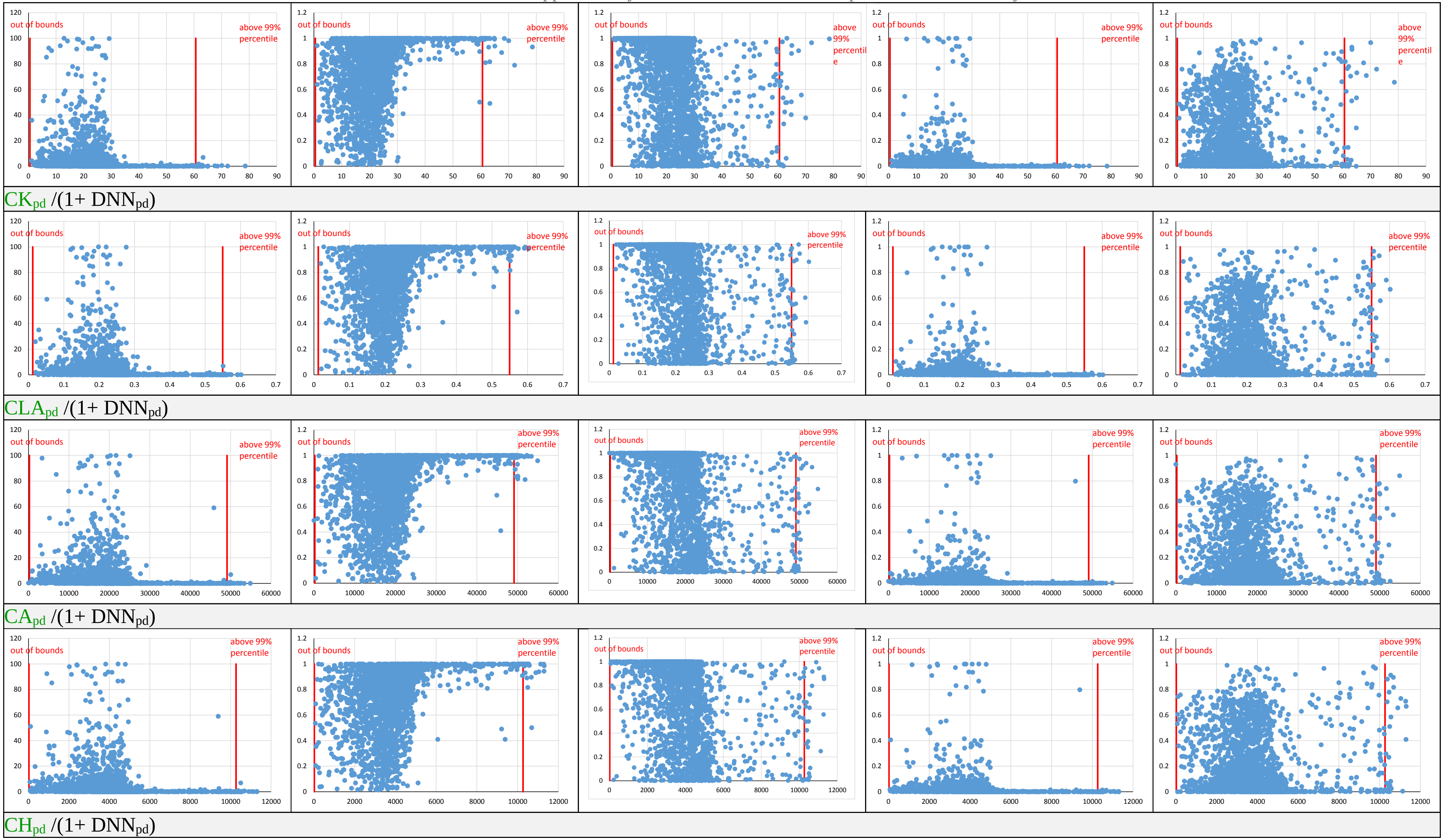
Neighbouring canopy median leaf height $CH50_{pd}$

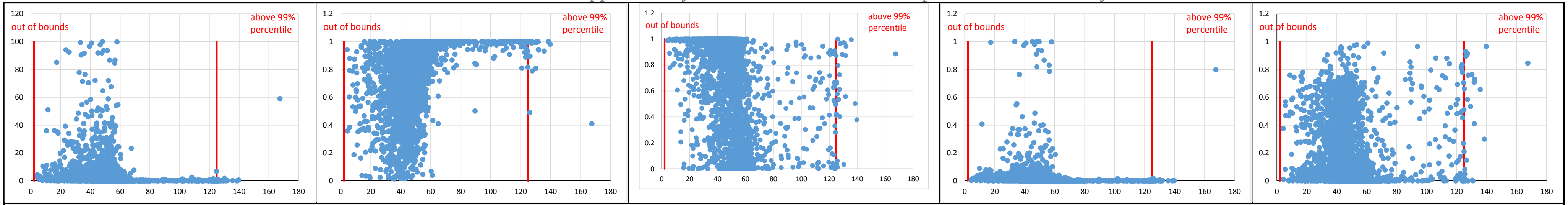


Distance to nearest neighbour DNN_{pd}

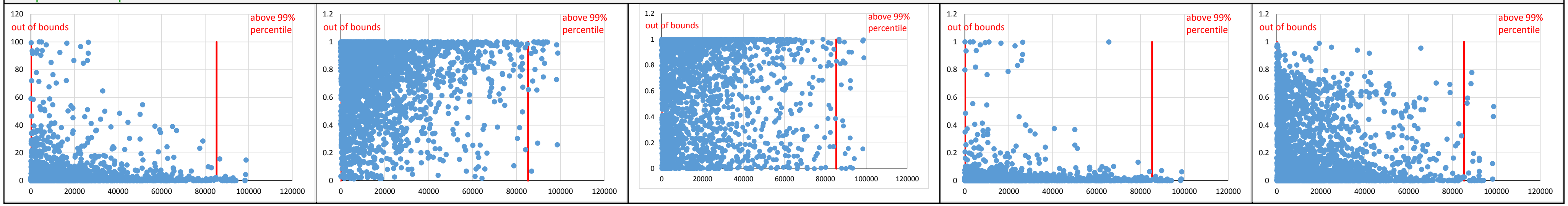


$CH50_{pd}$ /(1+ DNN_{pd})


out of bounds
above 99% percentile
CK_{pd} /(1+ DNN_{pd})
CLA_{pd} /(1+ DNN_{pd})
CA_{pd} /(1+ DNN_{pd})
CH_{pd} /(1+ DNN_{pd})


out of bounds
above 99% percentile

CD_{pd} Π CR_{pd}^2


out of bounds
above 99% percentile

1.5 References

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Annexe 6
Supplementary material of simplifying a complex model: sensitivity analysis and metamodelling of the complex mechanist model FLORSYS

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1 Supplementary materials for the evaluation of the metamodels

1.1 Evaluation criteria (Colbach et al., 2016)

1.1.1 Prediction error

For the evaluation, a series of evaluation indicators were used to compare N observed values (y_i) to simulated values ($\hat{y}_i$). Two complementary evaluation indicators were used in order to rank the tested scenarios, one assessing overall prediction error, the other the prediction quality of the model:

- The root square of the mean square error in predictions RMSEP= $\sqrt{\frac{\sum(y_i - \hat{y}_i)^2}{N}}$ (Wallach and Goffinet, 1987, 1989) was calculated for each location, scenario and for each weed and crop variable y (with y being dP, dPT, mP etc). RMSEP is the average prediction error and was divided here by ½[max-min observed values] to obtain the relative error RRMSEP which facilitates the comparison between variables and locations. Division by the middle of the range of variation was preferred to the usually used mean of observations because of the negative values resulting from log-transforming some y variables.

We moreover proposed two additional calculations of RMSEP to take account of the huge variability in observations and, to a lesser degree, in simulations in our data set:

- The RMSEP was corrected for variability in observations by subtracting the mean variance of observations over possible samples $\mathrm{var}_{\mathrm{obs}} = \frac{1}{DSQ}\sum_{dsq}\left(\mathrm{y}_{\mathrm{ds}} - \mathrm{y}_{\mathrm{dsq}}\right)^2$ from the MSEP before applying the root-square. At Epoisses and La Cage, $\mathrm{var}_{\mathrm{obs}}$ was calculated for each field and assessment date over the four assessment quadrats; for the other three sites, $\mathrm{var}_{\mathrm{obs}}$ was calculated for each cropping system, weed species and assessment date over all the fields with the crop x plough x tillage frequency belonging to the given cropping system. If MSEP is small or smaller than var_{obs}, the difference between observed and simulated values is mostly due to observation error.

- The RMSEP was corrected for variability due to stochasticity in simulations by subtracting the mean variance of simulations $\mathrm{var}_{\mathrm{sim}} = \frac{1}{DSR}\sum_{dsr}\left(\hat{\mathrm{y}}_{\mathrm{ds}} - \hat{\mathrm{y}}_{\mathrm{dsr}}\right)^2$ from MSEP. If MSEP is small or smaller than var_{obs}, the difference between observed and simulated values is mostly due to stochasticity.

As a result, RMSEP corrected for measurement error and model stochasticity becomes $\sqrt{\frac{\sum(w_i - \hat{w}_i)^2}{N} - \mathrm{var}_{obs} - \mathrm{var}_{sim}}$ (Wallach, 2006). To compare the prediction quality of different FLORSYS outputs and to determine the model's domain of validity in terms of variables and locations, we propose a synthetic graphical representation inspired by Coucheney *et al* (2015), (1) representing RMSEP vs. $\sqrt{\mathrm{var}_{obs}}$ for each variable y and location, both standardized by the standard-deviation in observations, i.e. STDEVobs= $\sqrt{\frac{\sum(y_i - \bar{y}_i)^2}{N}}$, with (2) the symbol size of each data point (variable x location) proportional to the Pearson correlation coefficient, and (3) vertical bars proportional to the prediction bias. Variable x location combinations are placed into performance classes ranging from "very good" to "bad" along the vertical axis, or into the "unclassifiable" area where observation error exceeds RMSEP.

1.1.2 Prediction quality

When testing the prediction quality, tree ranking indicators were used:

- The Pearson correlation coefficient between observed and simulated values $r = \frac{\Sigma(y_i - \bar{y})(\hat{y}_i - \bar{\hat{y}})}{\sqrt{\Sigma(y_i - \bar{y})^2}\sqrt{\Sigma(\hat{y}_i - \bar{\hat{y}})}^2}$. Pearson values close to 1 point to a positive correlation between observed and simulated data, but this correlation can differ from y=x (i.e. total fit between observed and simulated data), particularly in the case of a model bias.

- The modelling efficiency $EF = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2}$, where $\bar{y}$ is the mean of observations (Mayer and Butler, 1993), defines the ability of a model to predict the value of a variable. The closer EF is to 1, the better is the fit between observed and simulated data (Wallach, 2006). Negative EF values indicate that the mean observed value is a better predictor than the values predicted by the model; positive values are generally considered to indicate acceptable levels of model performance;
- The Spearman correlation coefficient, resulting from calculating the Pearson correlation coefficient with ranks of observed vs. simulated values instead of using the actual values. Spearman values close to 1 indicate that observed and simulated data are ranked similarly though actual values can differ considerably, both absolutely and relatively. When the Spearman coefficient exceeds the Pearson, ranks are better predicted than differences between values. When Pearson values exceed Spearman ones, ranks of similar values can be inverted.

For each outputs, maximal value of the three indicator constituted the prediction quality indicator.

1.2 Simulation time

Table 1: Simulation time for different voxel sizes and differents field sizes for different models (process based or metamodel) and the different methods to estimate the aggregated canopy variables. Numbers followed by the same letter are not significantly different at p=00.05

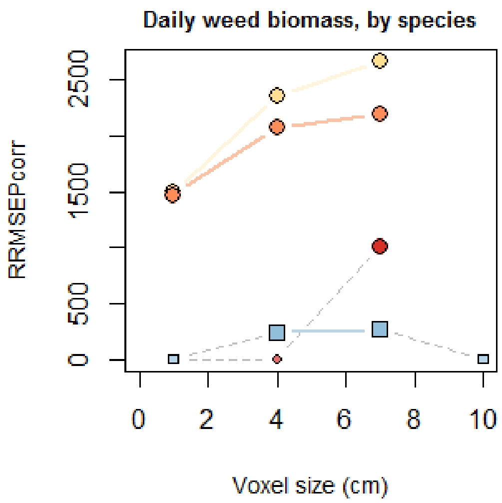
Voxel size(cm)	Area (m x m)	Log10	backtransformed	
1	6x3	4.82	65722	A
4	6x3	3.57	3674	B
10	6x3	3.39	2461	C
7	6x3	3.32	2105	D
7	3x3	3.29	1959	D
7	1x1	2.40	254	E

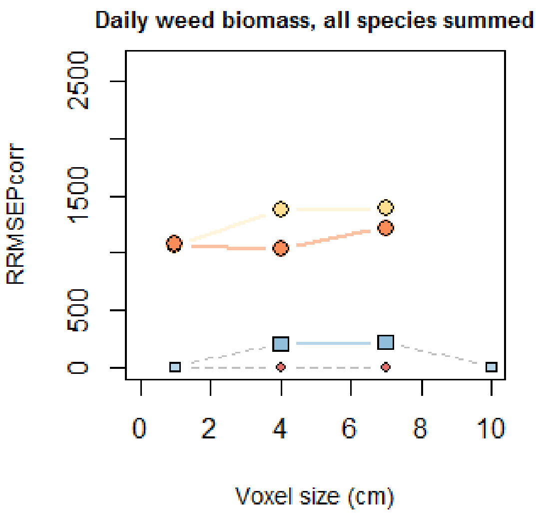
1.3 Prediction error

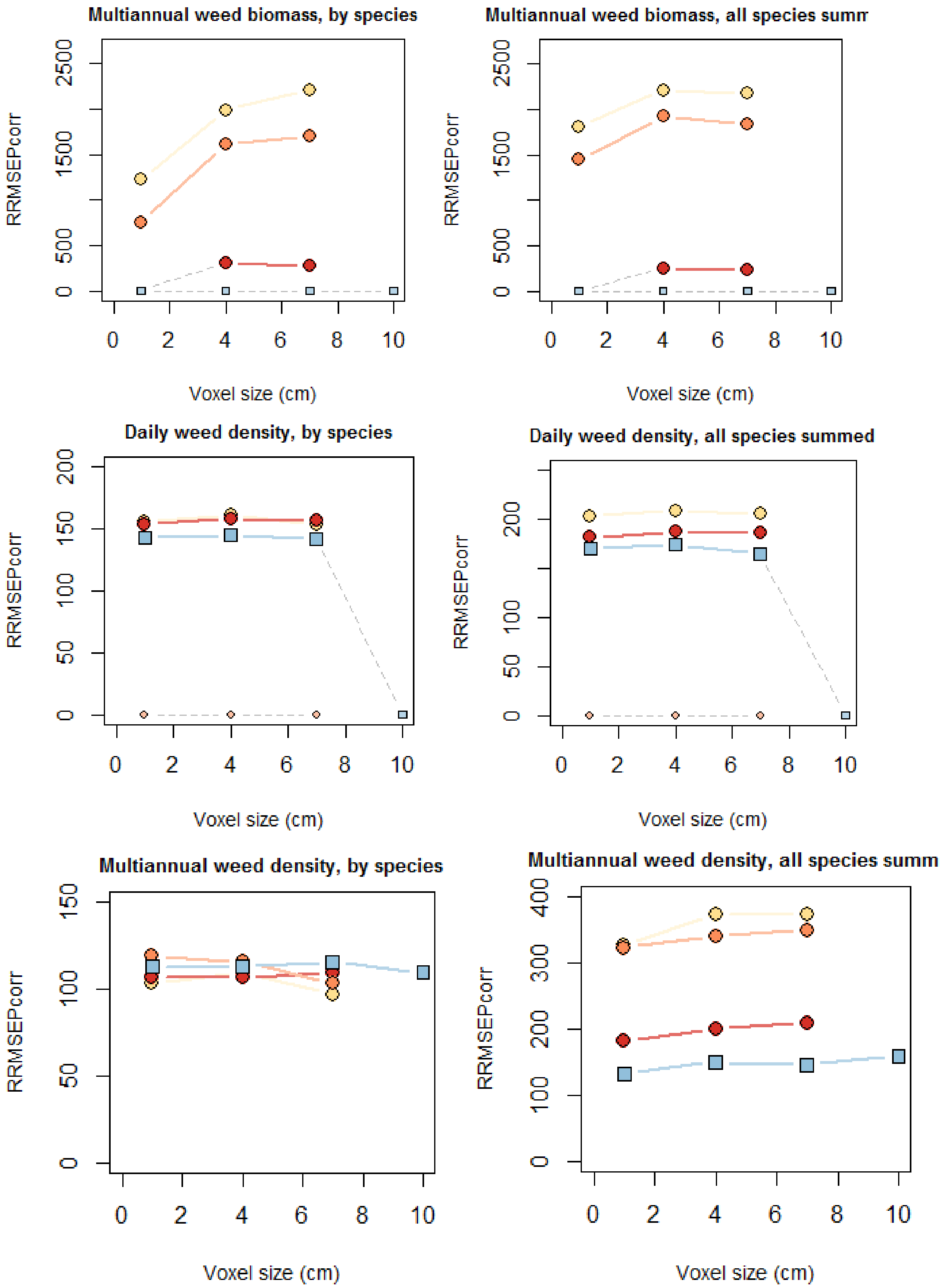
1.3.1 Depending on voxel size for all outputs

Figures to follow:

Prediction error (RRMSEP corrected, MJ·MJ-1) for the different outputs of FLORSYS. Blue squares are the process based simulations, circles are for the metamodels, red is when local neighbours are used for the aggregated canopy variable, yellow is when neighbours are averaged for the aggregated canopy variable and orange is a mix between local and average methods. Results are for a 3 m by 6 m virtual field. Grey dotted lines are insignificant results, i.e. variability in observations larger than prediction error which thus is close to nil. Metamodels were not simulated for a 10 cm voxel.







Multiannual weed biomass, by species
RRMSEPcorr
0
500
1500
2500
0
2
4
6
8
10
Voxel size (cm)
Multiannual weed biomass, all species summ
RRMSEPcorr
0
500
1500
2500
0
2
4
6
8
10
Voxel size (cm)
Daily weed density, by species
RRMSEPcorr
0
50
100
150
200
0
2
4
6
8
10
Voxel size (cm)
Daily weed density, all species summed
RRMSEPcorr
0
50
100
200
0
2
4
6
8
10
Voxel size (cm)
Multiannual weed density, by species
RRMSEPcorr
0
50
100
150
0
2
4
6
8
10
Voxel size (cm)
Multiannual weed density, all species summ
RRMSEPcorr
0
100
200
300
400
0
2
4
6
8
10
Voxel size (cm)

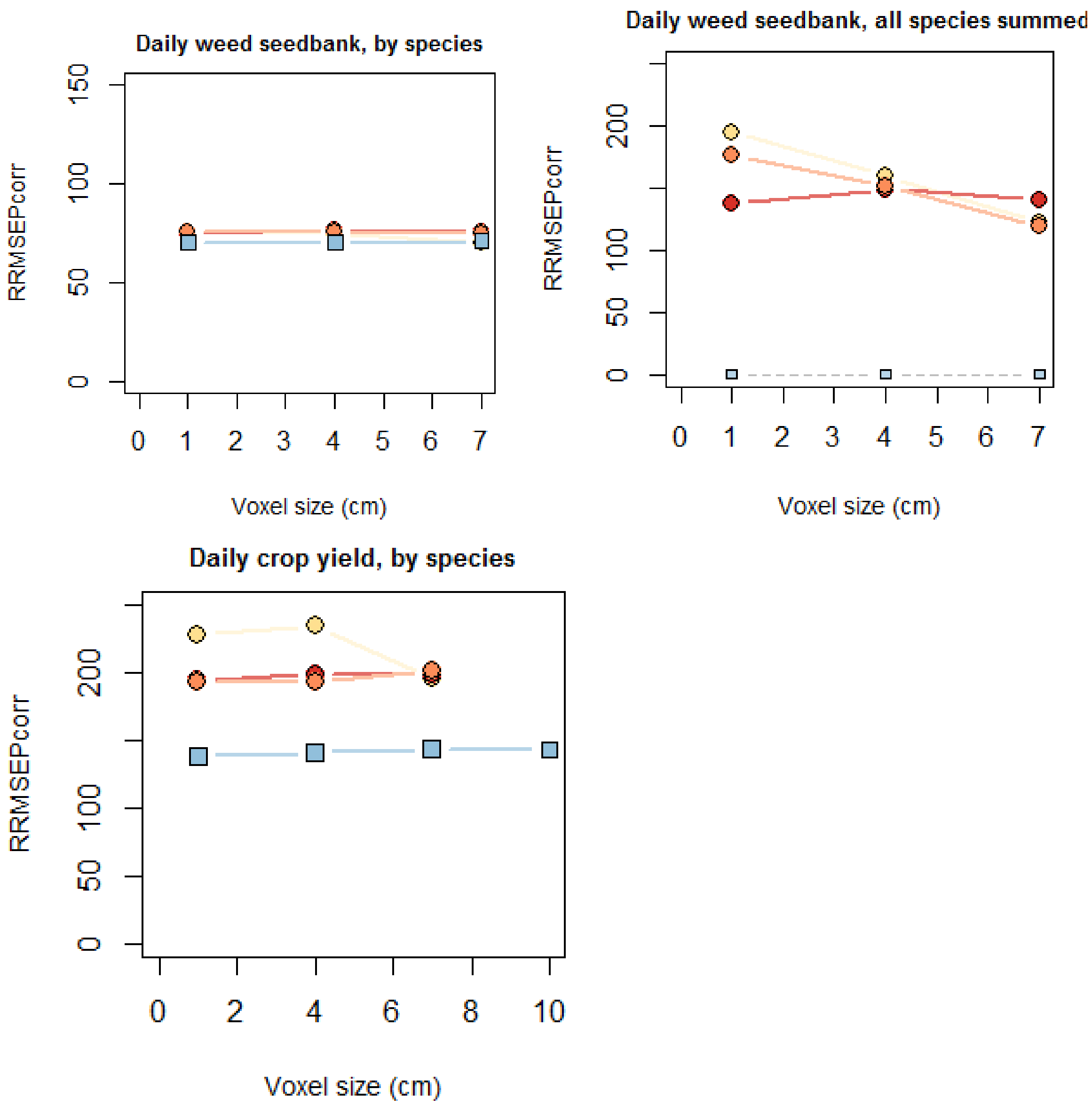


Figure 1: Prediction error (RRMSEP corrected, MJ·MJ^{-1}) for the different outputs of FLORSYS. Blue squares are the process based simulations, circles are for the metamodels, red is when local neighbours are used for the aggregated canopy variable, yellow is when neighbours are averaged for the aggregated canopy variable and orange is a mix between local and average methods. Results are for a 3 m by 6 m virtual field. Grey dotted lines are insignificant results, i.e. variability in observations larger than prediction error which thus is close to nil. Metamodels were not simulated for a 10 cm voxel.

1.3.2 Global comparison to show the least variable method for all outputs

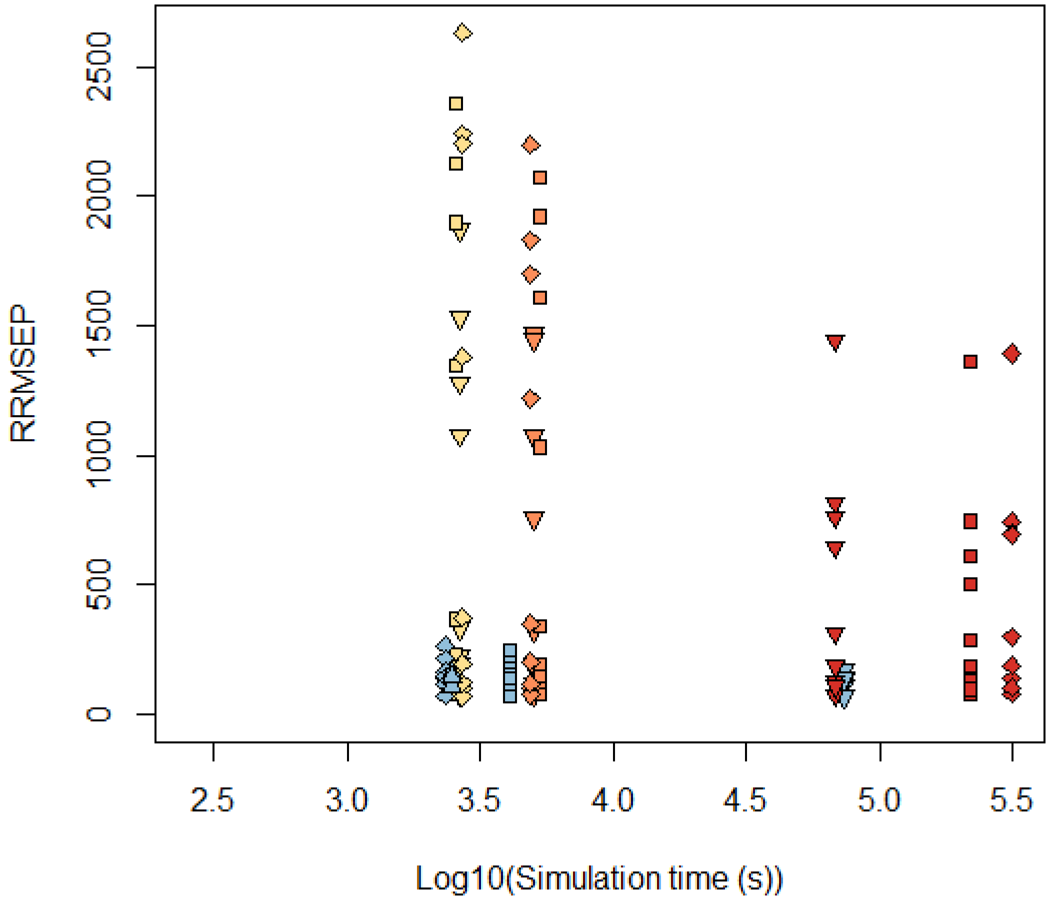


Figure 2: Prediction error (RRMSEP corrected, $MJ \cdot MJ^{-1}$) in function of the simulation time for the different types of metamodels and voxel sizes. The color of symbols represent different methods and the shapes represent different voxel sizes. Blue symbols: process based simulations, dark red symbols: local neighbours metamodel, light yellow symbols: averaged neighbours metamodel and orange symbols: mix between local and average metamodel. Triangle down: 1 cm voxel, squares: 4 cm voxel, triangles up: 7 cm voxel and diamond: 10 cm voxel. A log10 for the simulation time was chosen to show more the differences between the different methods.

1.3.3 Field size effect

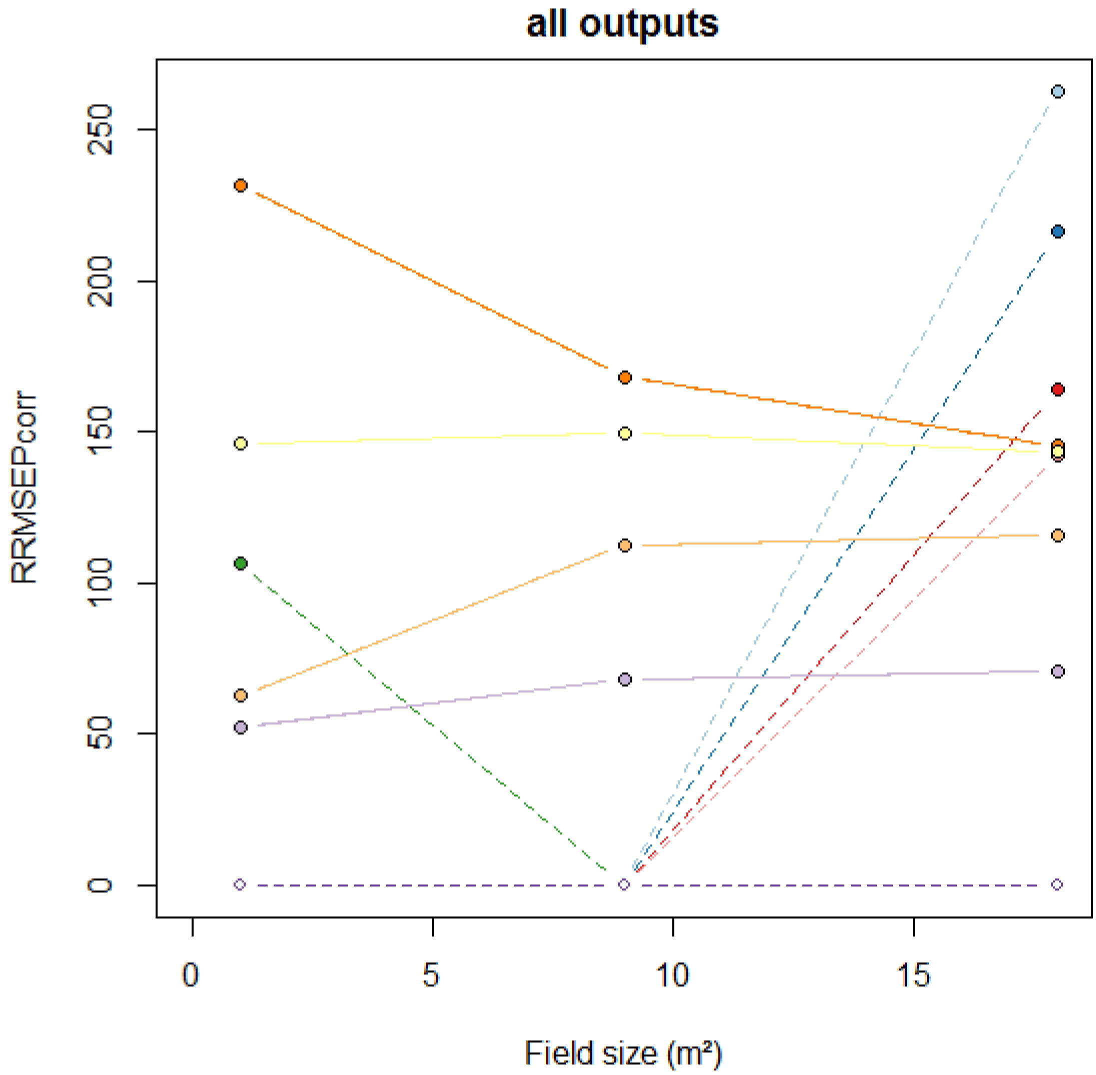


Figure 3: Prediction error (RRMSEP corrected, MJ·MJ^{-1}) in function of the size of the field for the different outputs in the process based model. The color of symbols represent different outputs listed below, dotted lines are when one value of the field size is non-significant, i.e. variability in observations larger than prediction error which thus is close to nil.

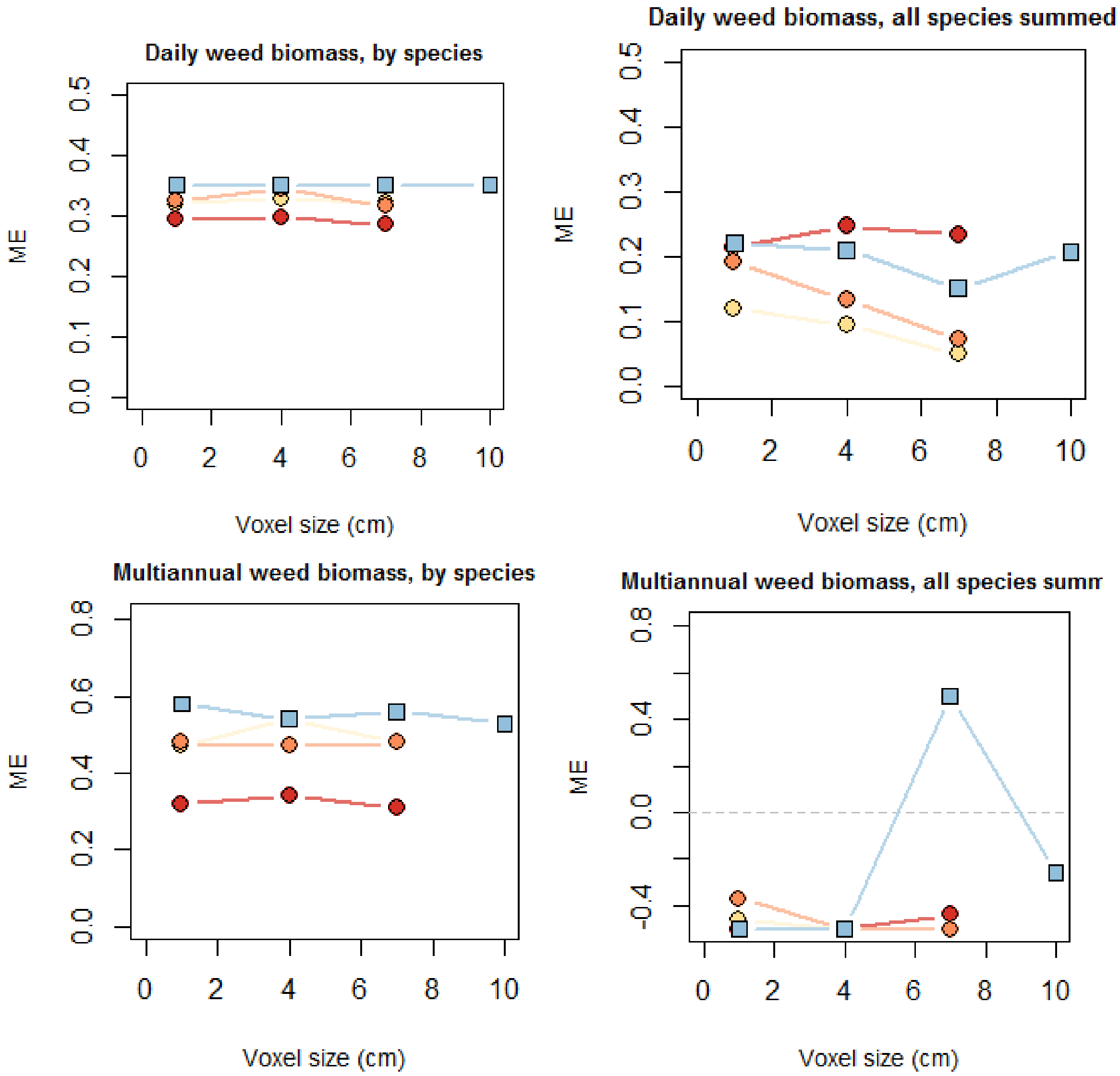
Colors legend:

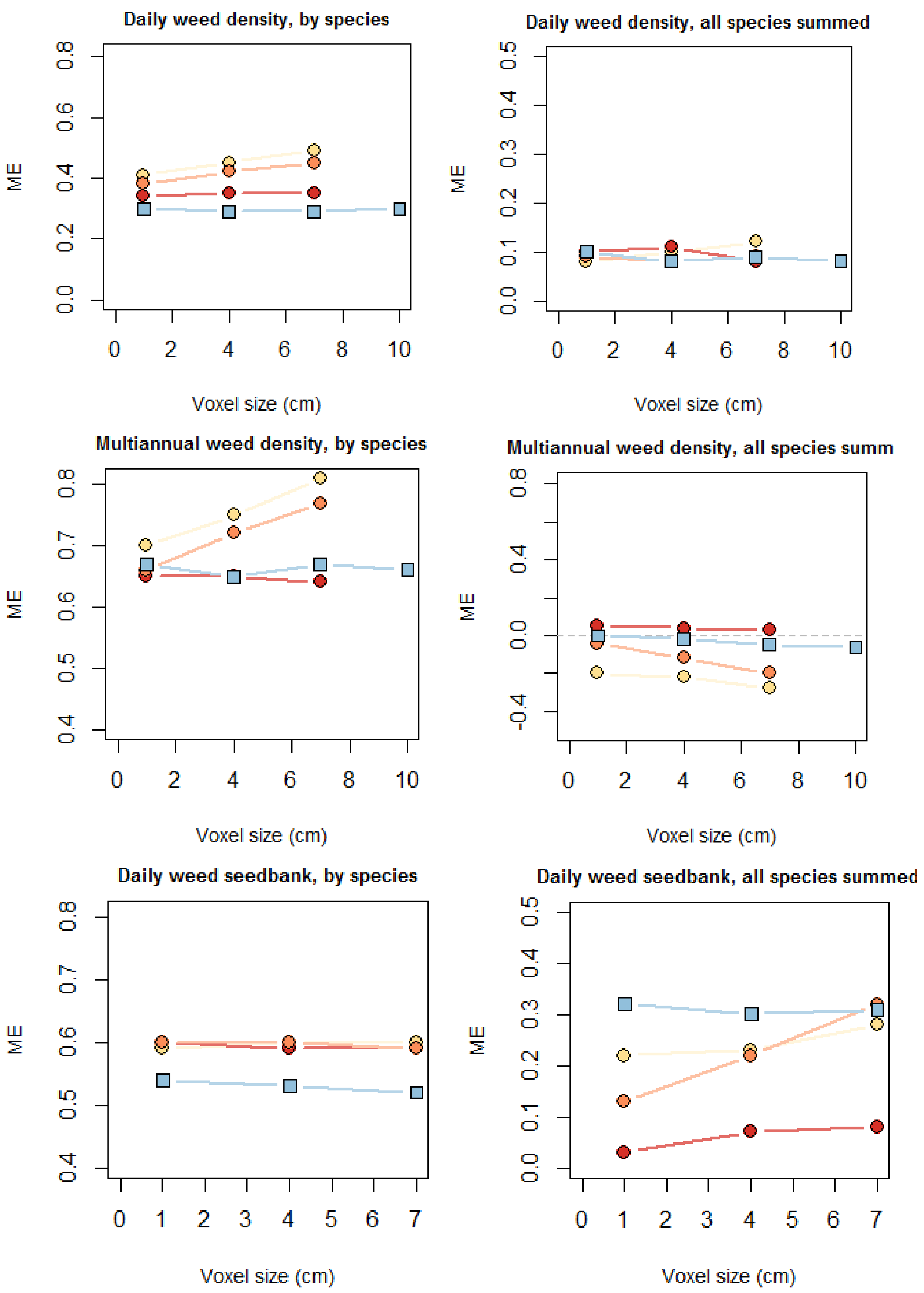
- Daily weed biomass, by species
- Daily weed biomass, all species summed
- Multiannual weed biomass, by species
- Multiannual weed biomass, all species summed
- Daily weed density, by species
- Daily weed density, all species summed
- Multiannual weed density, by species
- Multiannual weed density, all species summed
- Daily weed seedbank, by species
- Daily weed seedbank, all species summed
- Daily crop yield, by species

1.4 Modelling efficiency

1.4.1 Depending on voxel size for all outputs outputs

Figures to follow:
Modelling efficiency for the different outputs of FlorSys. Blue squares: process based simulations, circles: polynomials chaos metamodels, dark red: local neighbours metamodels, light yellow: average metamodels and orange: mix between local and average. Results are for a 3 m by 6 m virtual field. Grey dotted lines are insignificant results. Metamodels were not simulated for a 10 cm voxel.





Daily weed density, by species
Daily weed density, all species summed
Multiannual weed density, by species
Multiannual weed density, all species summ
Daily weed seedbank, by species
Daily weed seedbank, all species summed
ME
Voxel size (cm)

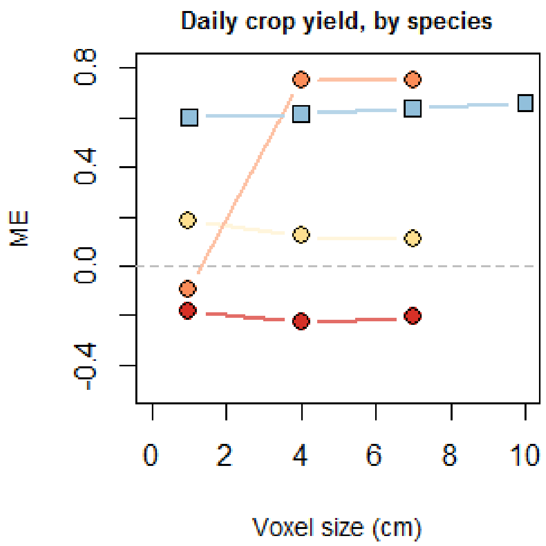


Figure 4: Modelling efficiency for the different outputs of FlorSys. Blue squares: process based simulations, circles: polynomials chaos metamodels, dark red: local neighbours metamodels, light yellow: average metamodels and orange: mix between local and average. Results are for a 3 m by 6 m virtual field. Grey dotted lines are insignificant results. Metamodels were not simulated for a 10 cm voxel.

1.4.2 Global comparison to show the less variable method for all outputs

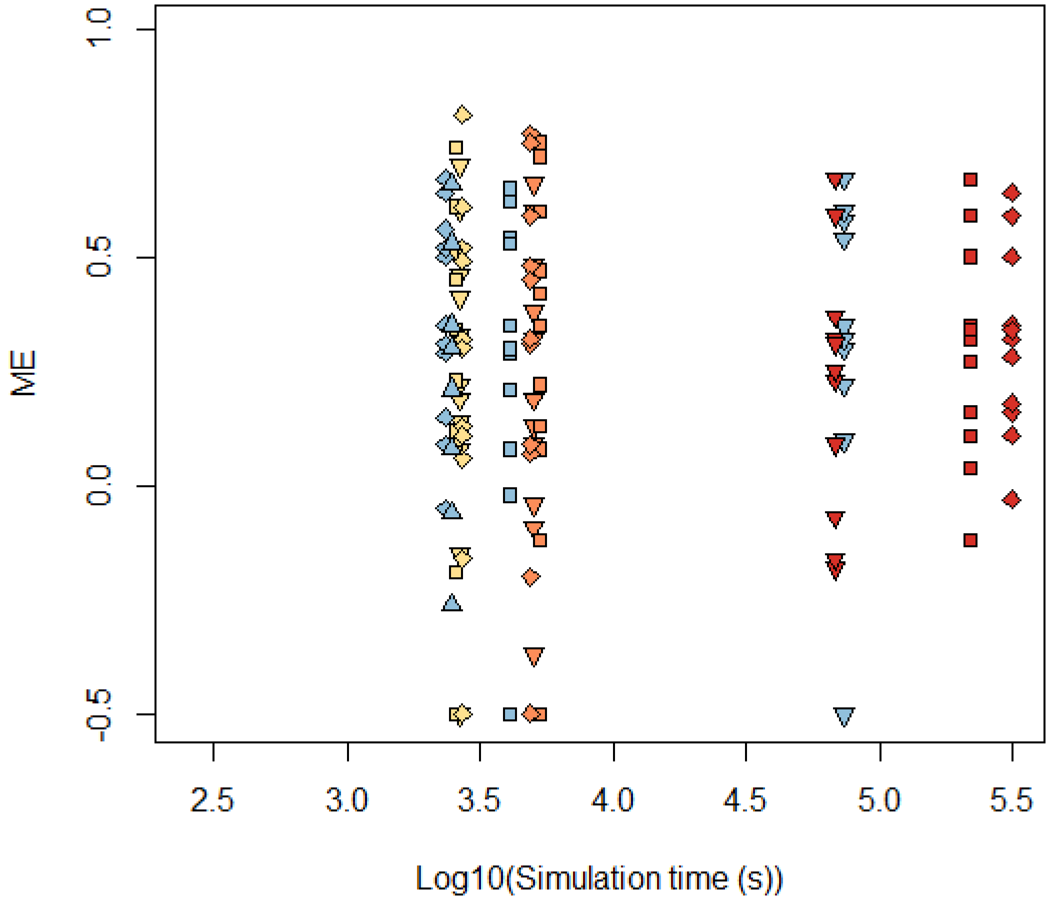


Figure 5: Modelling efficiency (ME) in function of the simulation time for the different types of metamodels and voxel sizes. The color of symbols represent different methods and the shapes represent different voxel sizes. Blue symbols: process based simulations, dark red symbols: metamodel with local neighbours, light yellow symbols: averaged neighbours and orange symbols: mix between local and average. Triangle down are for 1 cm voxels, squares are for 4 cm voxels, triangles up are for 7 cm voxels and diamond are for 10 cm voxels. A log10 for the simulation time was chosen to show more the differences between the different methods.

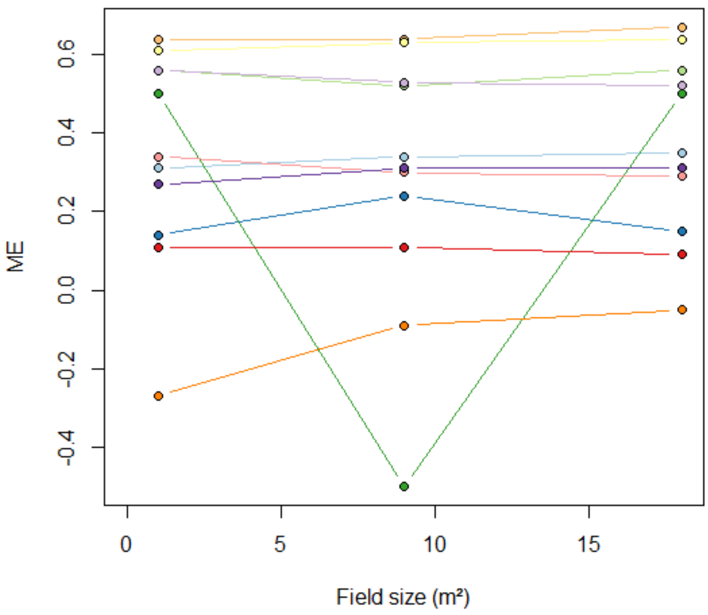


Figure 6: Modelling efficiency (ME) in function of the size of the field for the different outputs in the process based model. The color of symbols represent different outputs listed below.

- Daily weed biomass, by species
- Daily weed biomass, all species summed
- Multiannual weed biomass, by species
- Multiannual weed biomass, all species summed
- Daily weed density, by species
- Daily weed density, all species summed
- Multiannual weed density, by species
- Multiannual weed density, all species summed
- Daily weed seedbank, by species
- Daily weed seedbank, all species summed
- Daily crop yield, by species

1.5 References

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Annexe 7
Supplementary material of which cultural techniques drive weed dynamics and impact? Sensitivity analysis of a cropping system model to support integrated weed management

1 Short presentation of FLORSYS

Voir annexe A2 de la thèse.

2 Overview of the random cropping system created

The 3302 random cropping systems created were compared to the 142 standard systems.

2.1 Final cropping systems counts

Table 1 : Cropping systems counts by type, standard, no herbicides, no tillage and random ones

	Cropping system total count
Random cropping systems	2758
No herbicide cropping systems	201
No tillage cropping systems	201
Standard cropping systems	142
Sum	**3302**

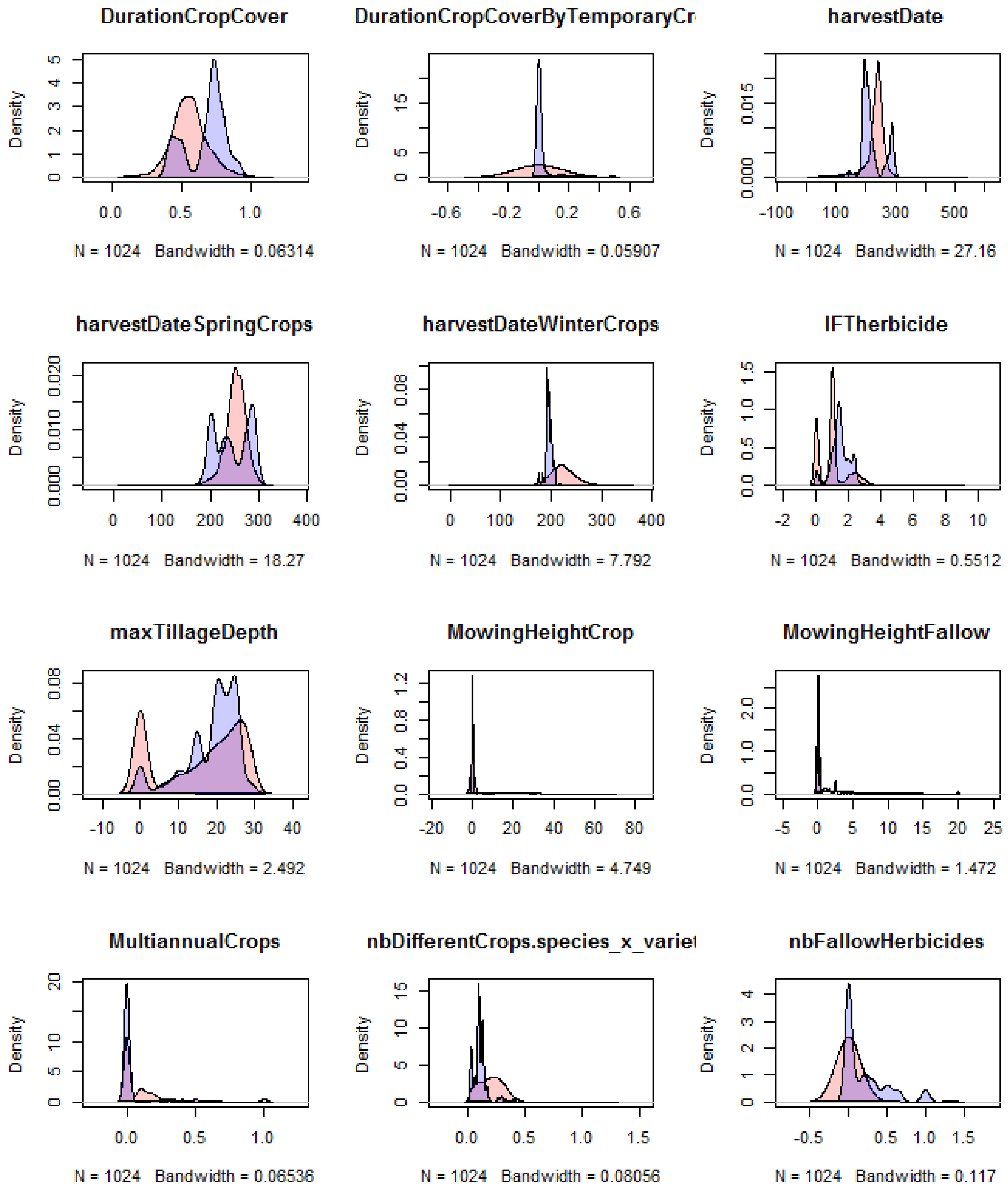
Table 2 : Counts of the number of climatic repetition that we were able to simulate with FlorSys for the random cropping in each production situation. To compare, the realistic cropping systems are also counted in each cropping situation, they all have 10 repetitions.

	Random cropping systems										**Realistic cropping systems**
Repetition count	1	2	3	4	5	6	7	8	9	10	10
PS.A	8	2	3	2	7	4	5	7	6	744	143
PS.B	0	0	0	0	0	0	0	0	0	0	91
PS.C	8	3	2	2	4	2	1		2	295	159
PS.D	6	7	3	3	6	4	6	8	10	686	30
PS.E	7	4	3	5	5	4	3	12	8	861	72
Sum	**29**	**16**	**11**	**12**	**22**	**14**	**15**	**27**	**26**	**2586**	**495**

In random cropping systems the10 climatic repetition were not always possible, some weather events causing bugs.

2.2 Overview of the random cropping systems

Figures to follow: Kernel density estimation of the cropping systems descriptors. Density function against the cropping systems descriptors whose information can be found in the Appendix (§ III.2.7). Random cropping systems in red and real-life systems in blue, purple shows overlaps. The bandwidth correspond to smoothing parameter (the higher, the smother the curve will be compared to the data points).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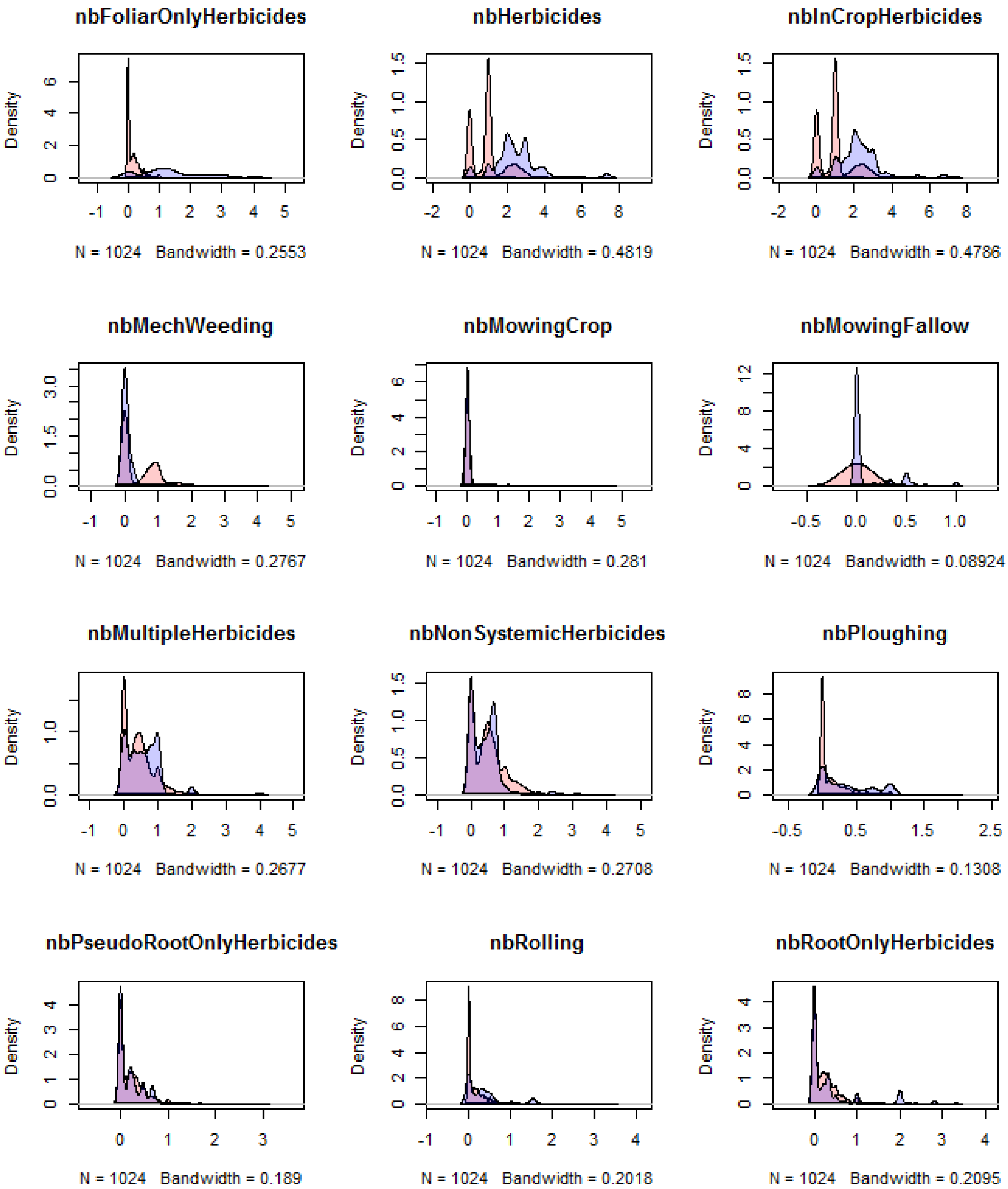
Density
N = 1024 Bandwidth = 0.06314
DurationCropCoverByTemporaryCr
Density
N = 1024 Bandwidth = 0.05907
harvestDate
Density
N = 1024 Bandwidth = 27.16
harvestDateSpringCrops
Density
N = 1024 Bandwidth = 18.27
harvestDateWinterCrops
Density
N = 1024 Bandwidth = 7.792
IFTherbicide
Density
N = 1024 Bandwidth = 0.5512
maxTillageDepth
Density
N = 1024 Bandwidth = 2.492
MowingHeightCrop
Density
N = 1024 Bandwidth = 4.749
MowingHeightFallow
Density
N = 1024 Bandwidth = 1.472
MultiannualCrops
Density
N = 1024 Bandwidth = 0.06536
nbDifferentCrops.species_x_variet
Density
N = 1024 Bandwidth = 0.08056
nbFallowHerbicides
Density
N = 1024 Bandwidth = 0.117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Density
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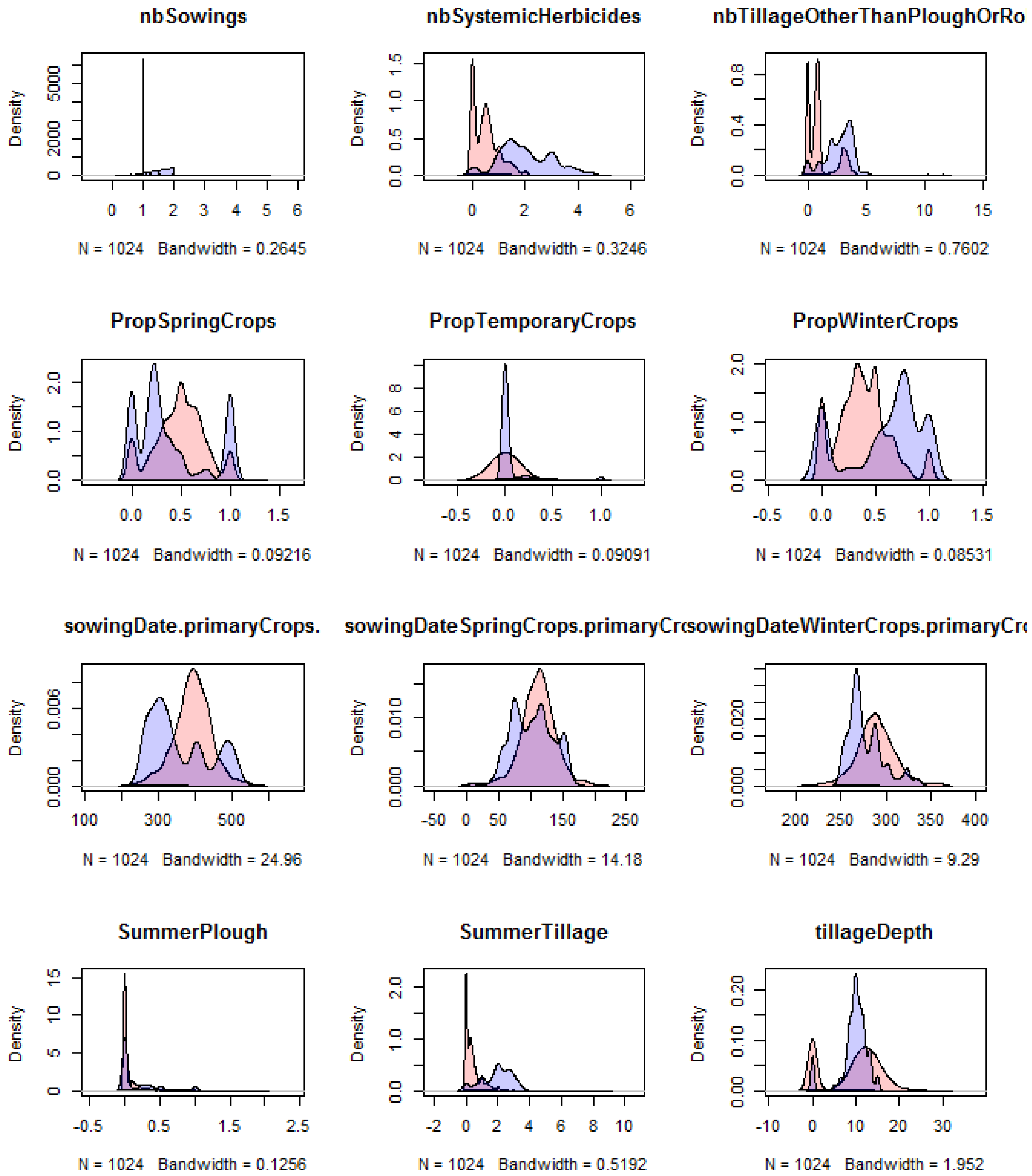
nbHerbicides
Density
N = 1024 Bandwidth = 0.4819
nbInCropHerbicides
Density
N = 1024 Bandwidth = 0.4786
nbMechWeeding
Density
N = 1024 Bandwidth = 0.2767
nbMowingCrop
Density
N = 1024 Bandwidth = 0.281
nbMowingFallow
Density
N = 1024 Bandwidth = 0.08924
nbMultipleHerbicides
Density
N = 1024 Bandwidth = 0.2677
nbNonSystemicHerbicides
Density
N = 1024 Bandwidth = 0.2708
nbPloughing
Density
N = 1024 Bandwidth = 0.1308
nbPseudoRootOnlyHerbicides
Density
N = 1024 Bandwidth = 0.189
nbRolling
Density
N = 1024 Bandwidth = 0.2018
nbRootOnlyHerbicides
Density
N = 1024 Bandwidth = 0.2095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nbSystemicHerbicides
Density
N = 1024 Bandwidth = 0.3246
nbTillageOtherThanPloughOrRo
Density
N = 1024 Bandwidth = 0.7602
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Density
N = 1024 Bandwidth = 0.09216
PropTemporaryCrops
Density
N = 1024 Bandwidth = 0.09091
PropWinterCrops
Density
N = 1024 Bandwidth = 0.08531
sowingDate.primaryCrops.
Density
N = 1024 Bandwidth = 24.96
sowingDateSpringCrops.primaryCr
Density
N = 1024 Bandwidth = 14.18
sowingDateWinterCrops.primaryCr
Density
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Density
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SummerTillage
Density
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tillageDepth
Density
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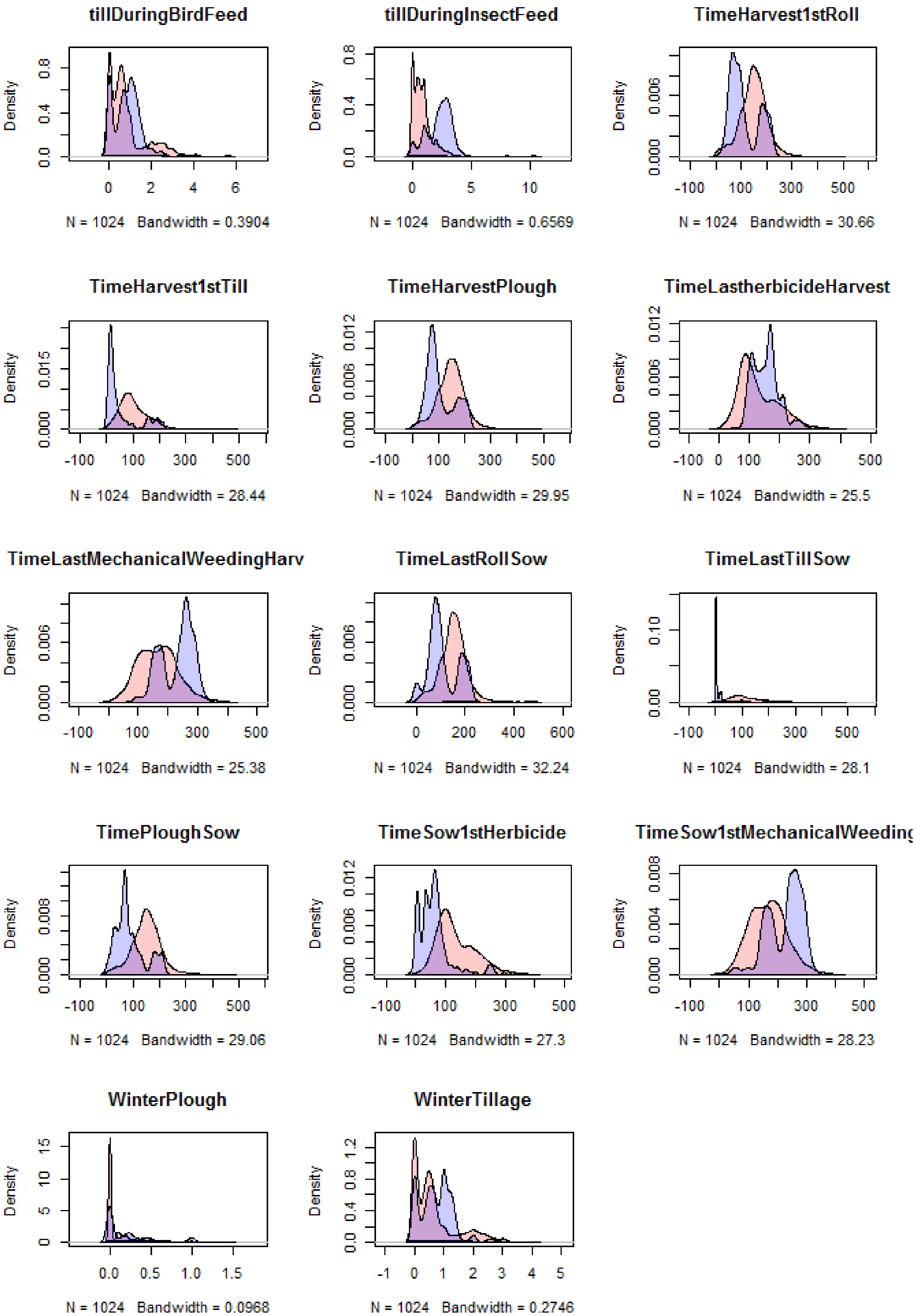
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tillDuringInsectFeed
N = 1024 Bandwidth = 0.6569
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N = 1024 Bandwidth = 30.66
TimeHarvest1stTill
N = 1024 Bandwidth = 28.44
TimeHarvestPlough
N = 1024 Bandwidth = 29.95
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TimeLastMechanicalWeedingHarv
N = 1024 Bandwidth = 25.38
TimeLastRollSow
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TimeLastTillSow
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TimeSow1stMechanicalWeeding
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WinterPlough
N = 1024 Bandwidth = 0.0968
WinterTillage
N = 1024 Bandwidth = 0.2746
Density

Figure S. 1 Kernel density estimation of the cropping systems descriptors. Density function against the cropping systems descriptors whose information can be found in the Appendix (§ III.2.7). Random cropping systems in red and real-life systems in blue, purple shows overlaps. The bandwidth correspond to smoothing parameter (the higher, the smother the curve will be compared to the data points).

2.3 Correlations between inputs variables

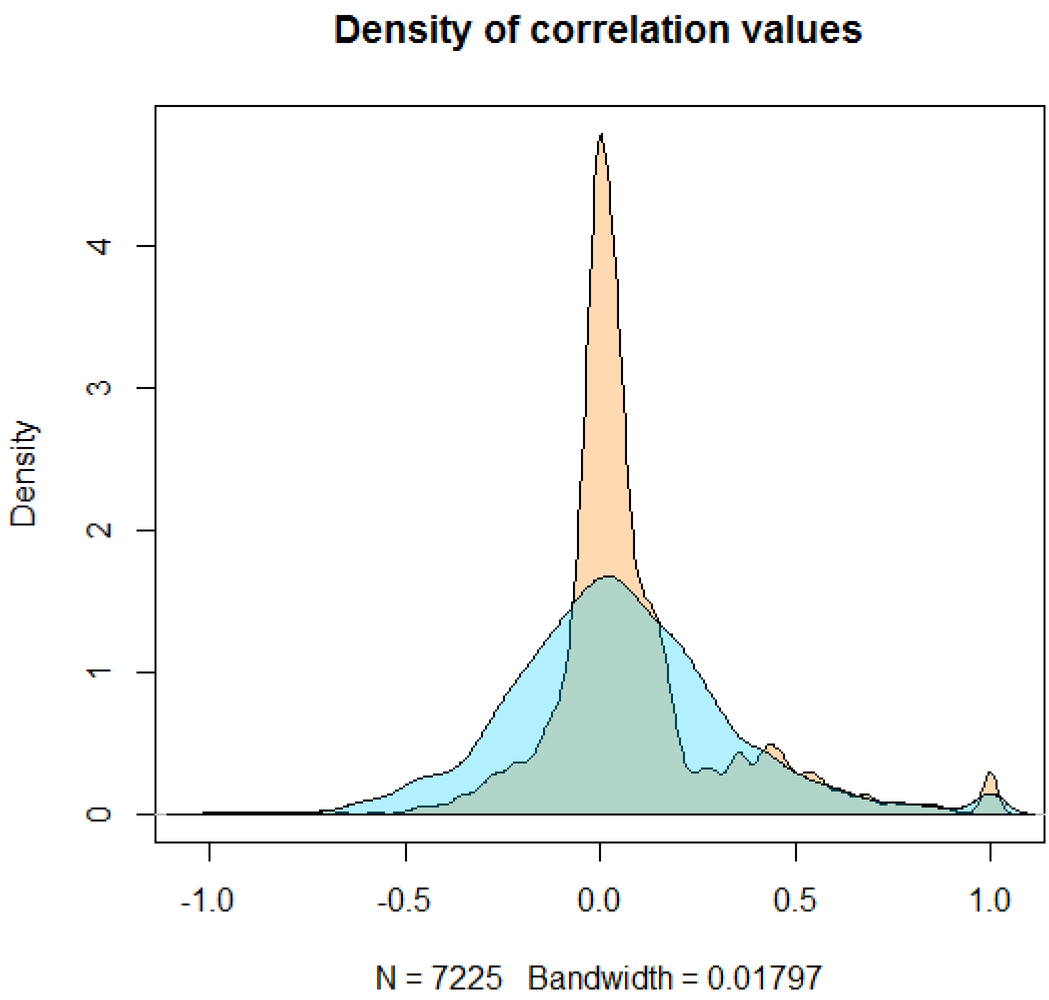


Figure S. 2 Kernel density estimation (density function) of Spearman correlation coefficients among cropping system. In blue: realistic cropping systems, in orange: random cropping systems. The random cropping systems are dispersed than the realistic ones. The bandwidth correspond to smoothing parameter (the higher, the smother the curve will be compared to the data points).

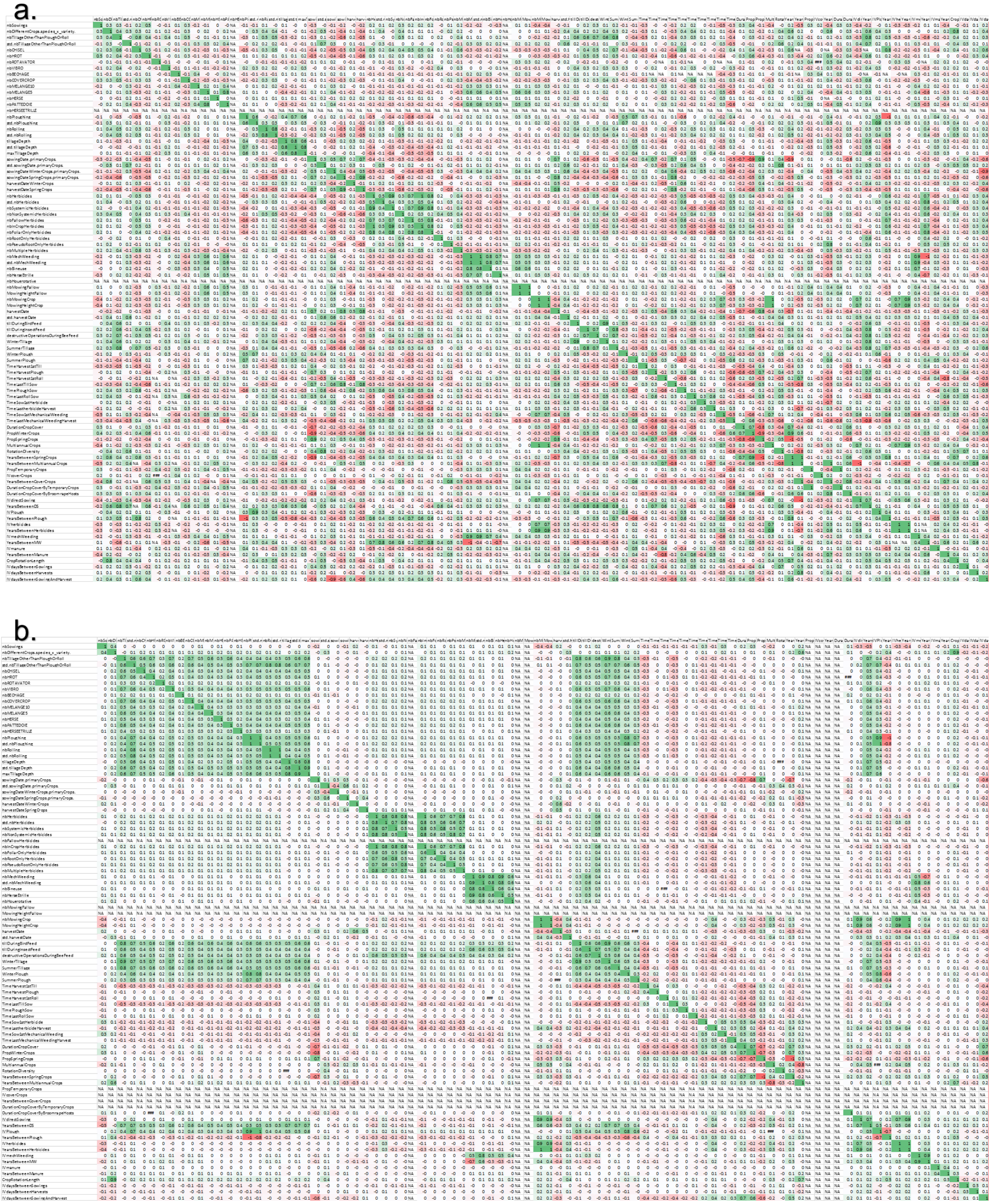


Figure S. 3 Overview of Spearman correlation coefficients among cropping system descriptors. Cells are coloured from dark red for -1, to dark green for 1 and passing by white for 0. (a.) real-life cropping systems and (b.) random cropping systems. In the random cropping systems, the green rectangles show positive correlations for the use of tillage and mechanical weeding tools.

3 PCA and correlations

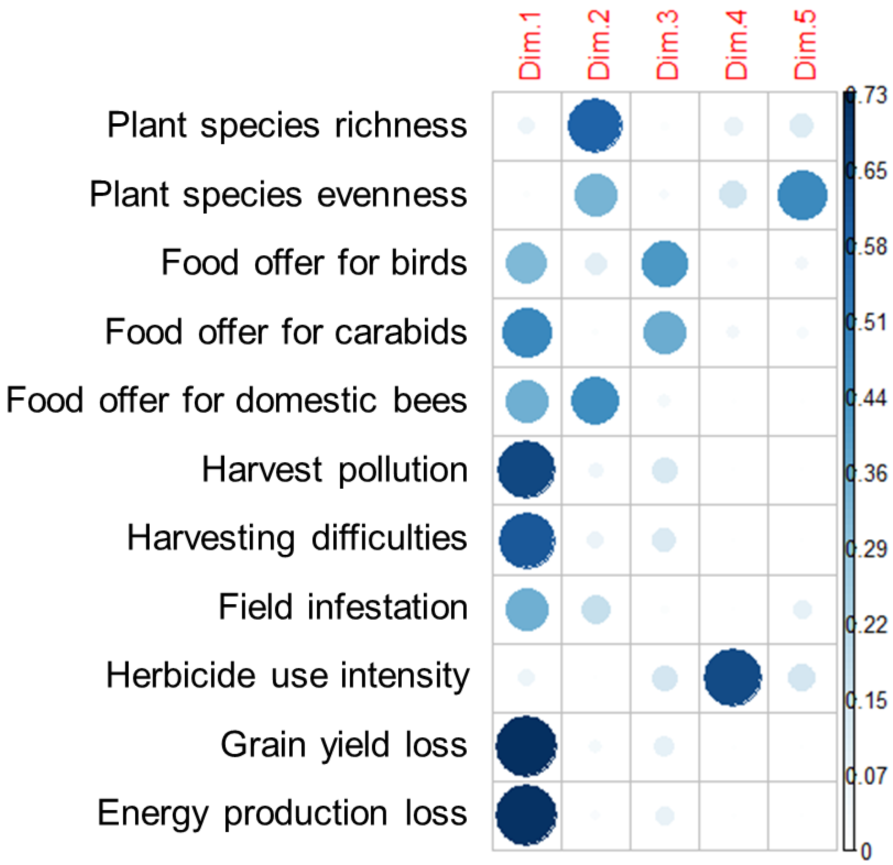


Figure 1Correlation plot of the weed impact indicators. First dimension represent more the nuisibility indicators when the second one represent more biodiversity indicators.

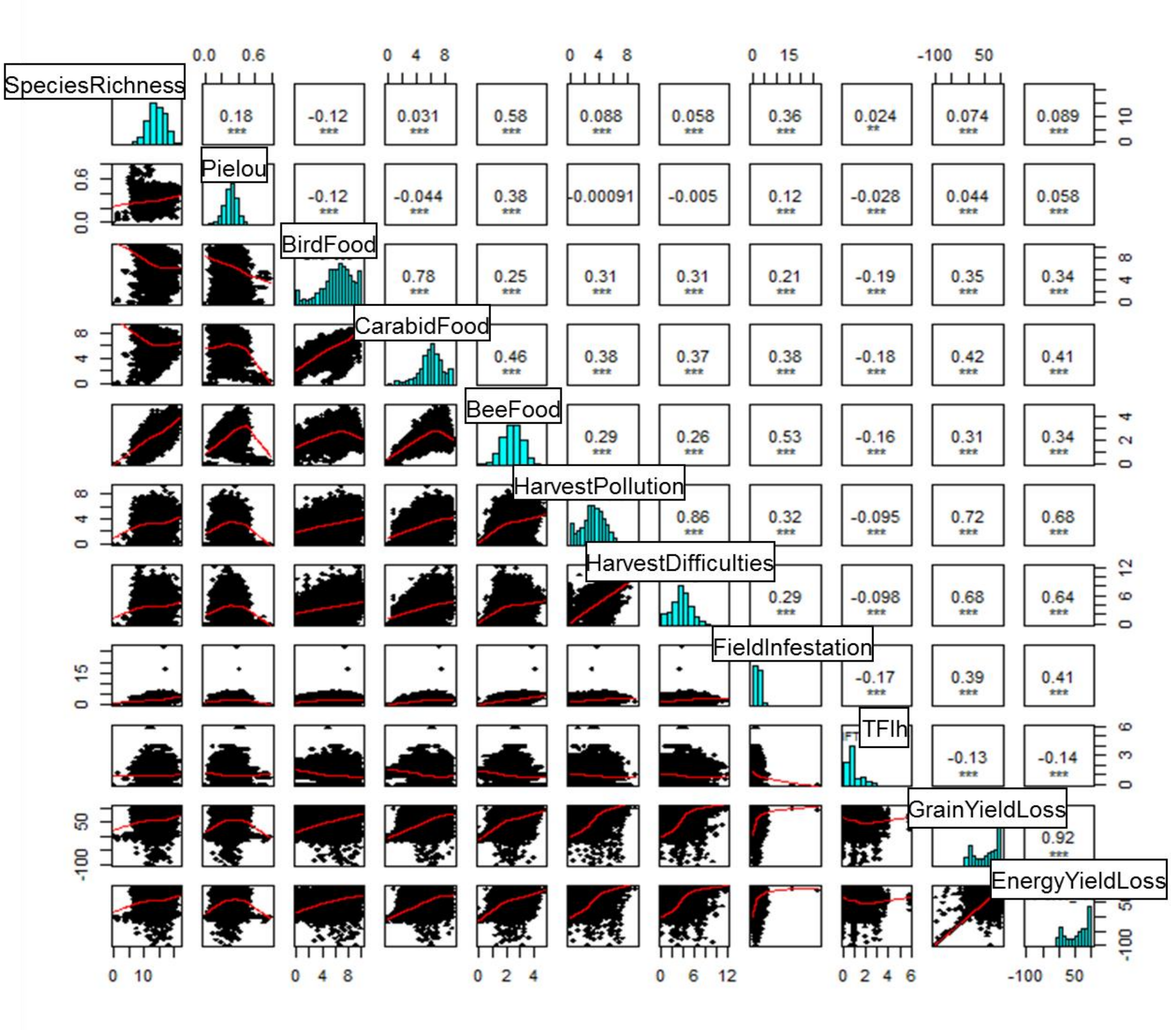


Figure 2 : In between indicators spearman correlations.

4 Correlation analysis between indicators

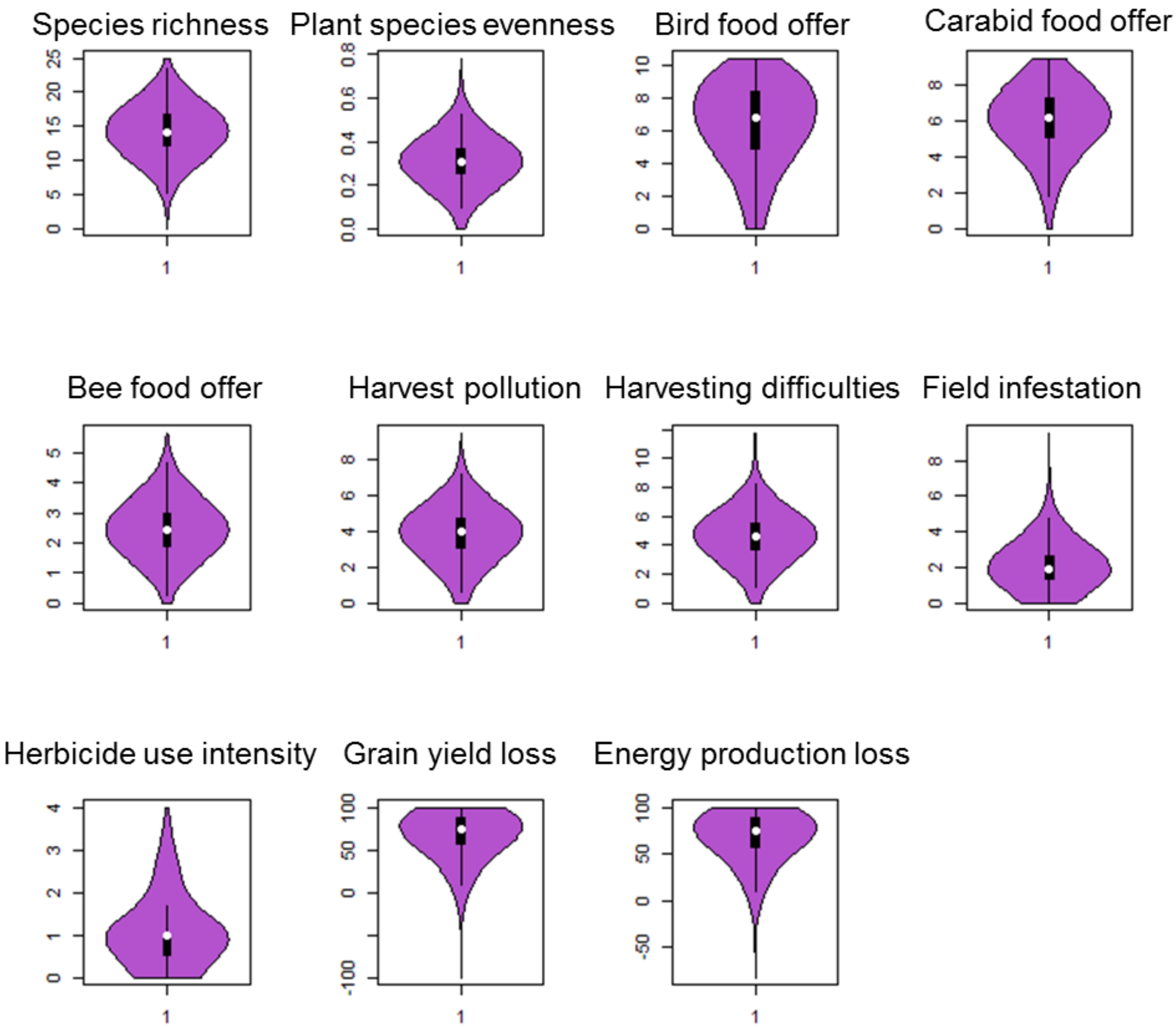


Figure 3 : Violin plots representing the distribution of all indicators values (kernel density), with the width representing the frequency, the white dot is the median, the thick black line is the interquartile range and the thin line is the 95% confidence interval.

Table S. 1 Details of the distribution of weed impact indicator values for all the cropping systems of the learning dataset.

	Plant species richness (nb plant)	**Plant species evenness** (no unit)	**Bird food offer** (seeds.m-2.day-1)	**Carabid food offer** (seed.m-2.day-1)	**Bee food offer** (plants·m-².day-1)	**Harvest pollution** (no unit)	**Harvesting difficulties** (no unit)	**Field infestation** (t.ha-1.day-1)	**Herbicide use intensity** (no unit)	**Grain yield loss** (% of g·m-²)	**Energy production loss** (% of MJ.ha-1)
Mean	14.27	0.31	6.40	6.04	2.46	3.83	4.58	2.05	1.02	69.19	69.22
Standard deviation	3.14	0.09	2.53	1.75	0.80	1.31	1.41	1.08	0.83	24.63	24.50
Min	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-100.0	-82.95
1stQ	12.09	0.25	4.90	5.05	1.91	3.07	3.74	1.32	0.55	56.73	56.86
Median	14.20	0.31	6.76	6.18	2.45	3.97	4.66	1.93	1.00	75.11	75.12
3rdQ	16.68	0.36	8.38	7.22	3.01	4.72	5.52	2.68	1.00	88.12	88.04
Max	25.00	0.78	10.43	9.46	5.68	9.54	11.79	9.57	4.00	100.00	100.00

5 Variation in crop yield loss due to stochasticity

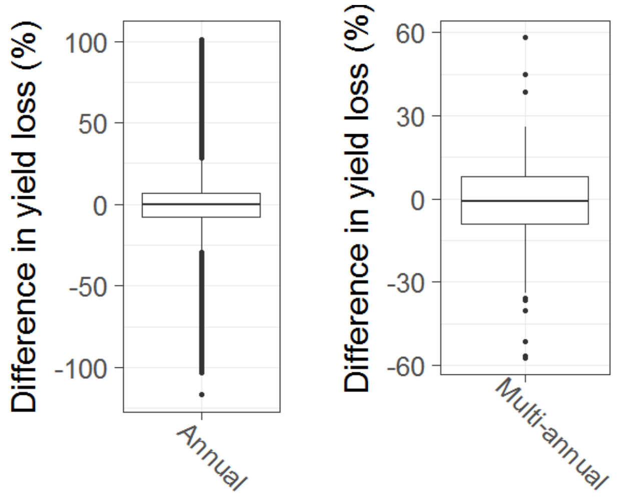


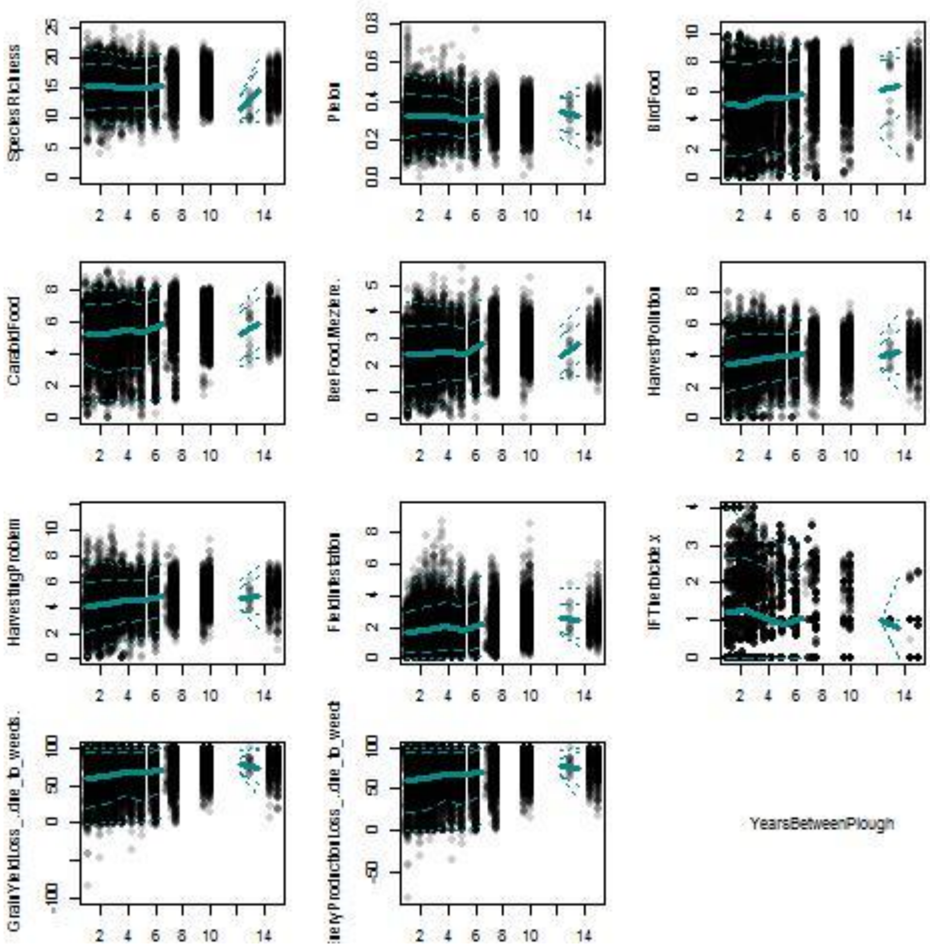
Figure 4. Difference in crop yield loss (%) in two successive series of simulations, without any change in input variables. Example of herbicide-free cropping systems.

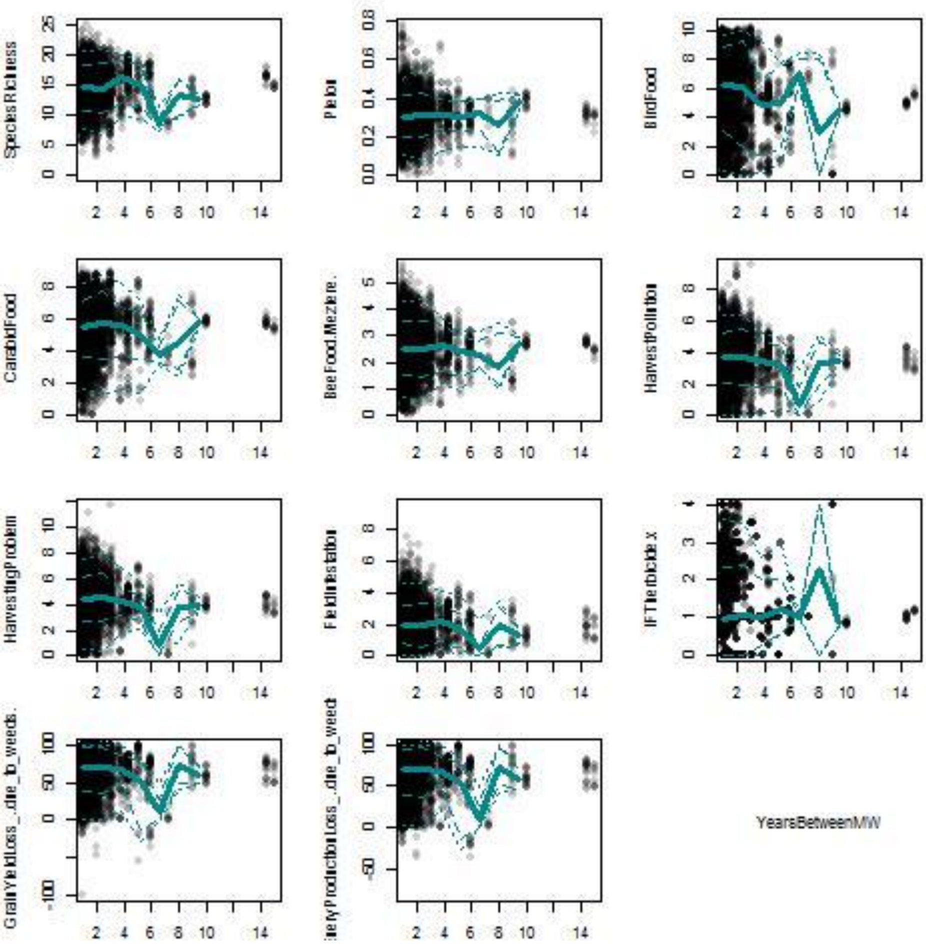
Table 3. Difference in crop yield loss (%) in two successive series of simulations, with any change in input variables. Example of herbicide-free cropping systems.

Scale	Min.	1st Quartile	Median	Mean	3rd Quartile	Max.
Annual	-116.8	-7.7	0.0	-0.8	6.7	101.3
Multi-annual	-57.5	-8.9	-0.9	-1.7	8.0	58.3

Figures to follow:

Weed impact indicator values depending on the cropping system descriptors. Dots are indicator value averaged over all simulated years of a cropping system x weather repetition. In blue, moving mean and quantiles, for 10 points (or 5 for (*) marked figures), mean in bold, 0.01 and 0.99 quantiles in dotted line and 0.1 and 0.9 quantiles in dashed line.




SpeciesRichness
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BirdFood
CarabidFood
BeeFood.Mezlere.
HarvestPollution
HarvestingProblem
FieldInfestation
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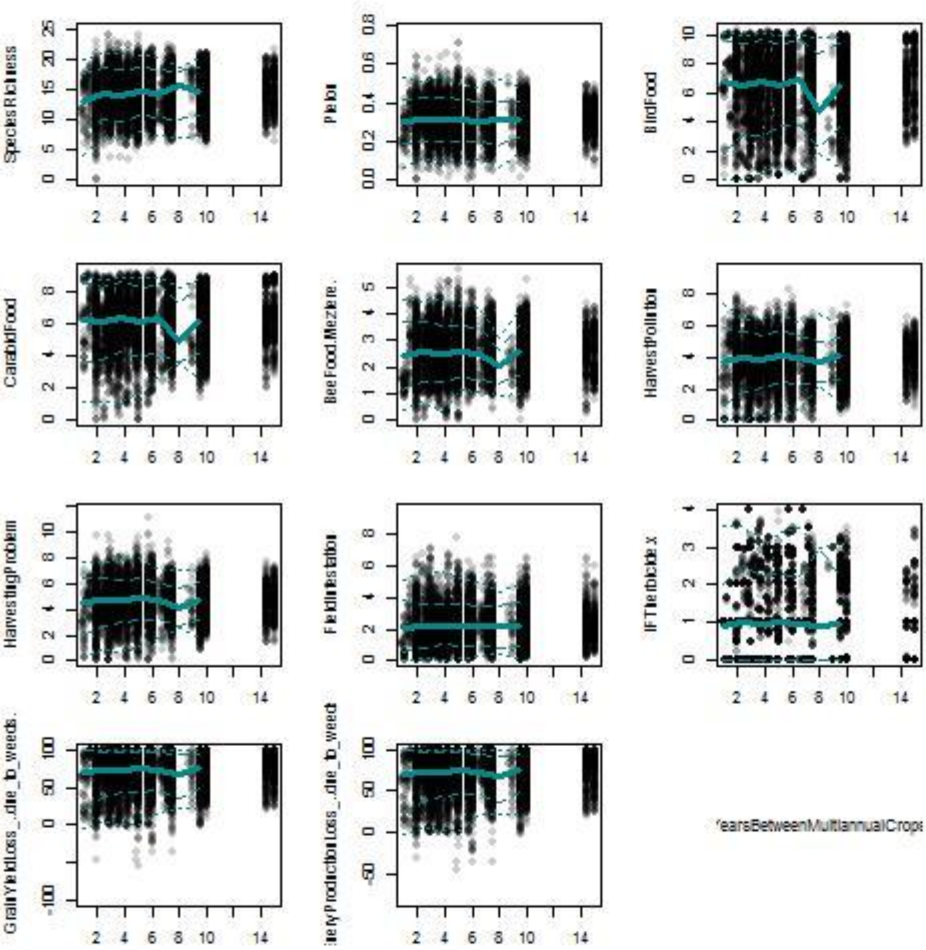
ietyProductionLoss_.due_to_weed
YearsBetweenMW


SpeciesRichness
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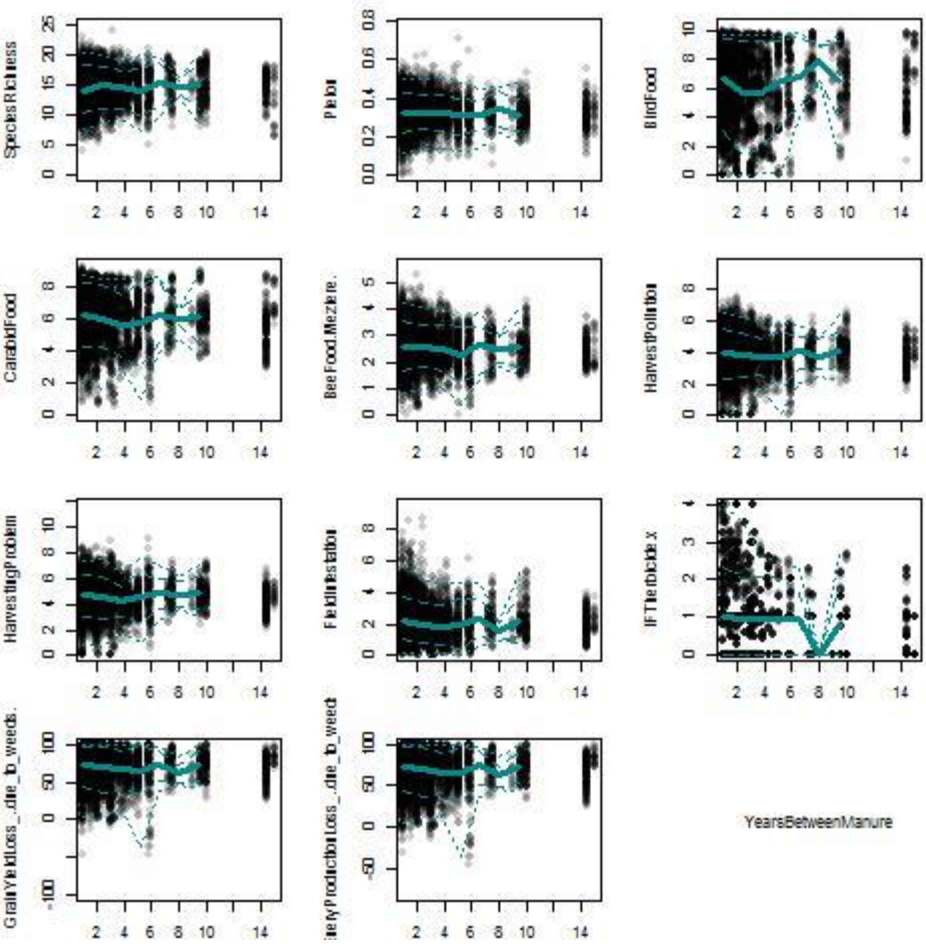
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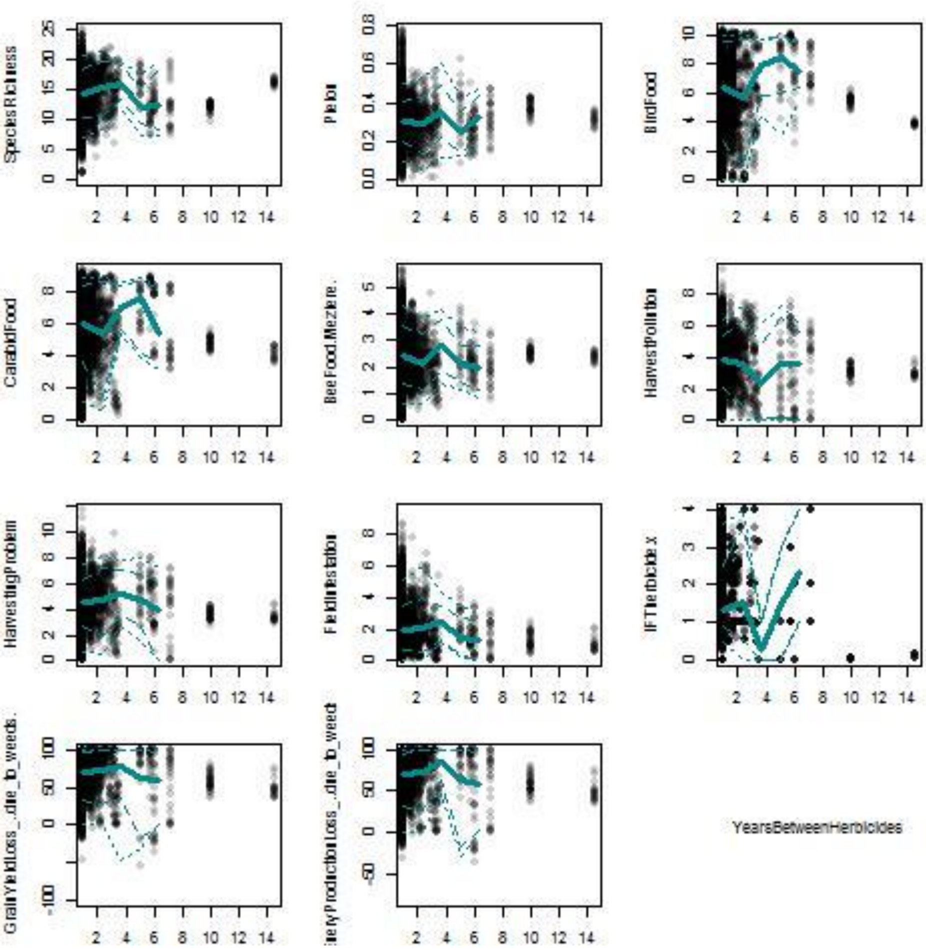
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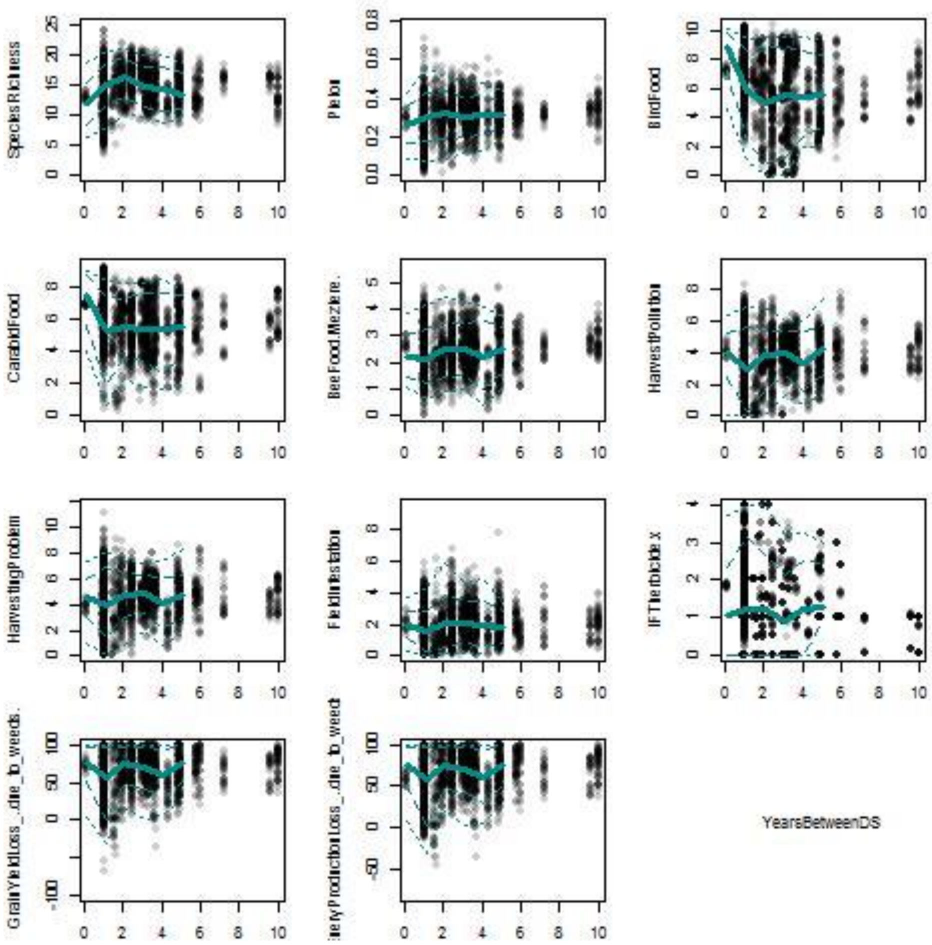
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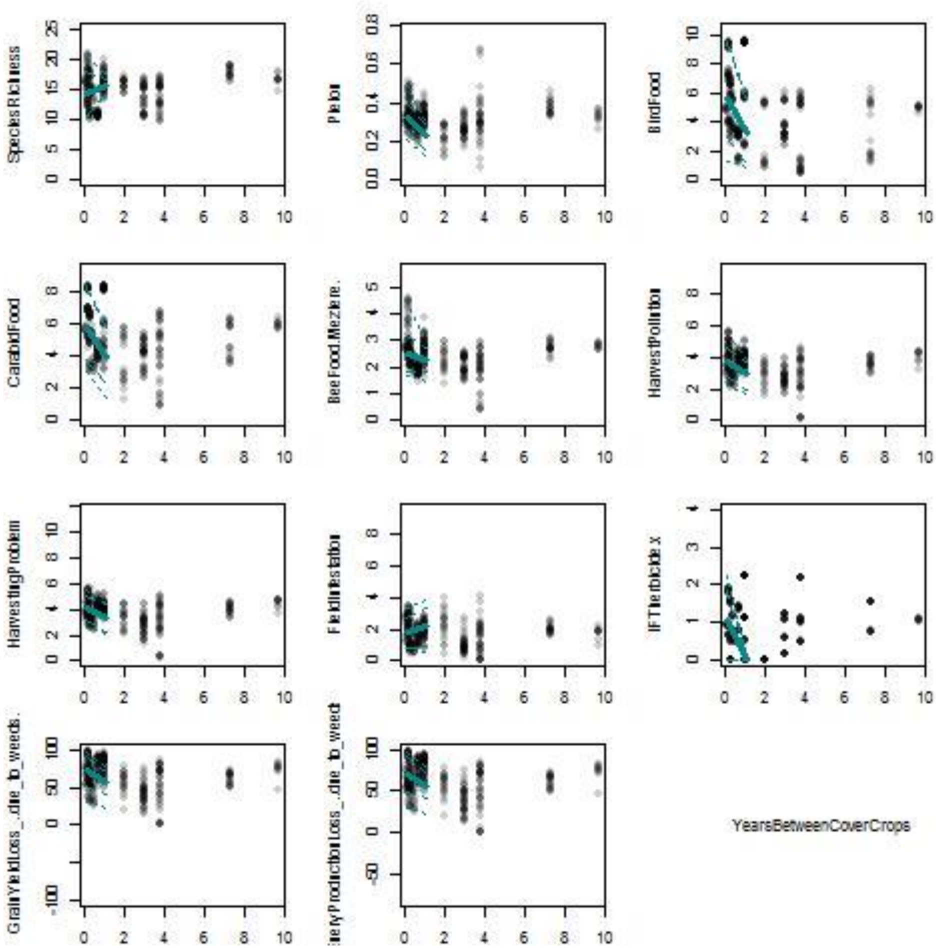
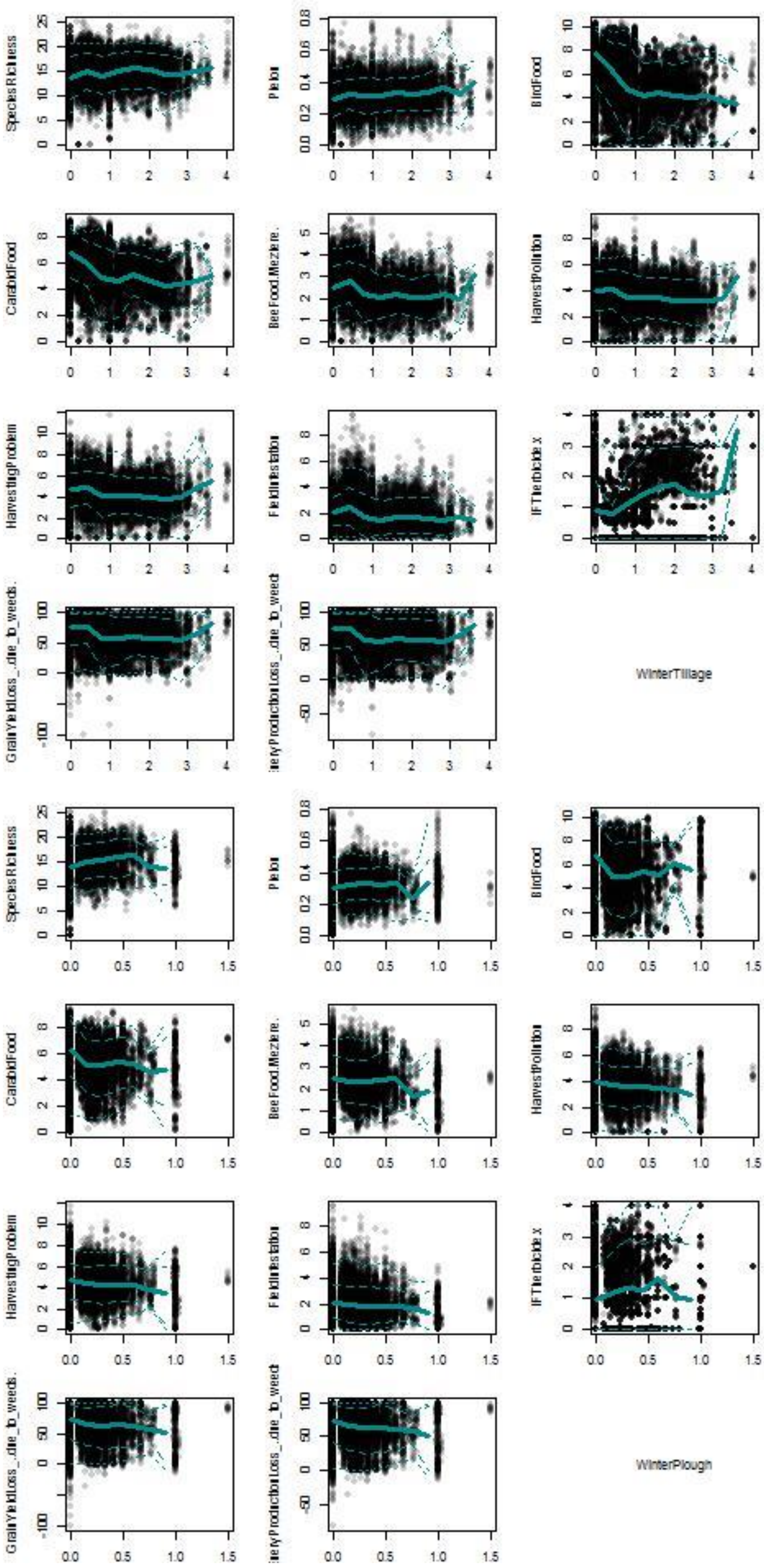
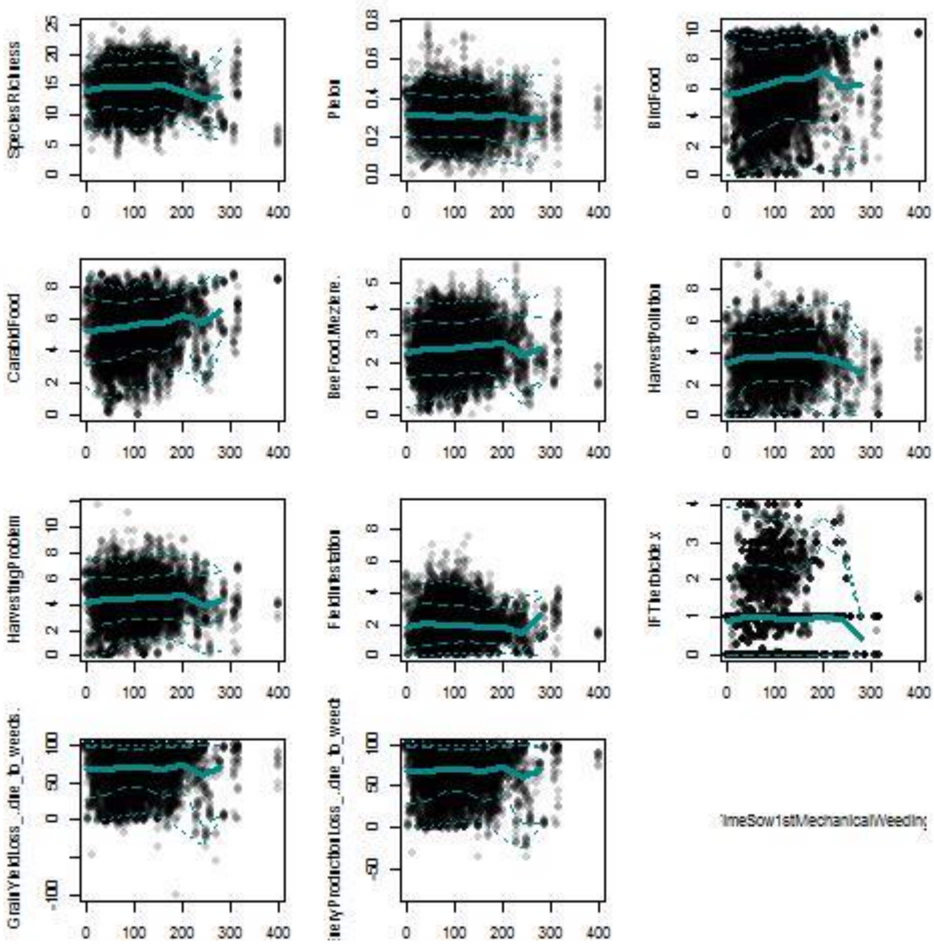

YearsBetweenCoverCrops


WinterTillage
WinterPlough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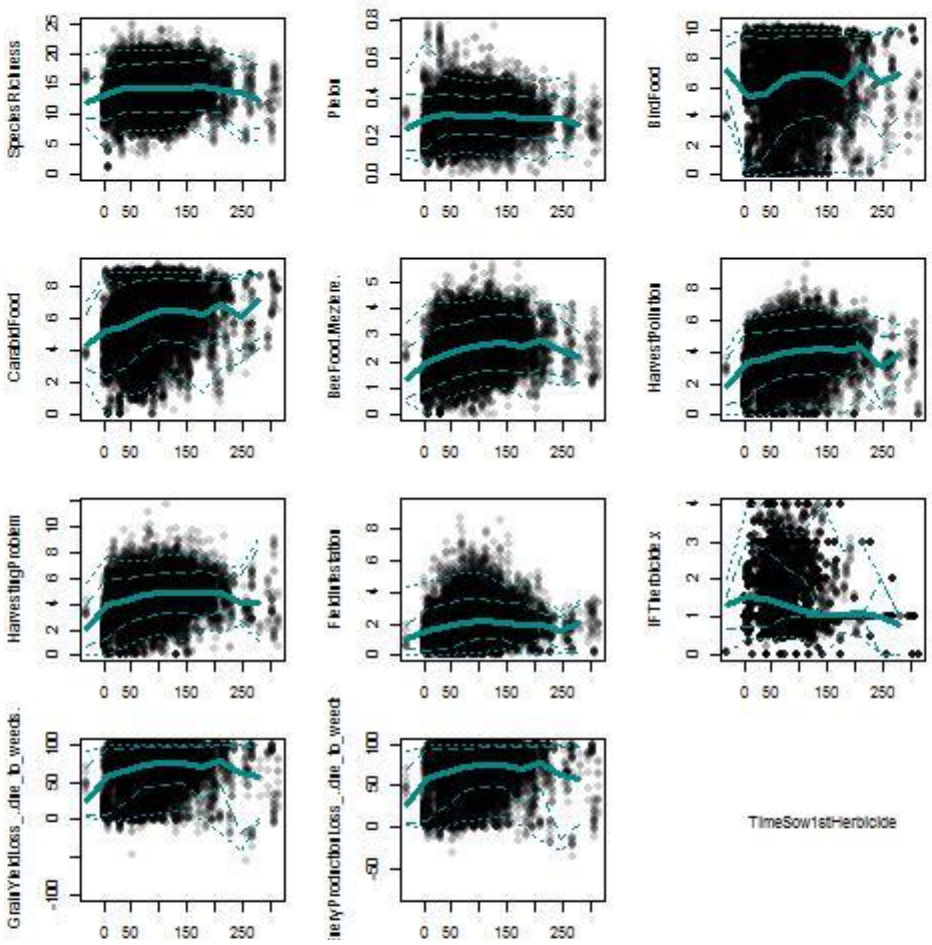
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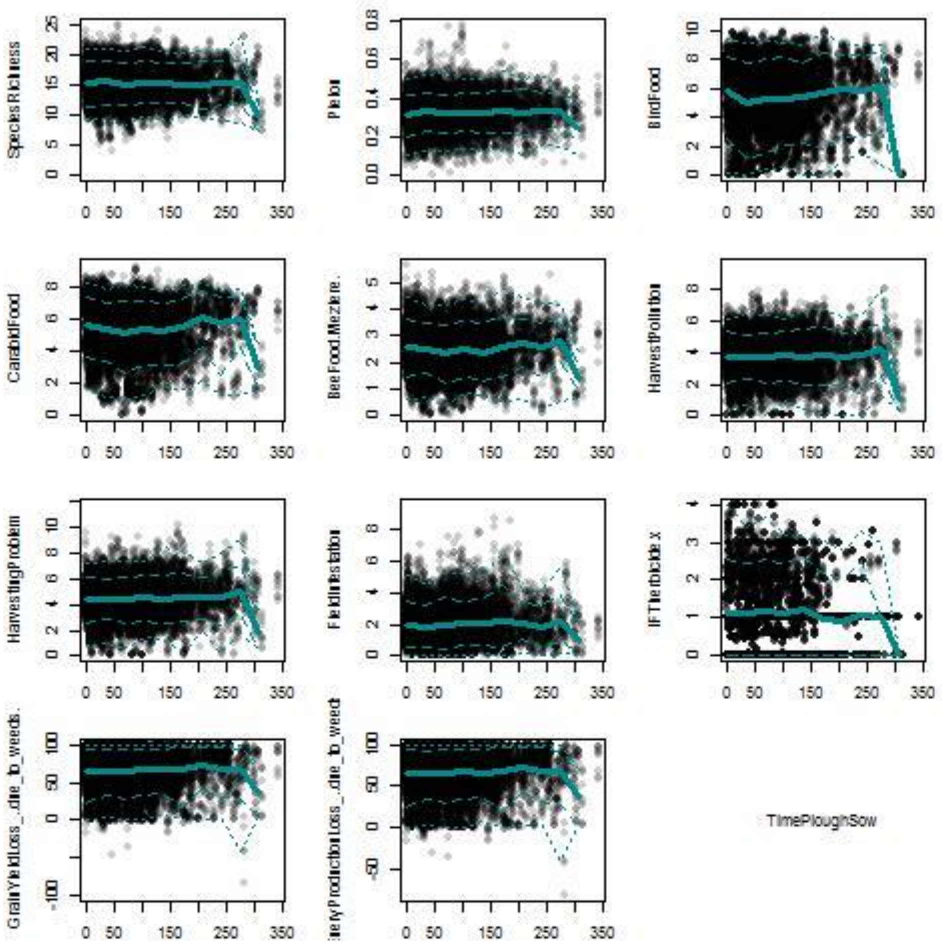
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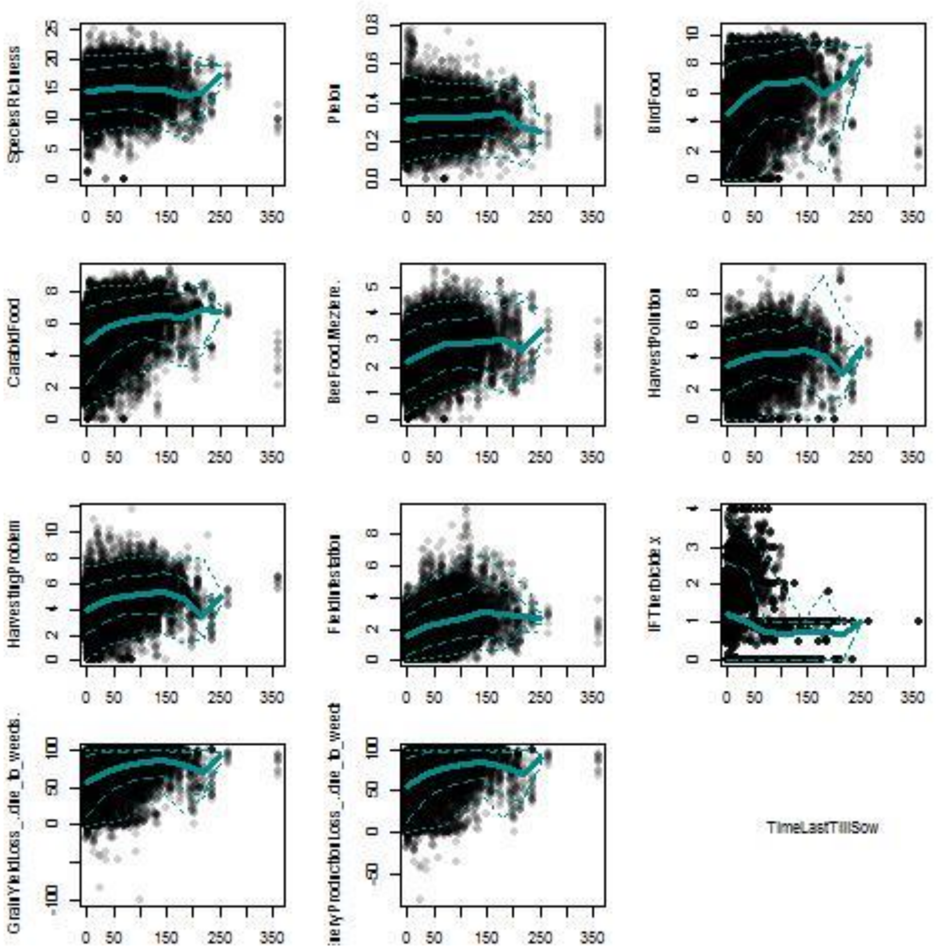
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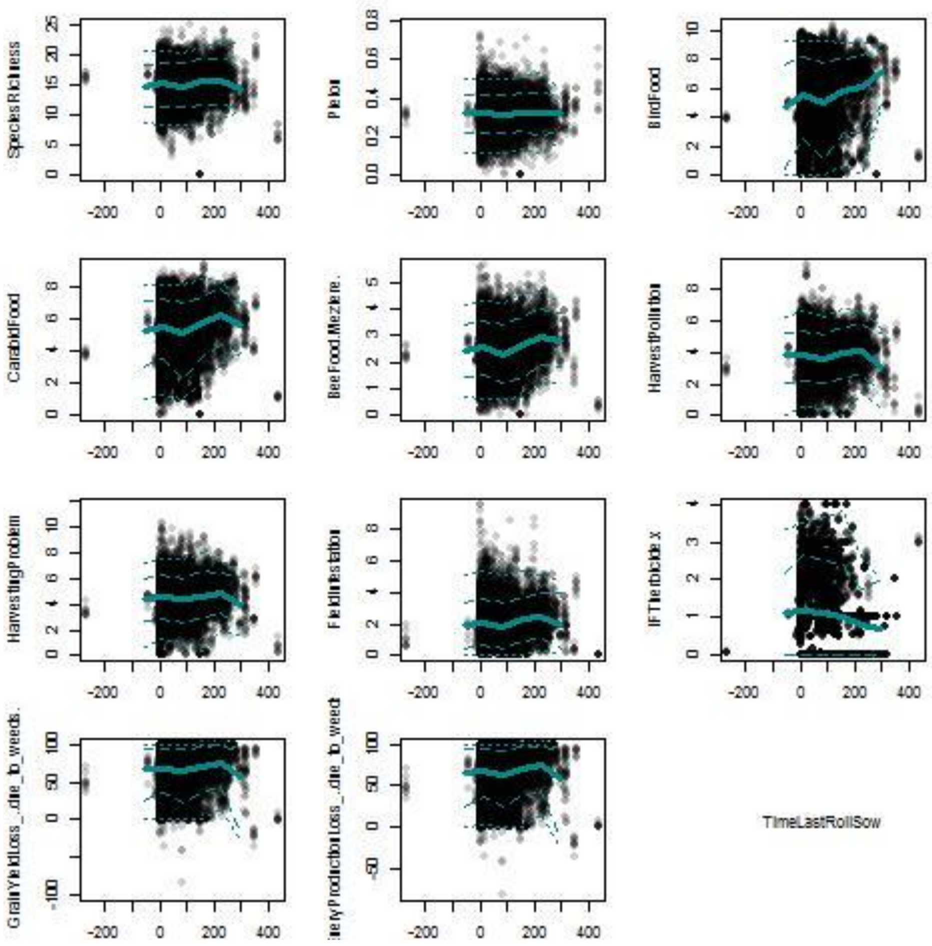
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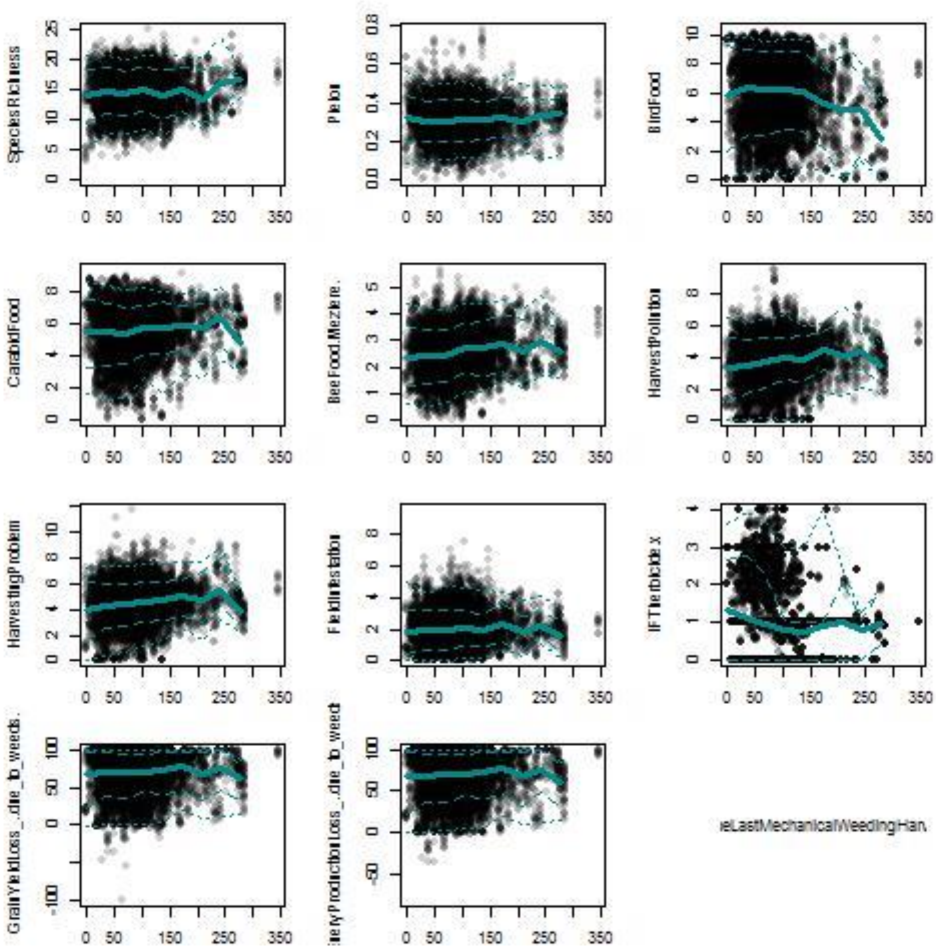
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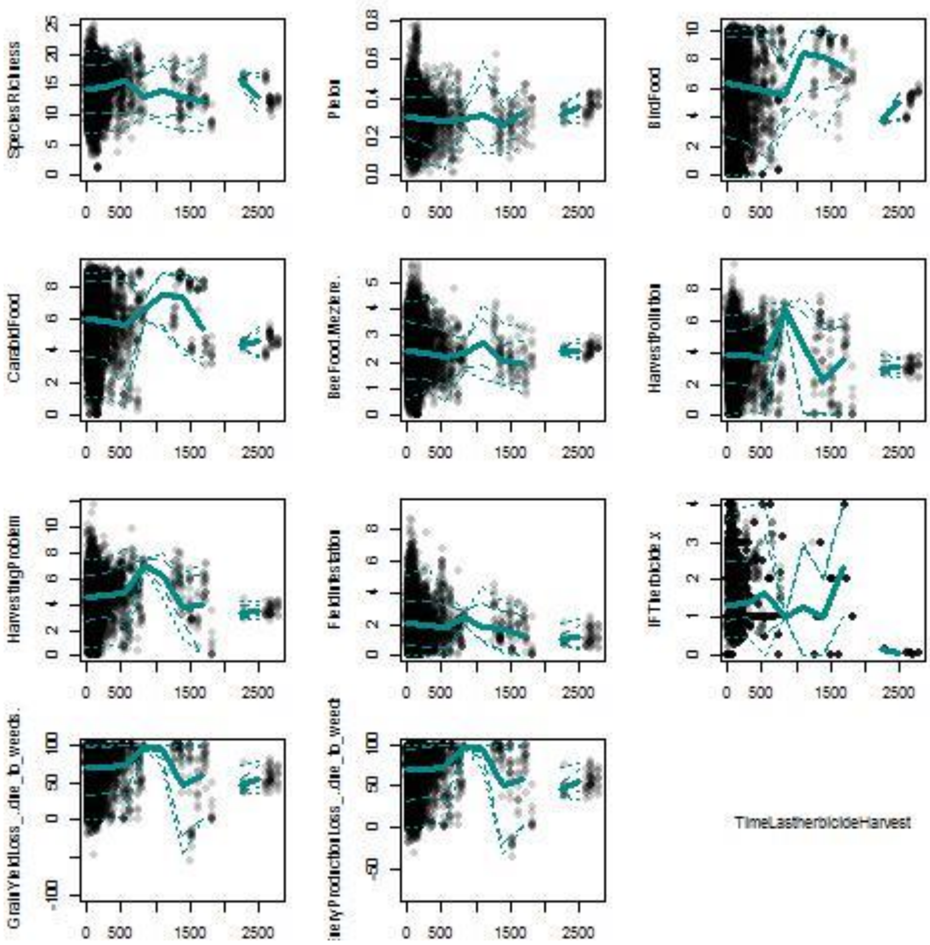
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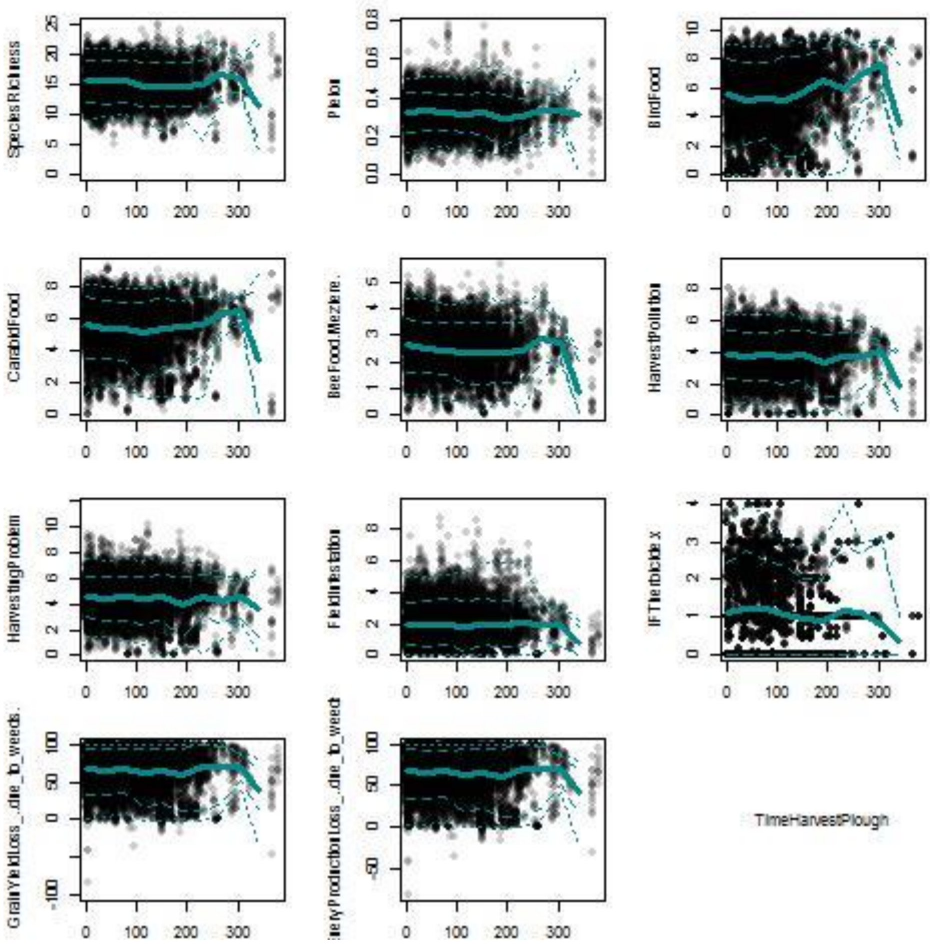
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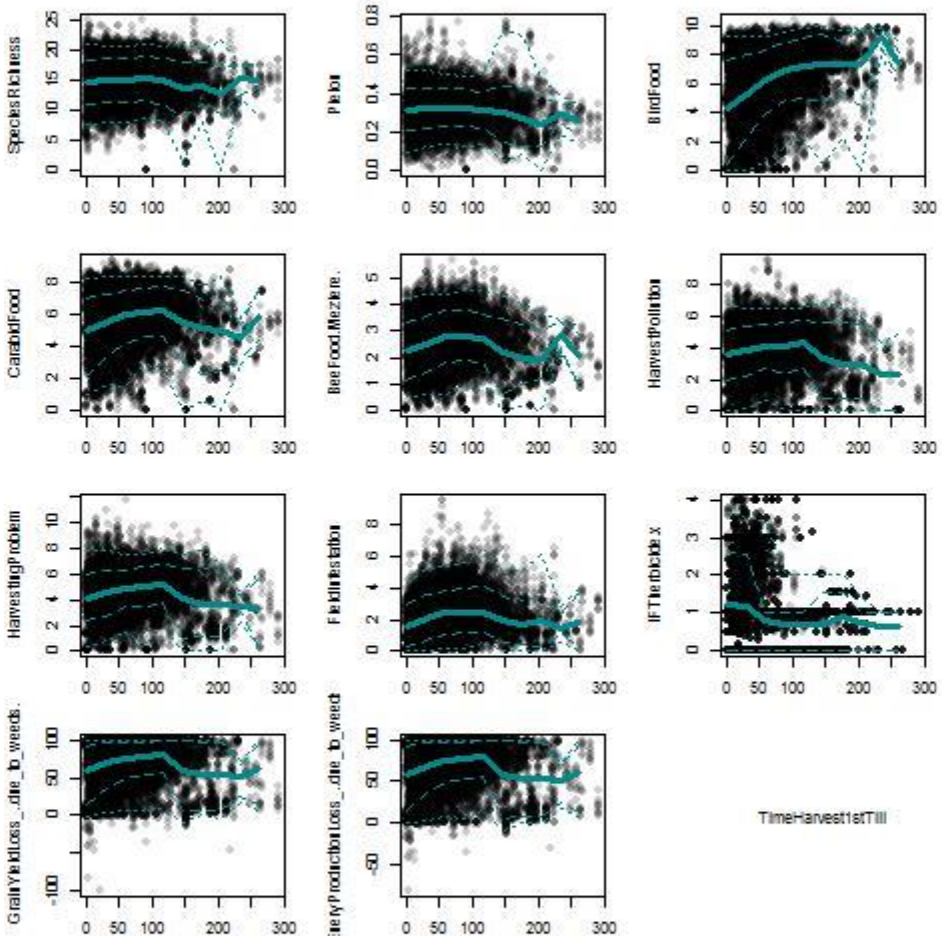
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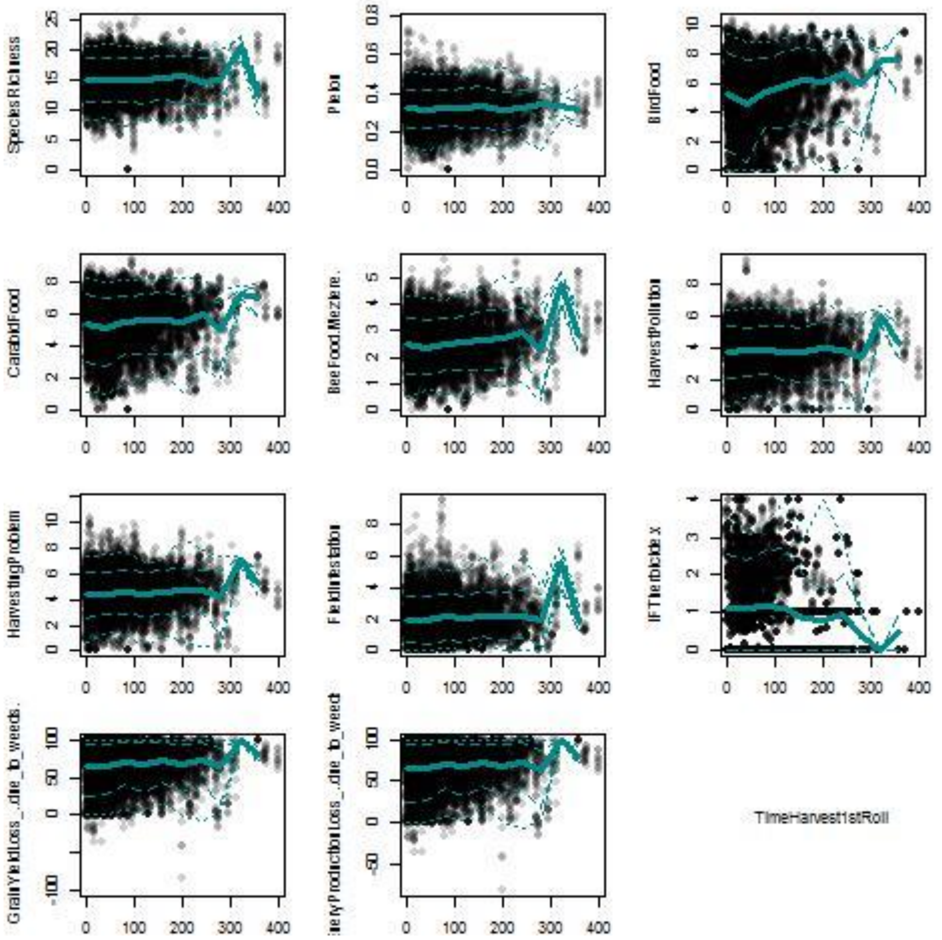
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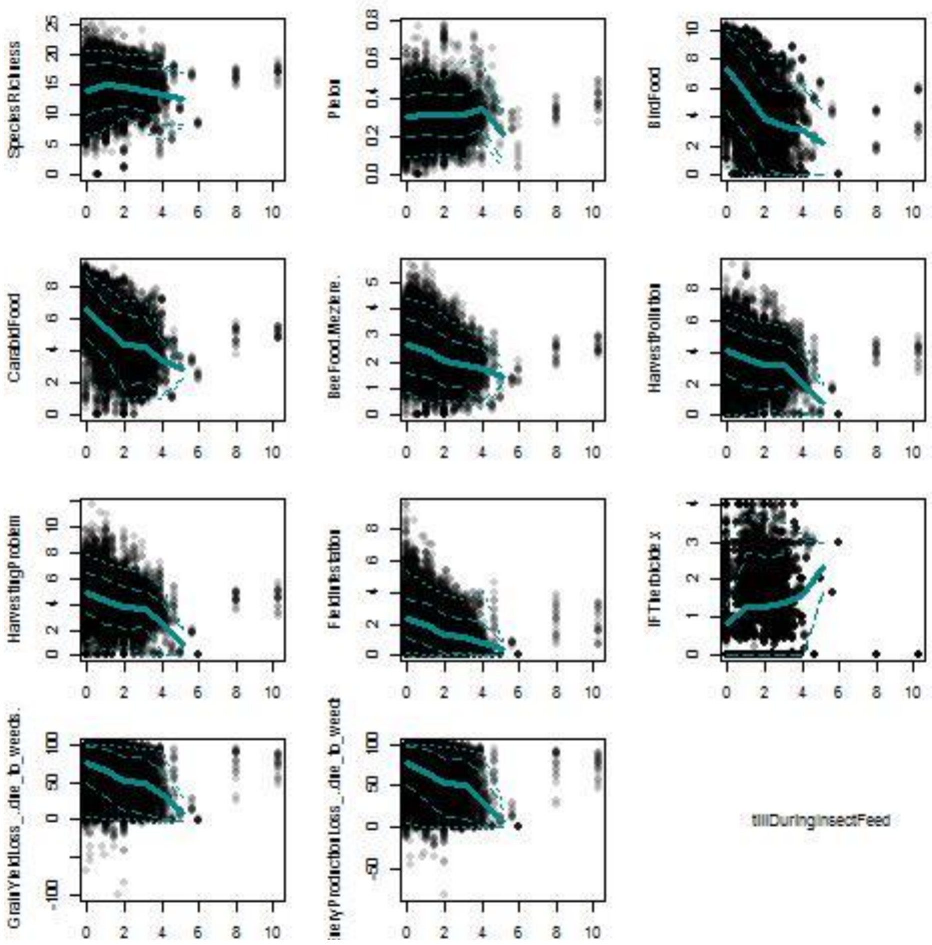
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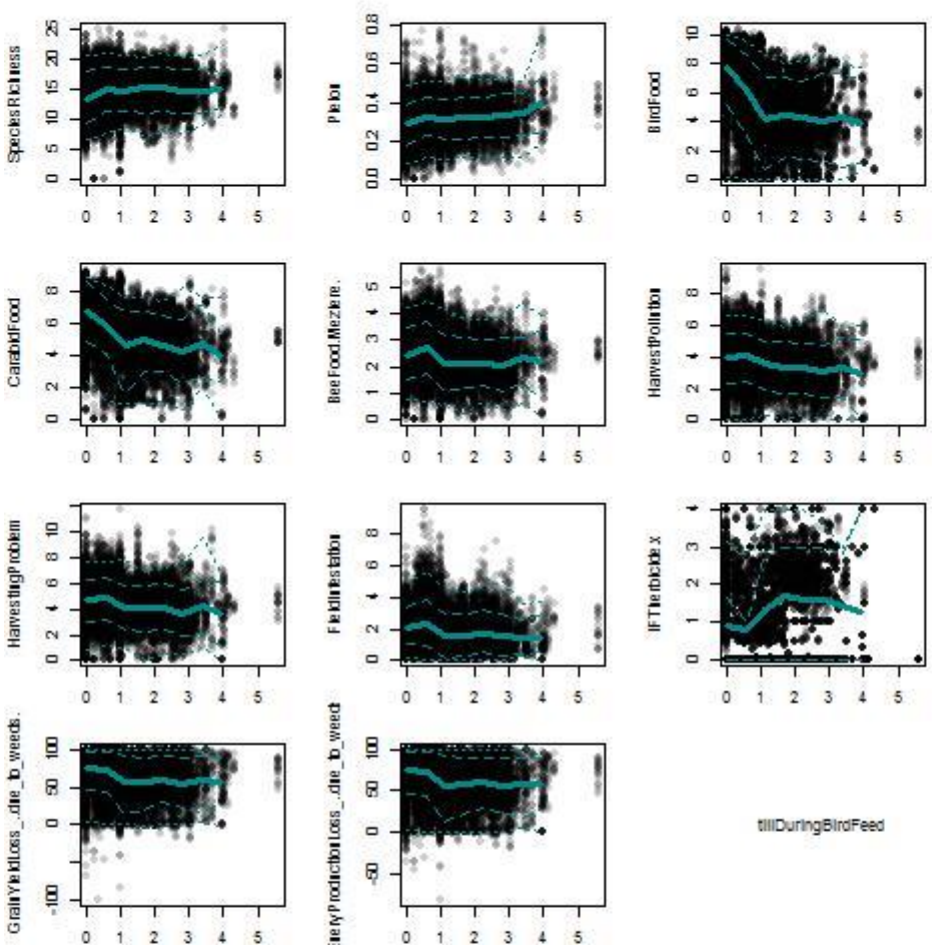
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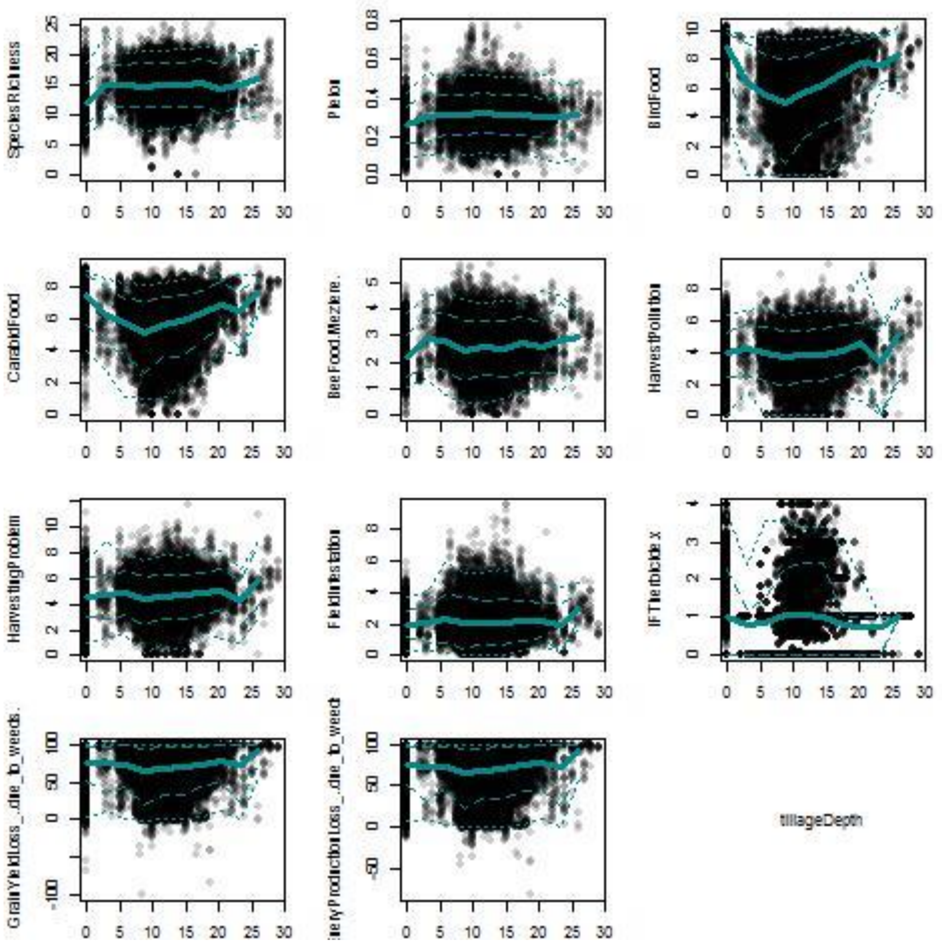
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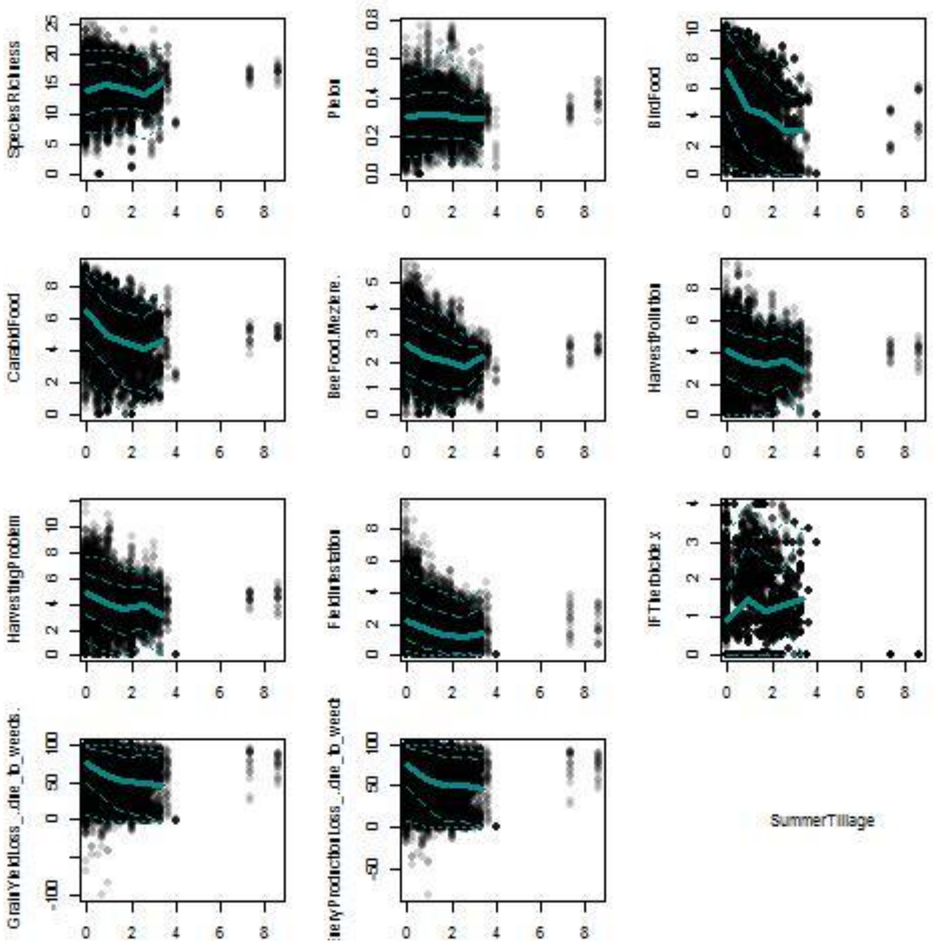
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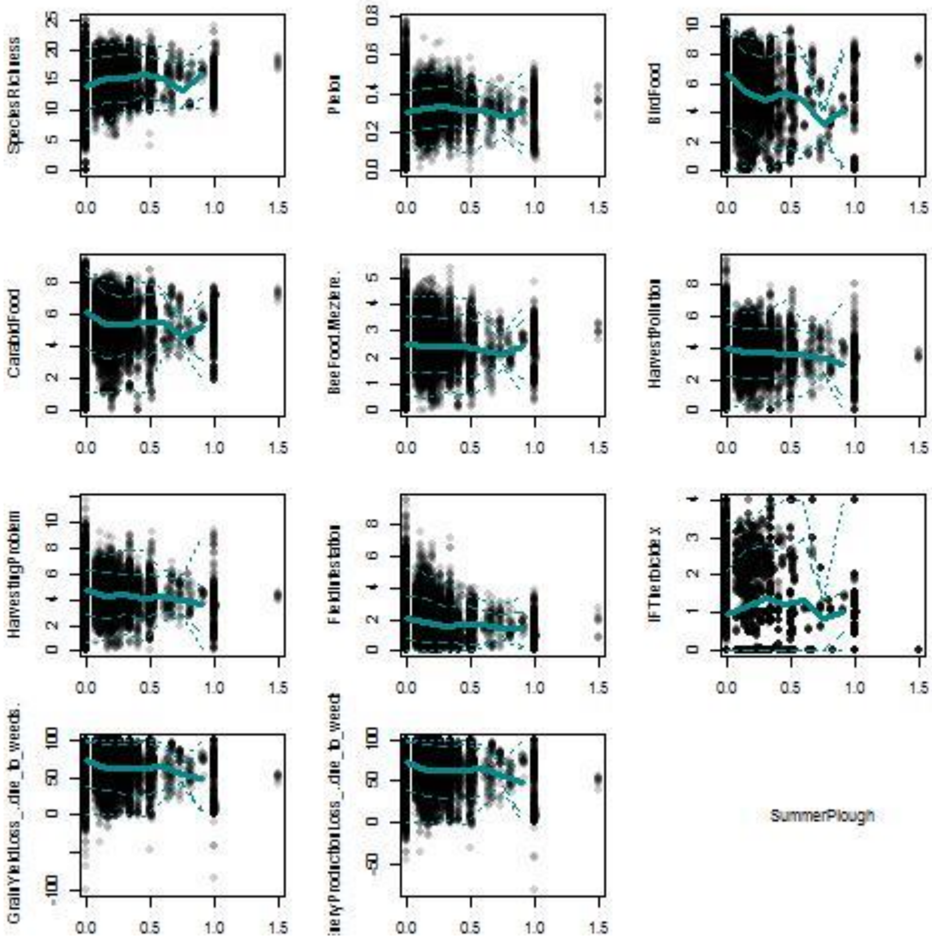
SummerTillage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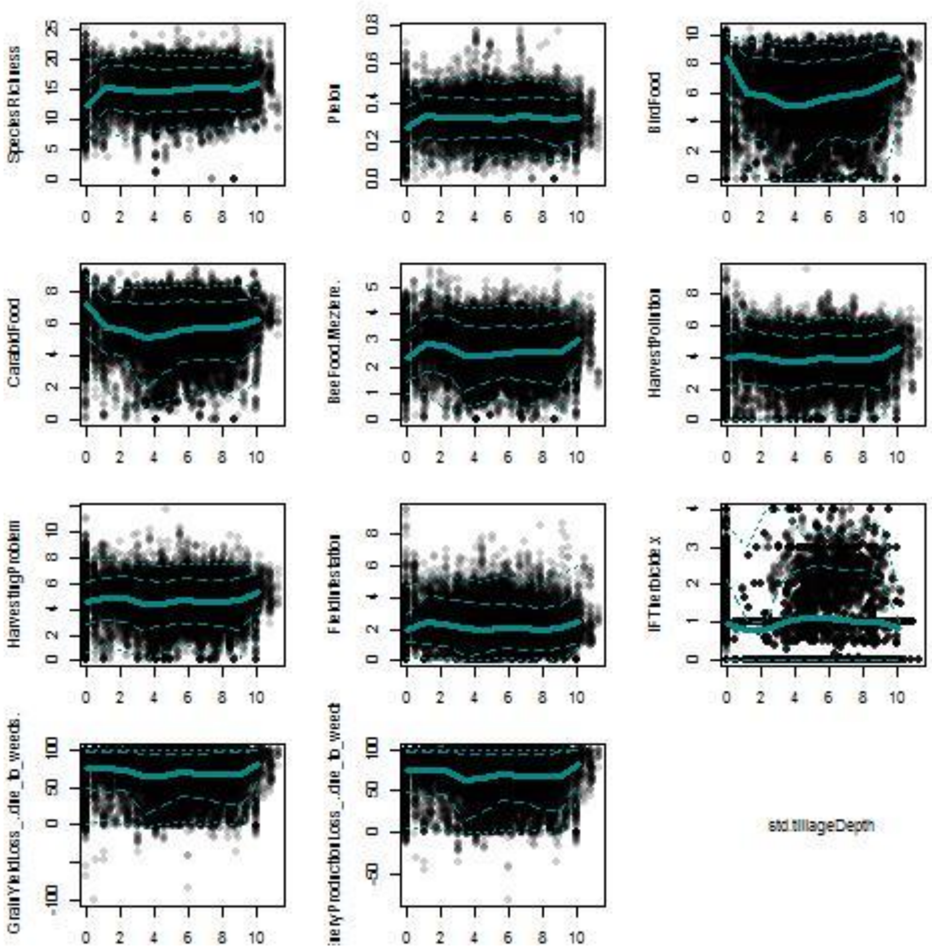
SummerPlough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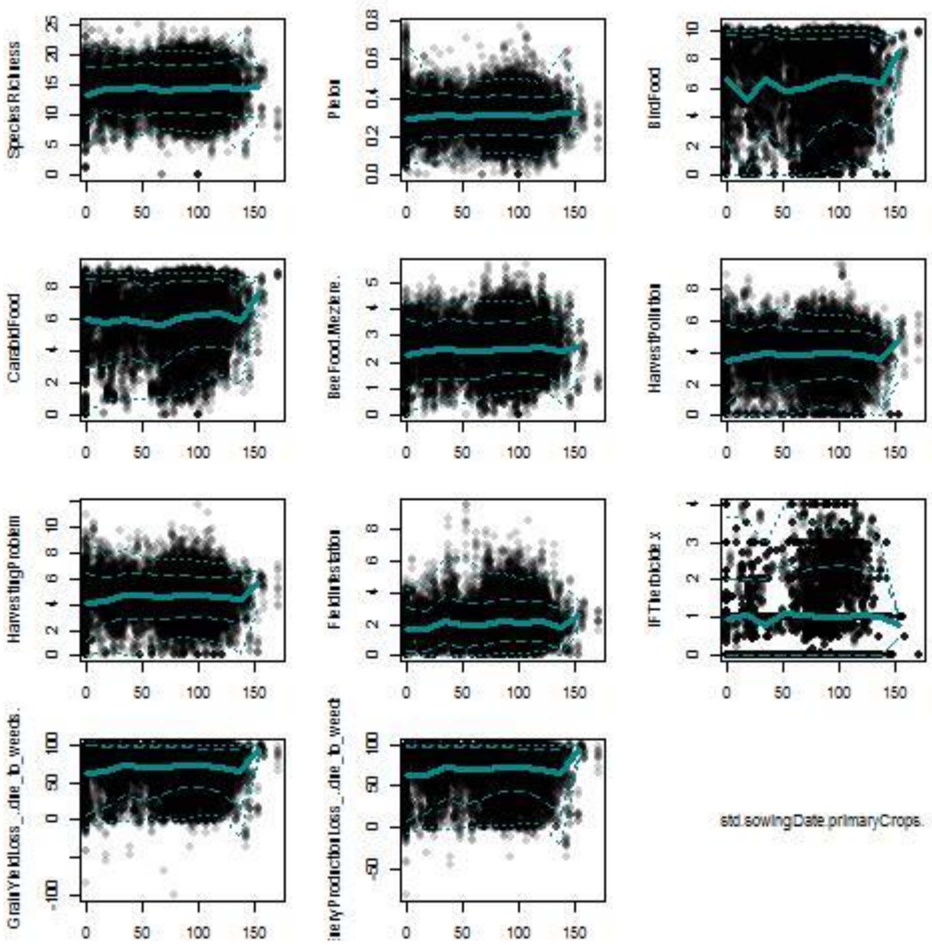
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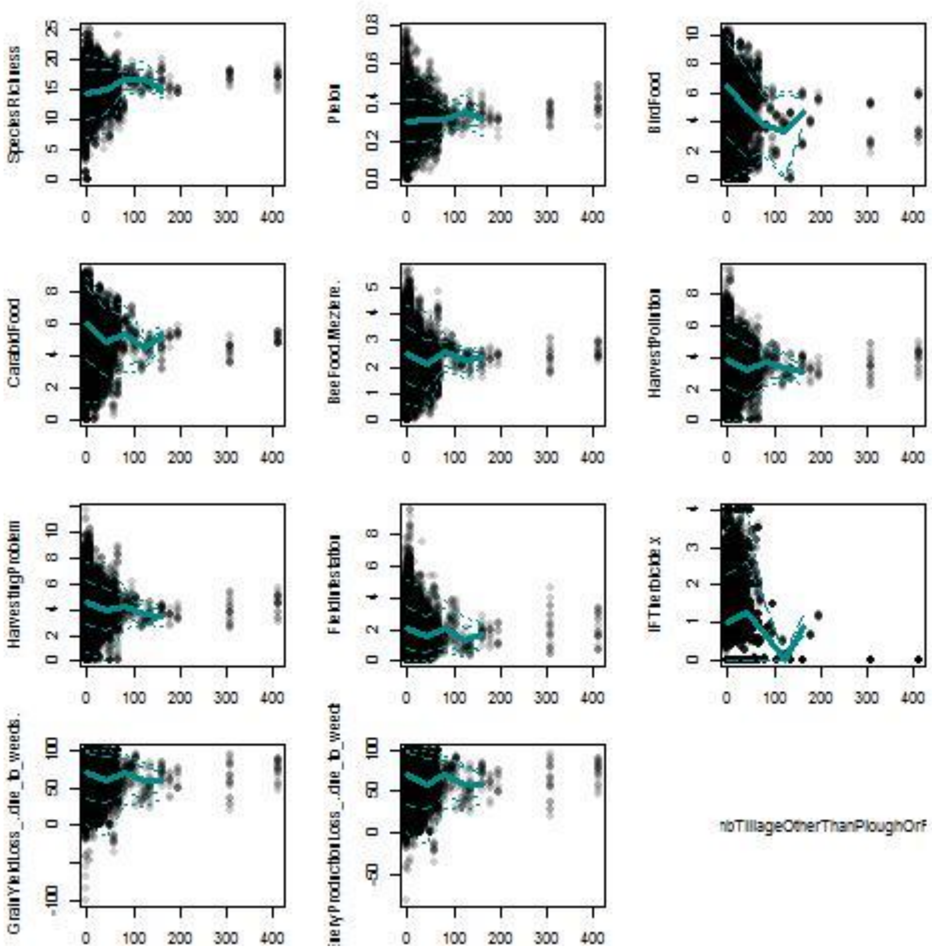
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IFTherbicide.x
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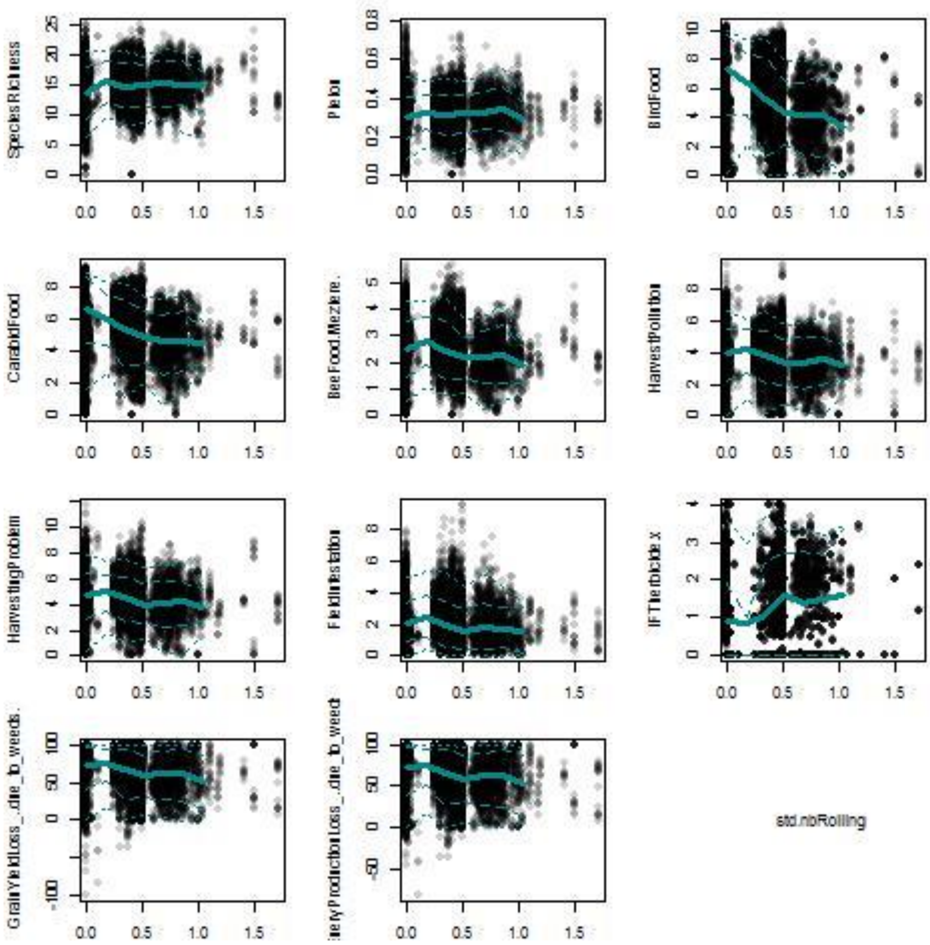
nbTillageOtherThanPloughOrF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CarabidFood
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FieldInfestation
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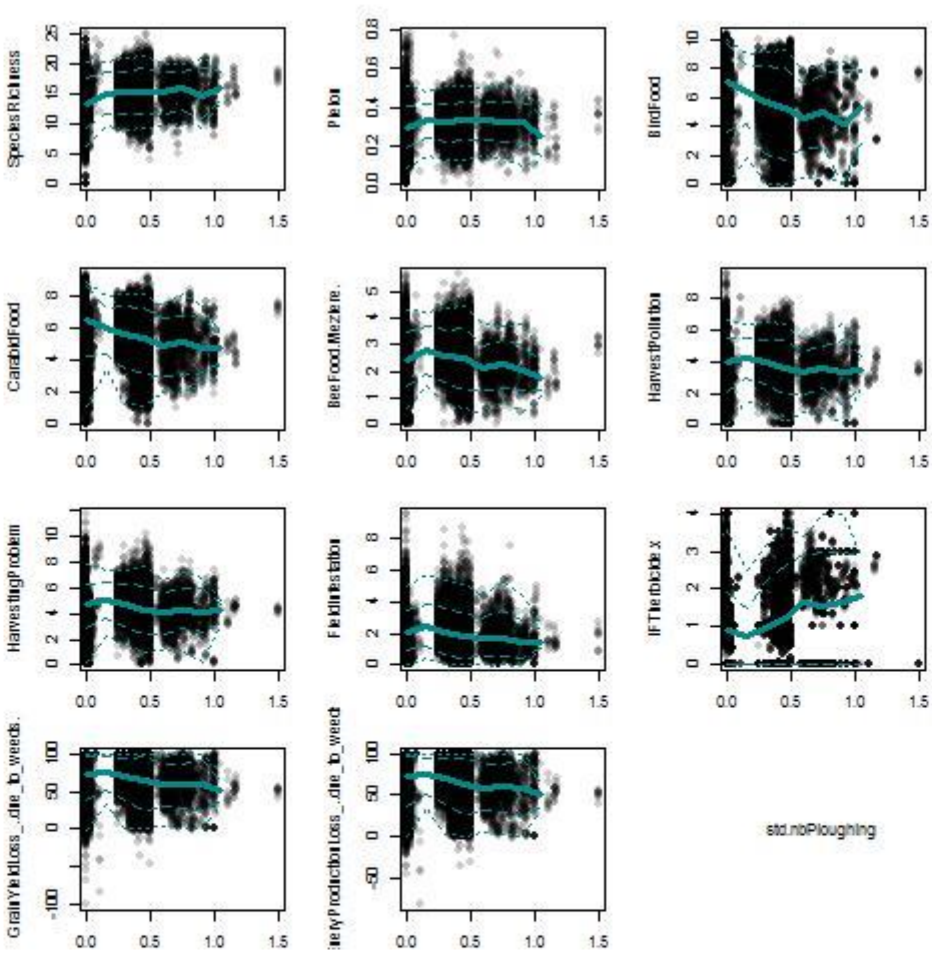
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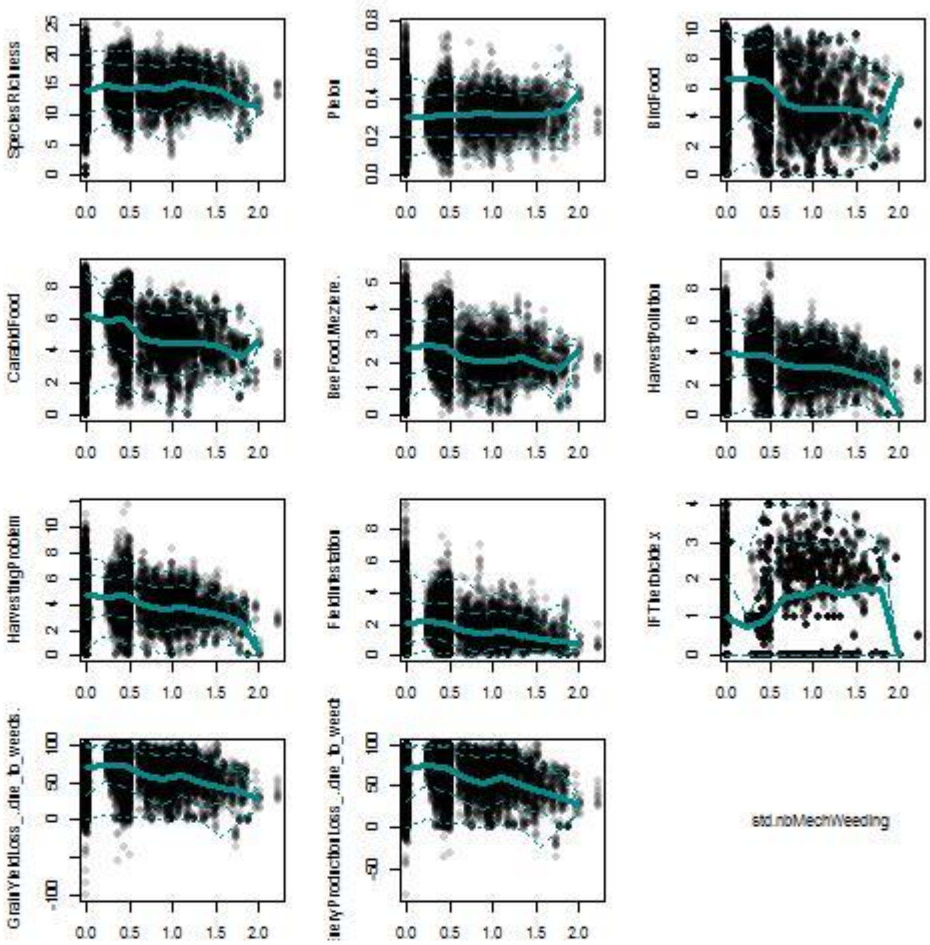
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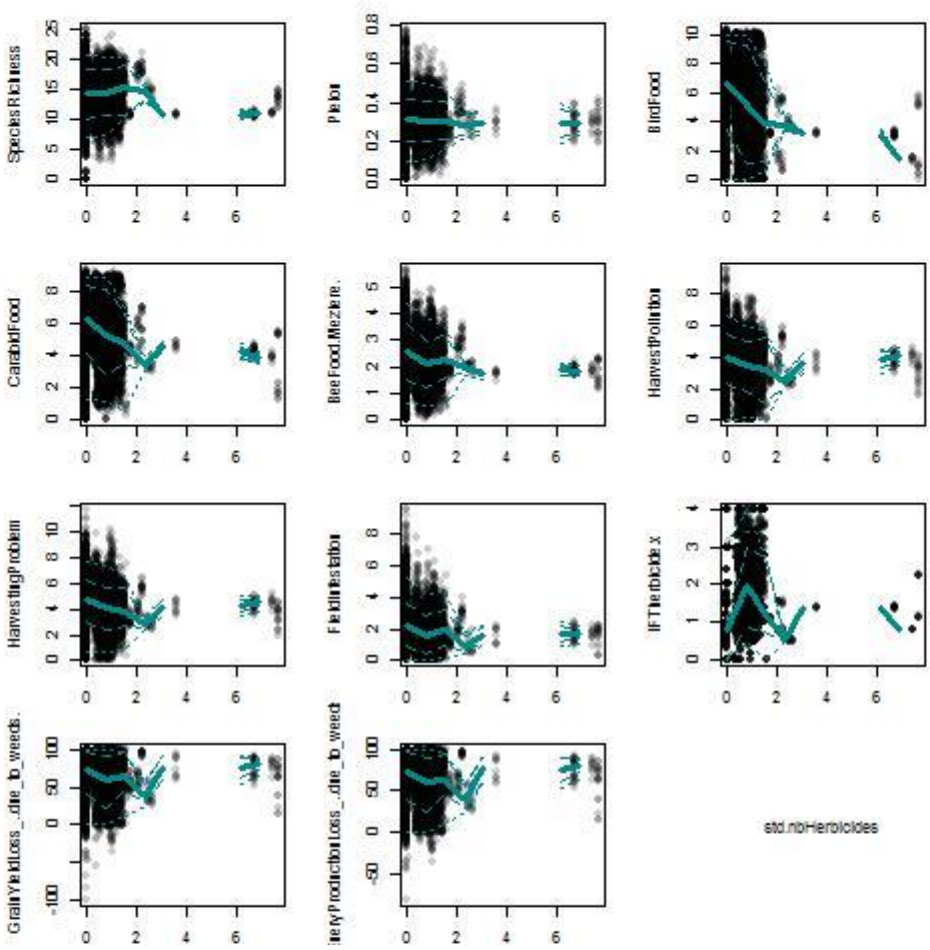
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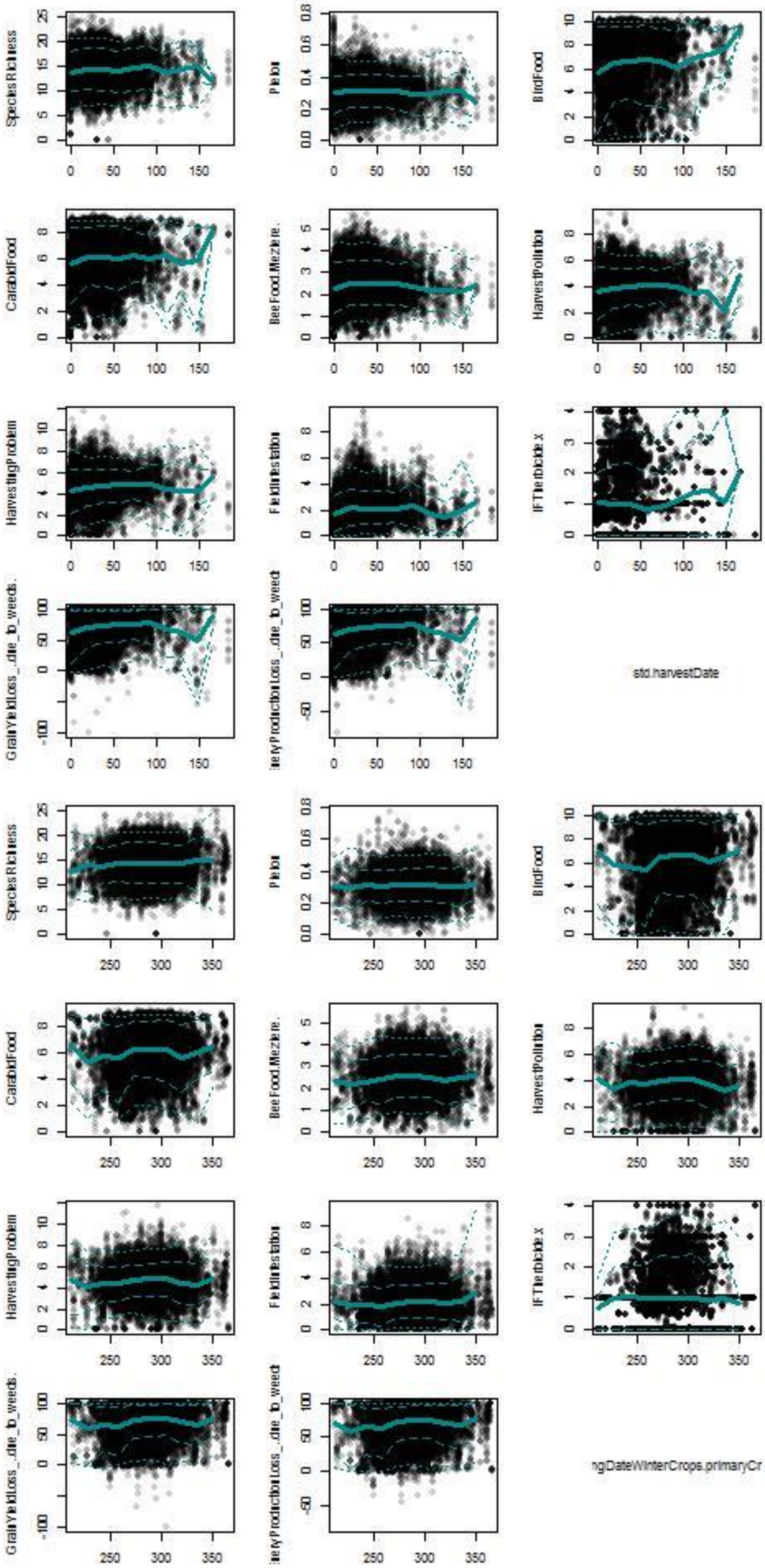
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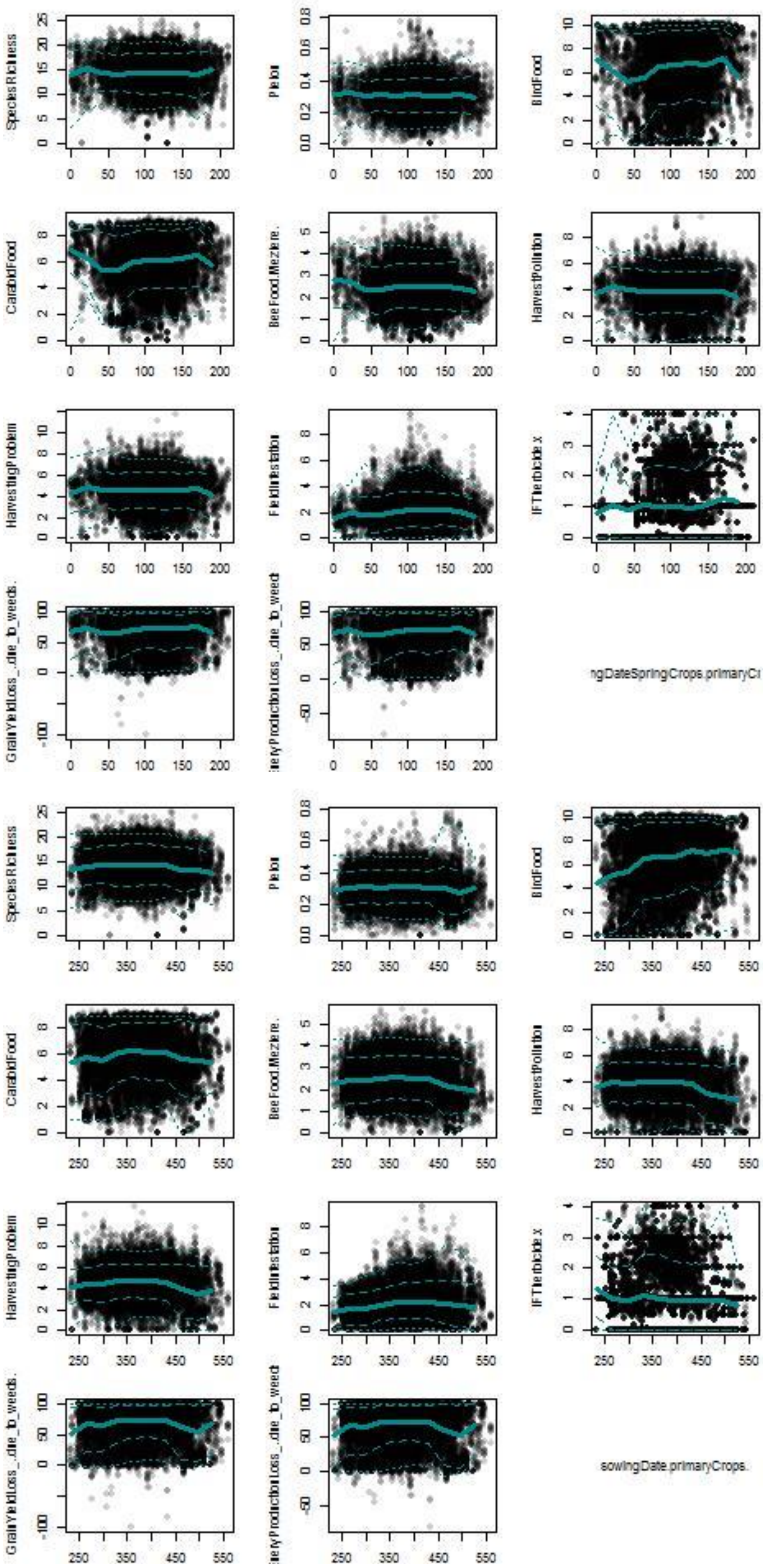
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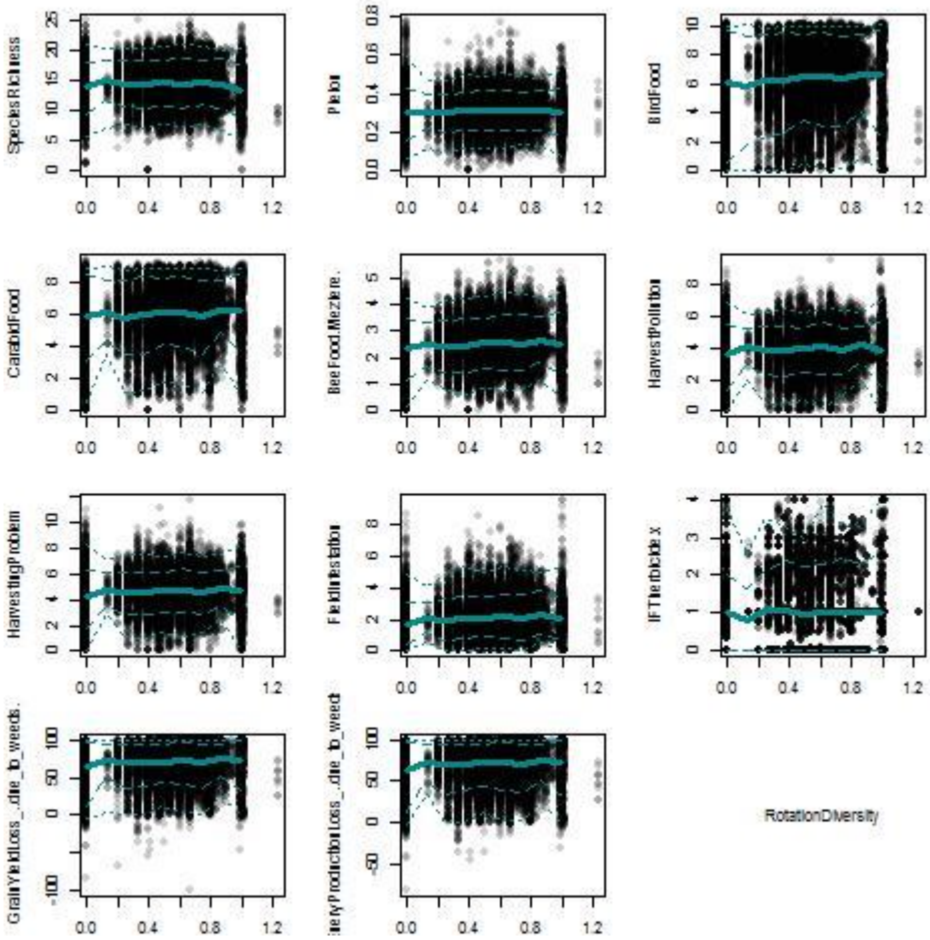
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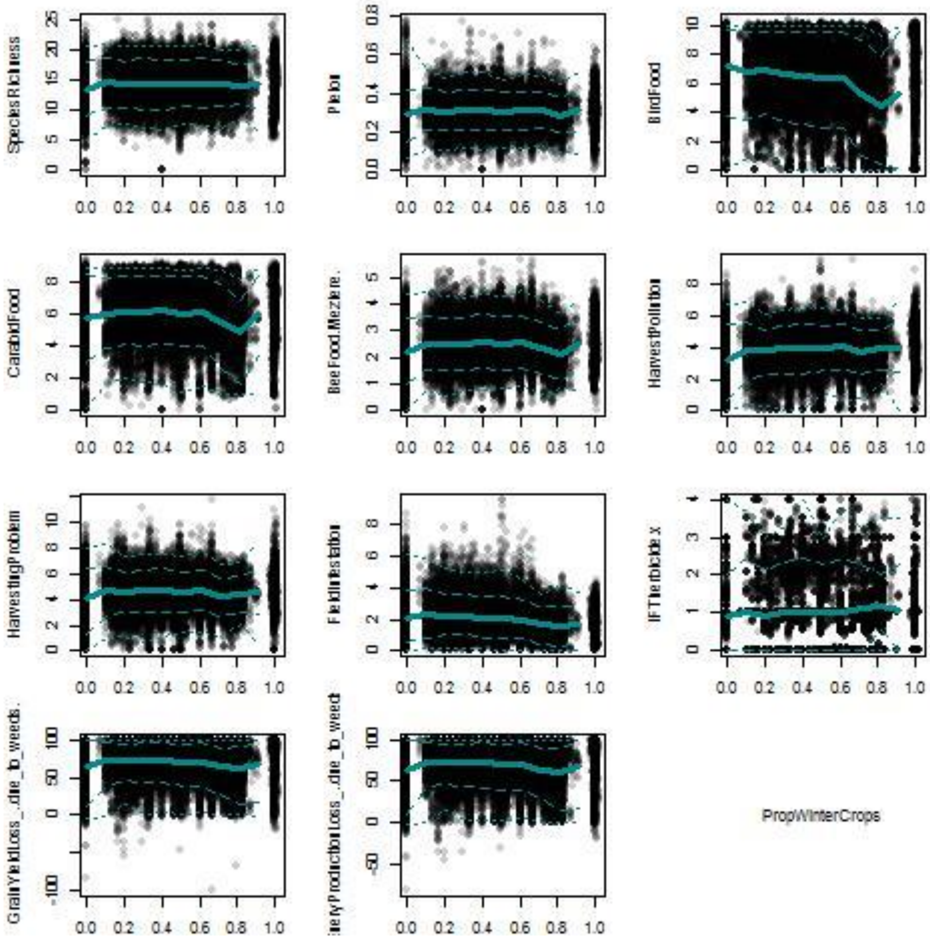
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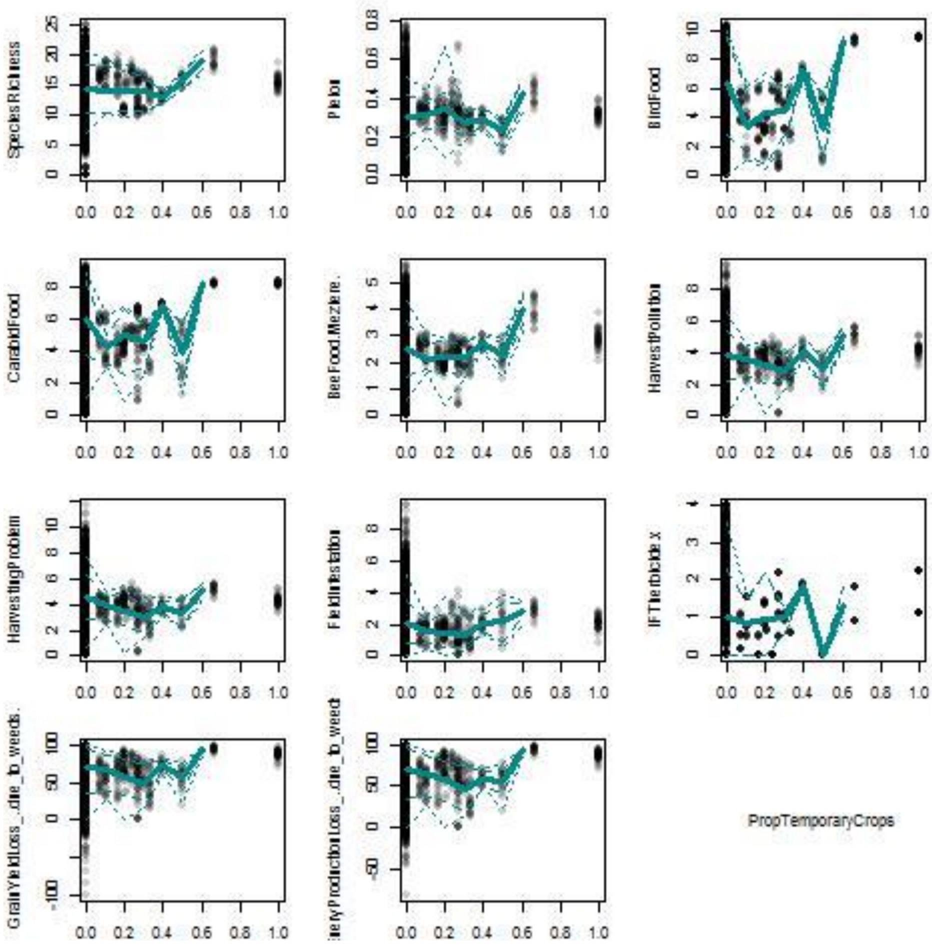
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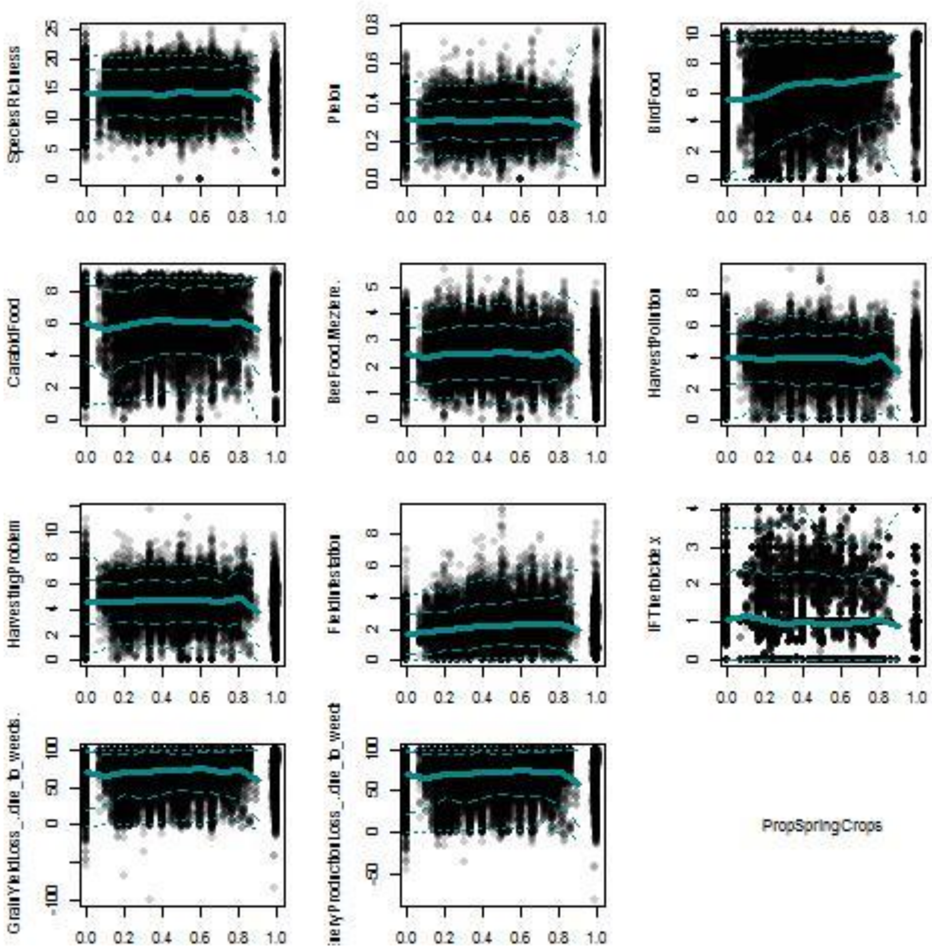
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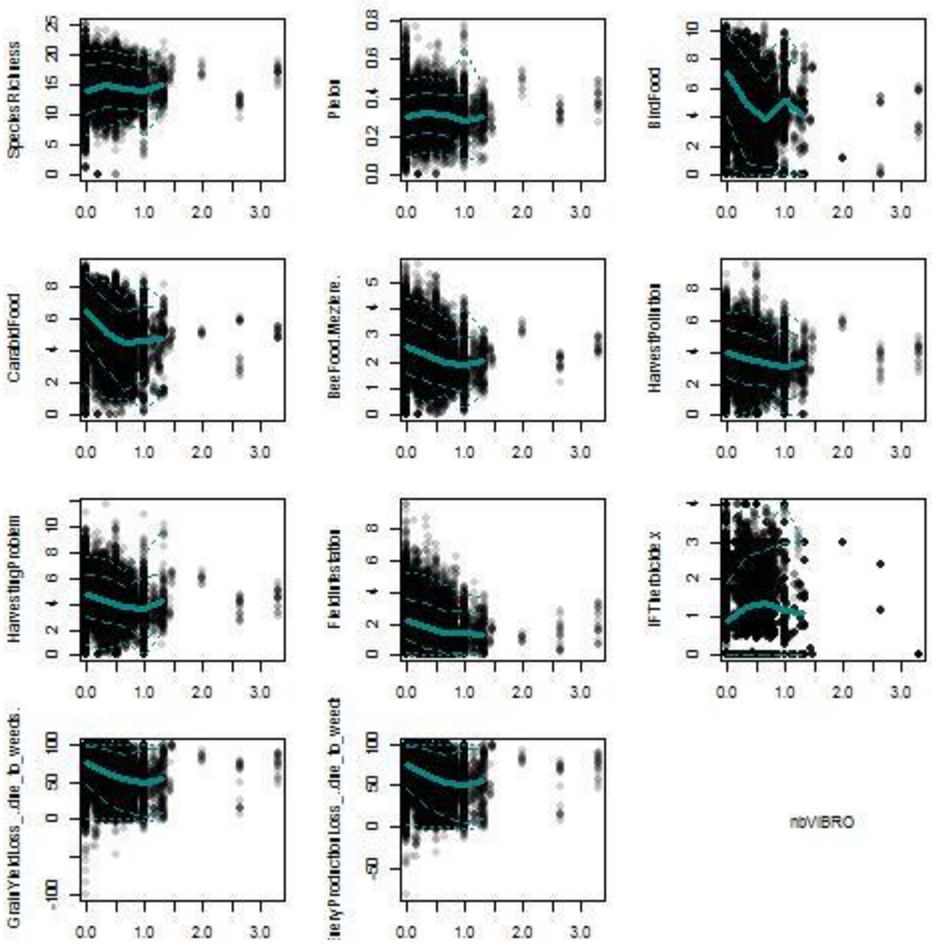

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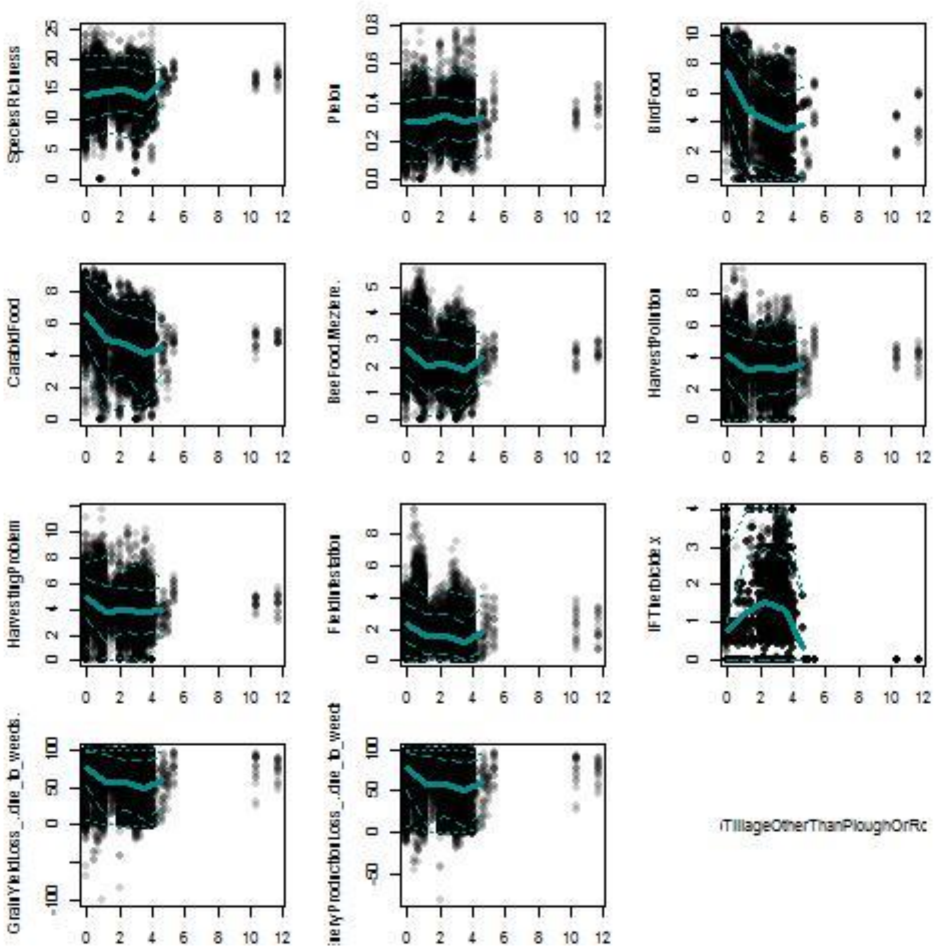

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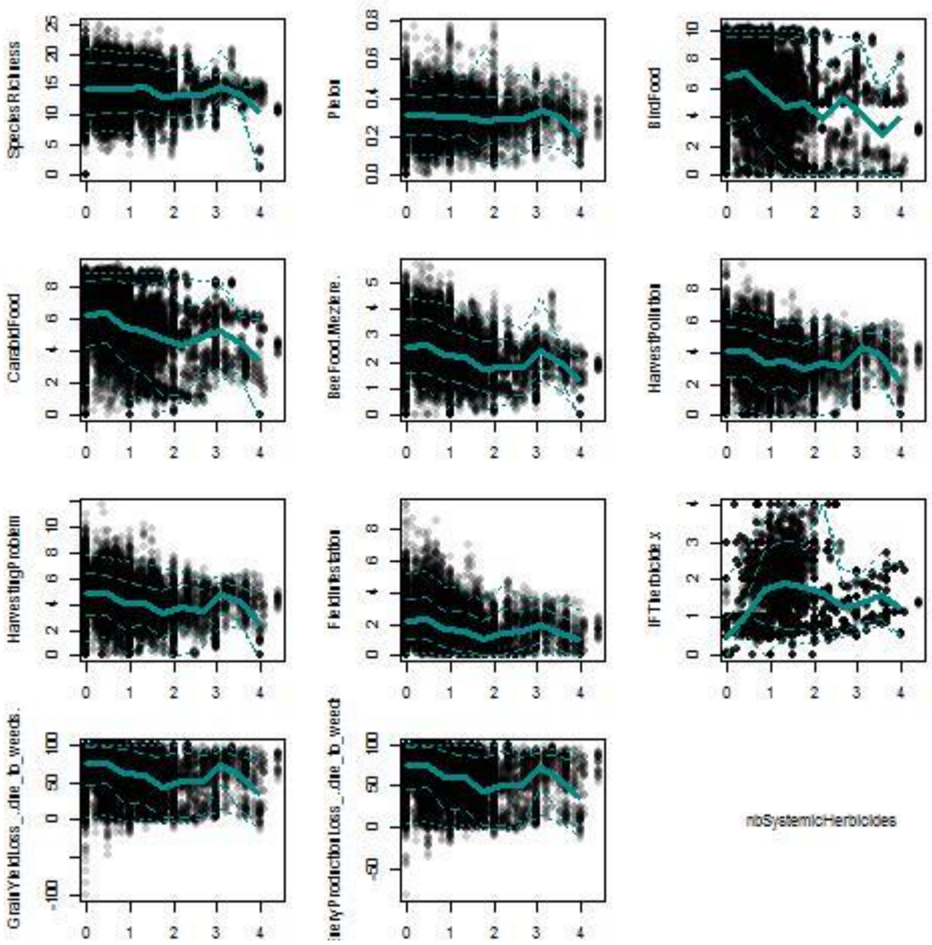
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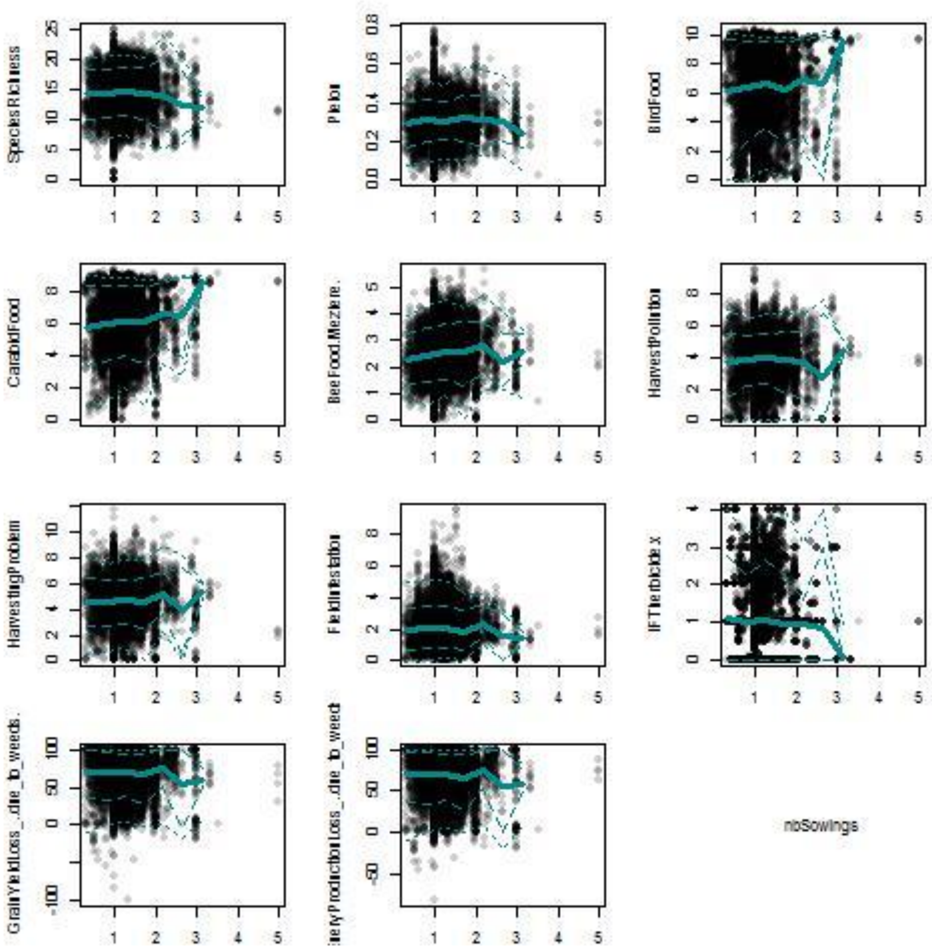
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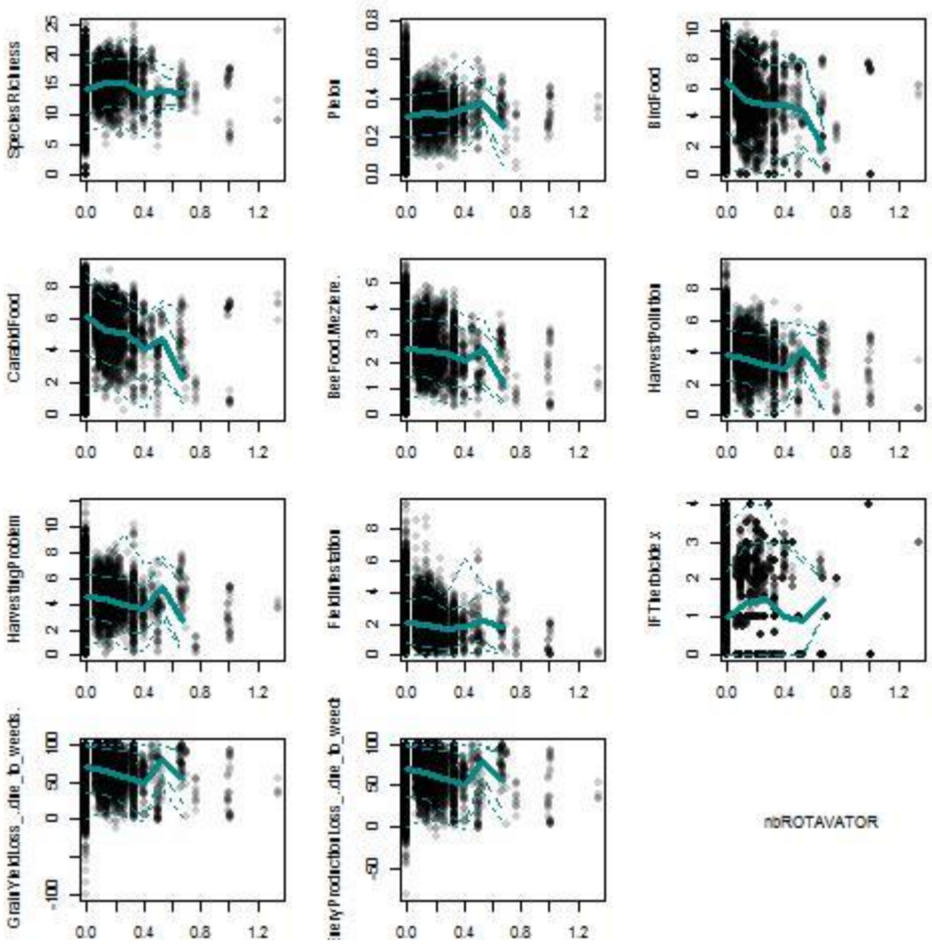
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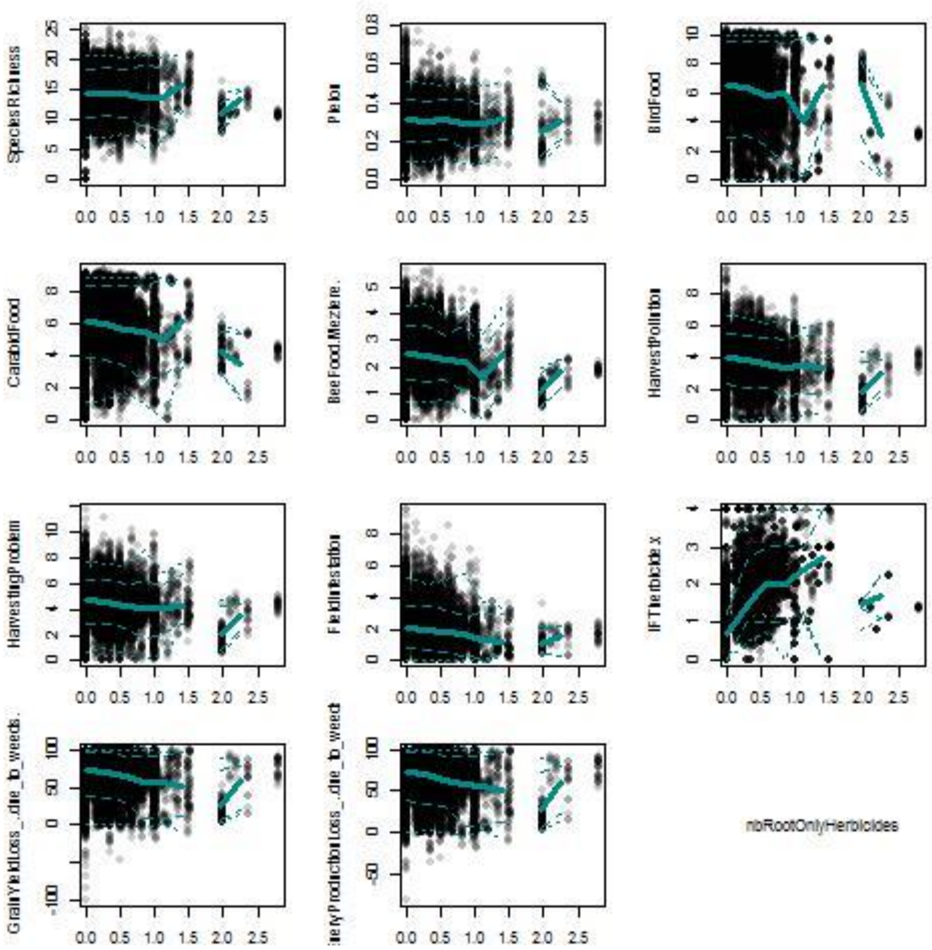
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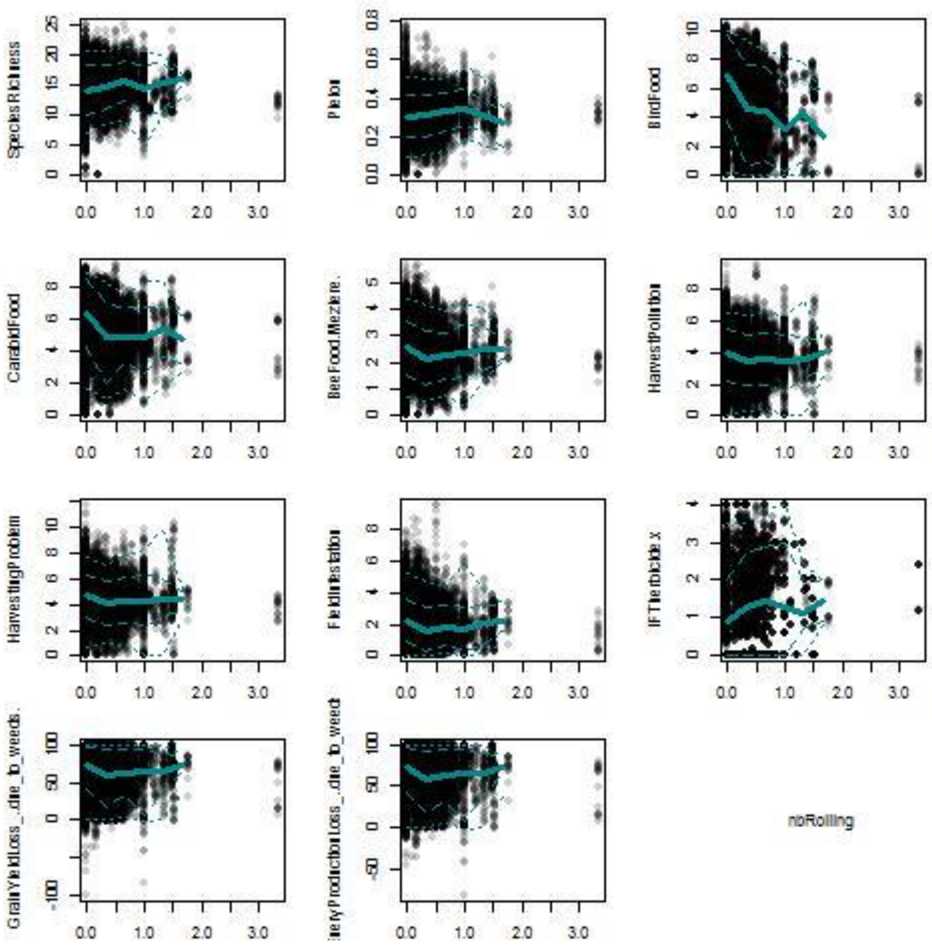
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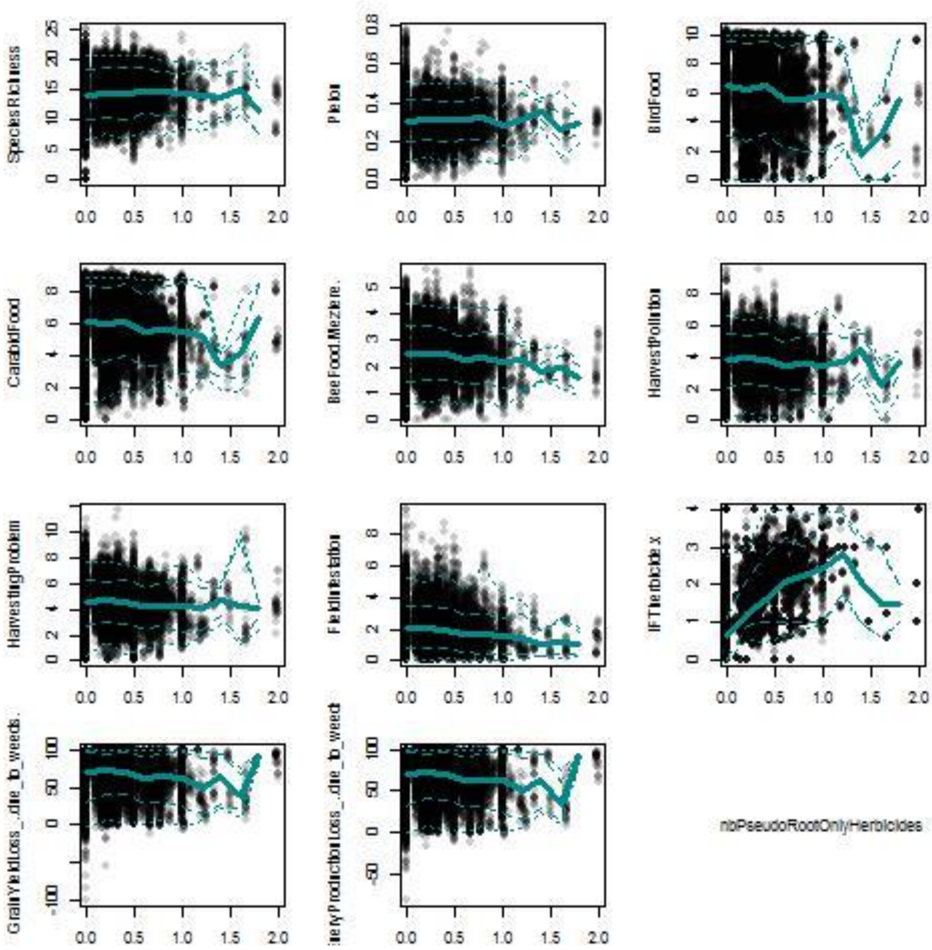
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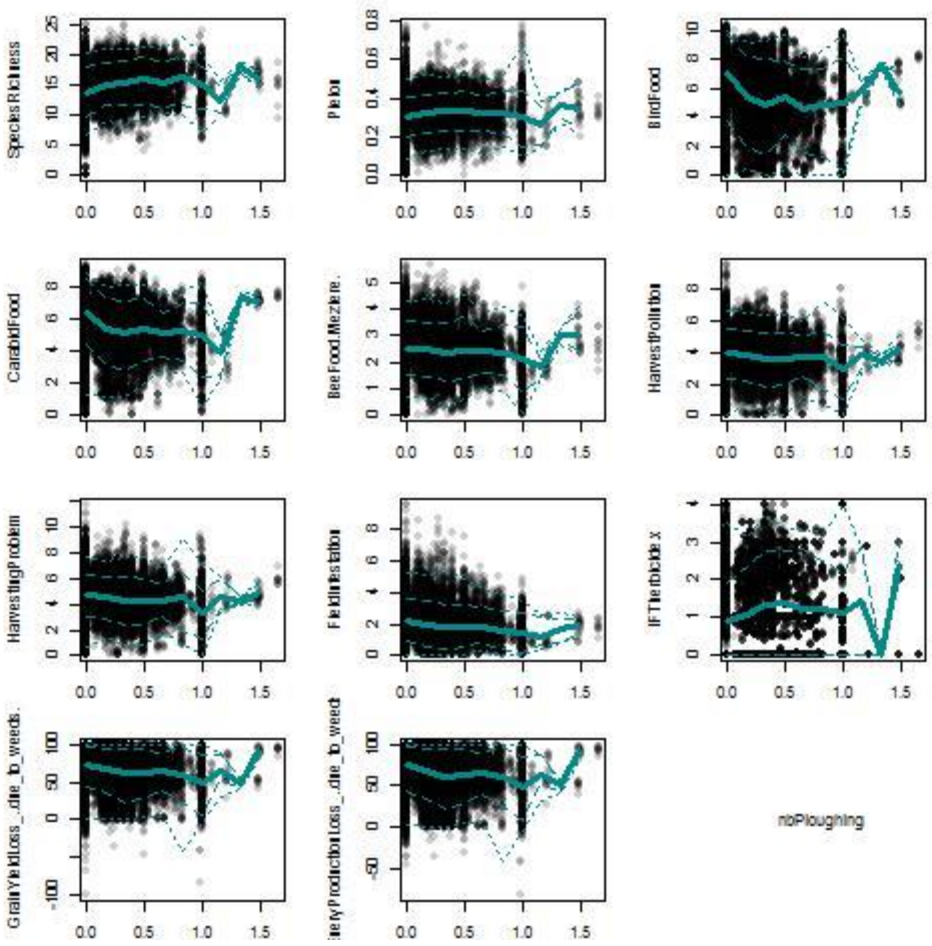

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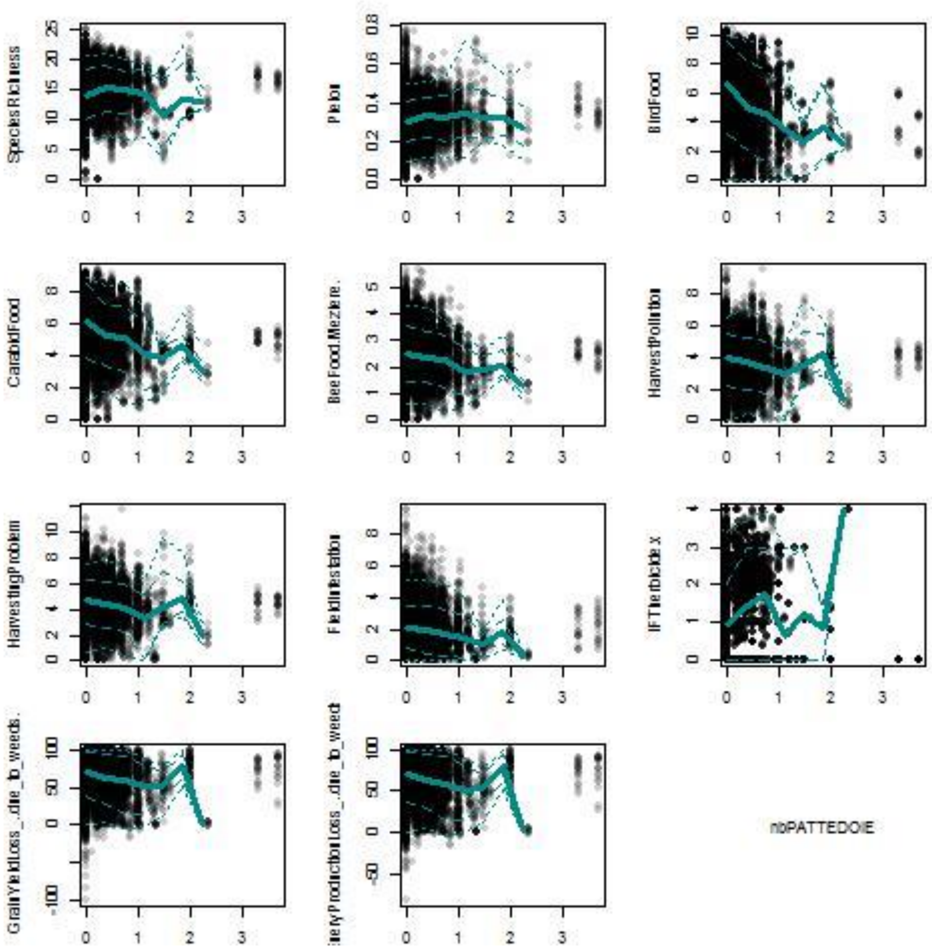

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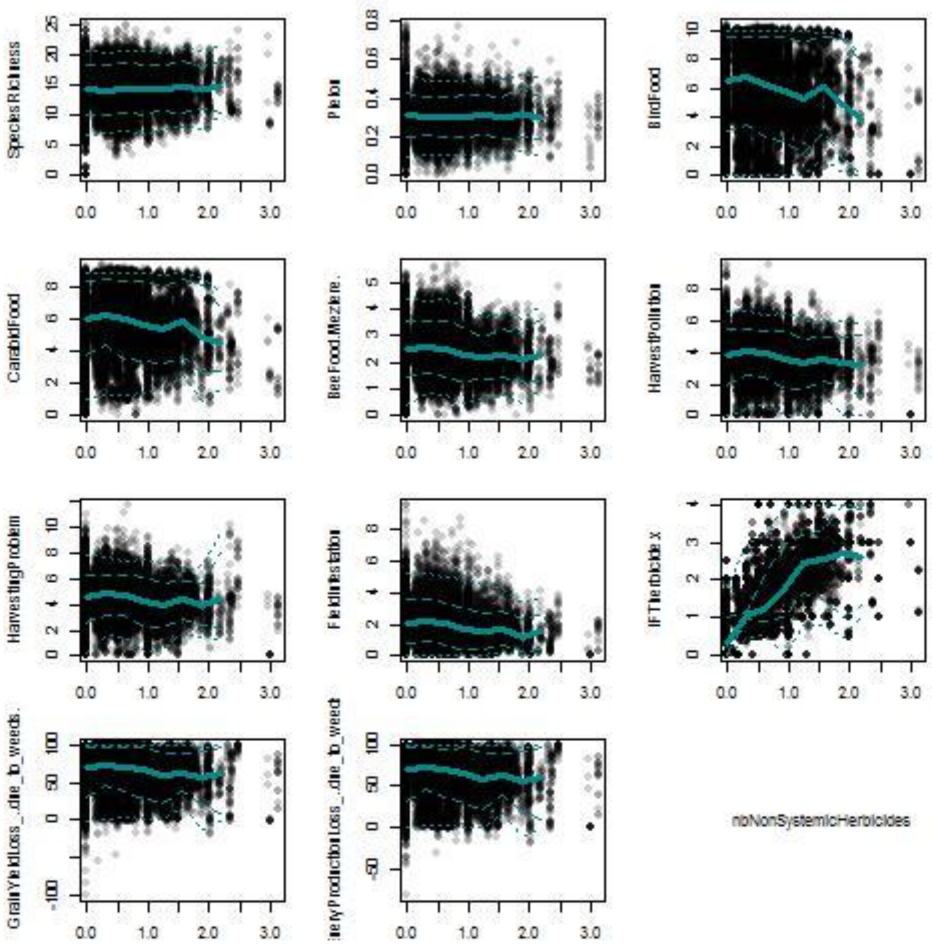
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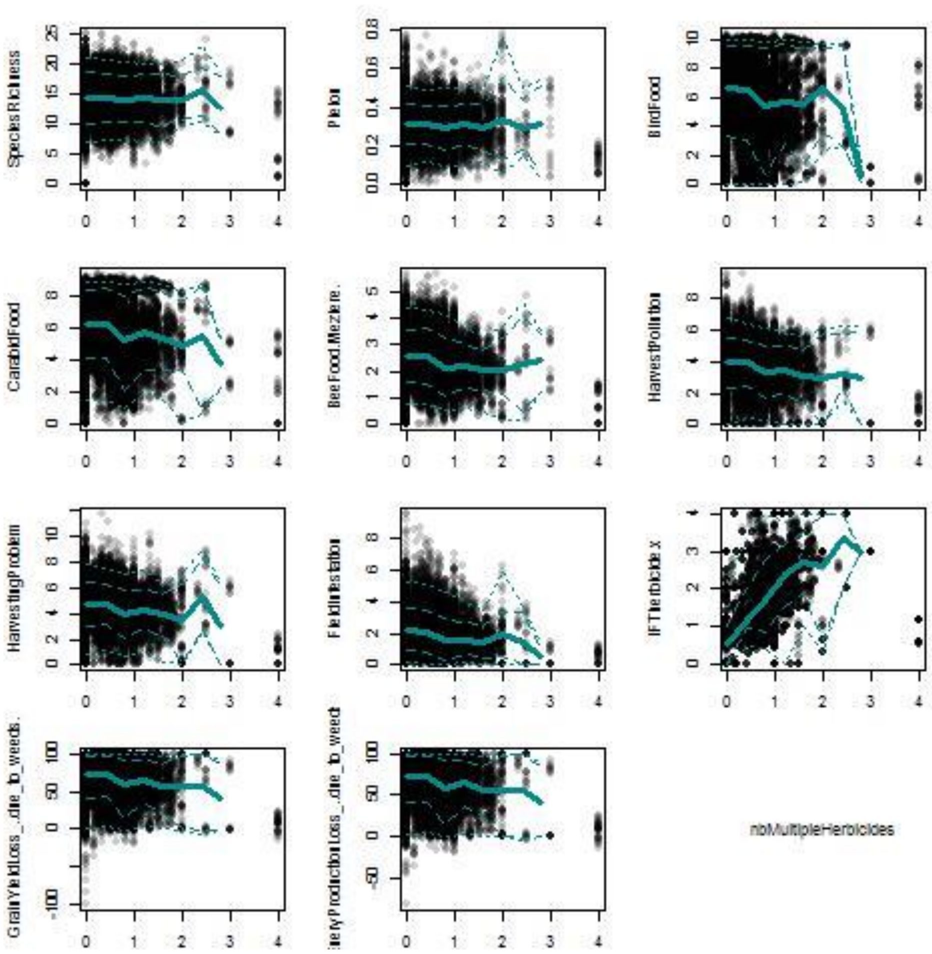
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FieldInfestation
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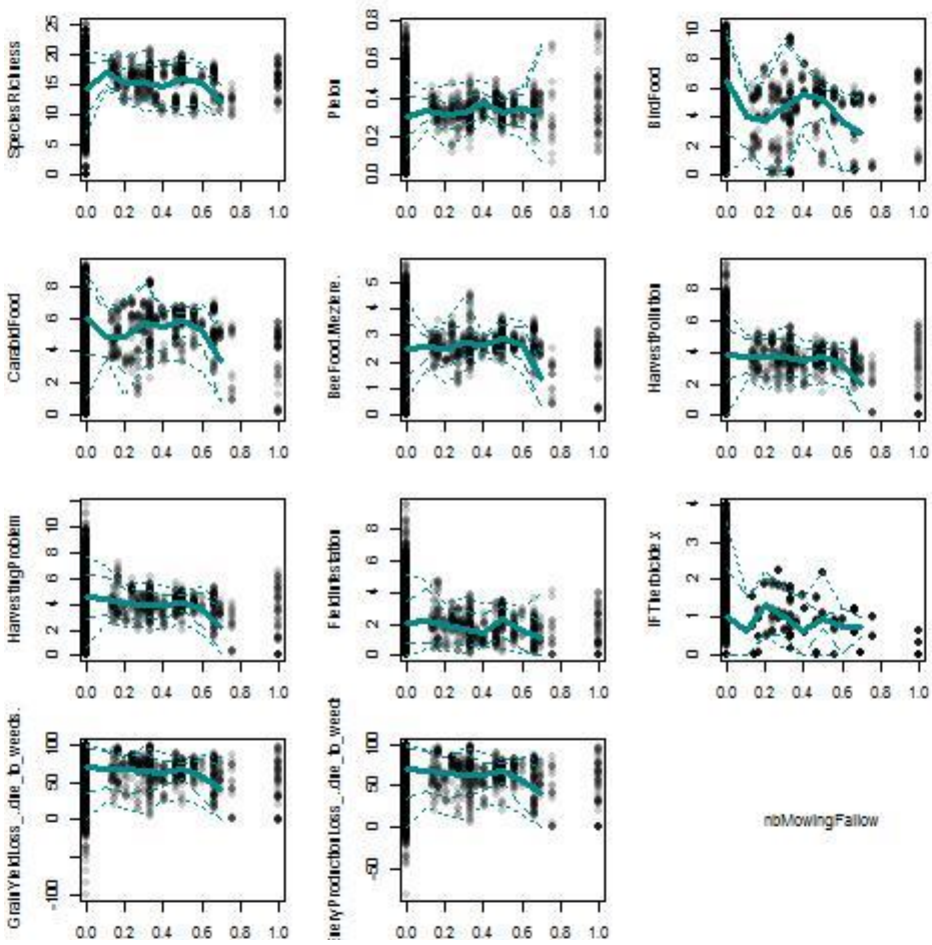
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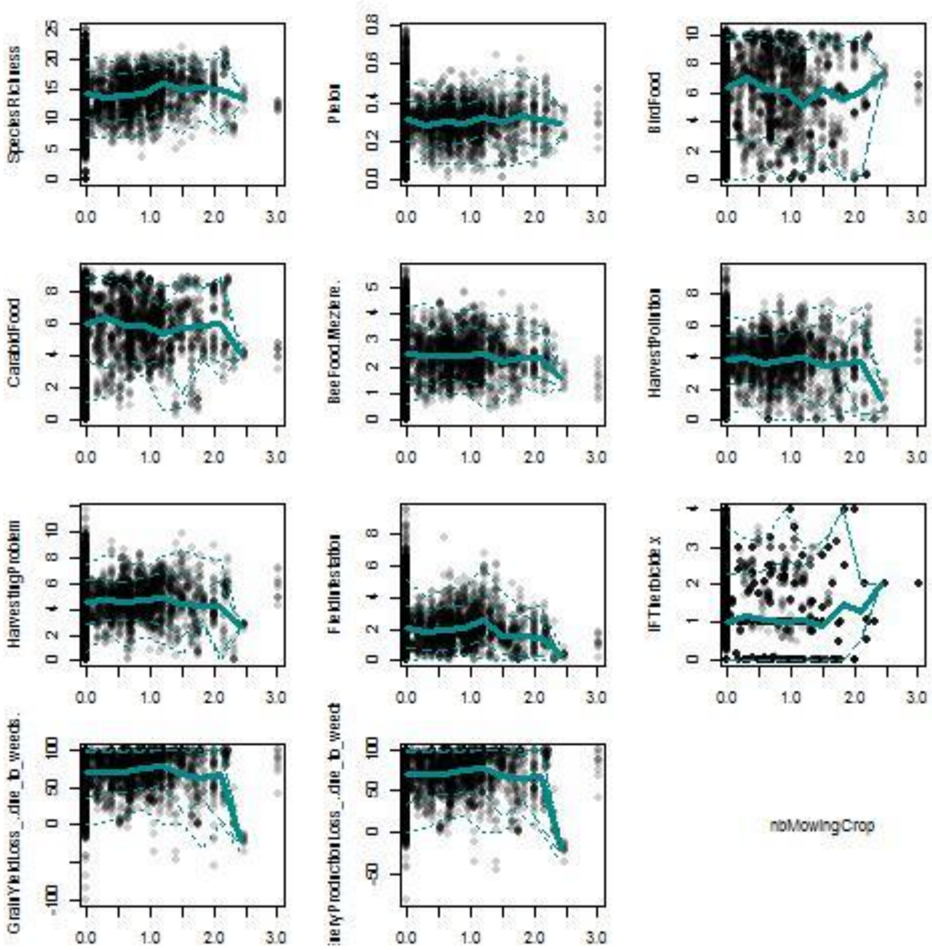
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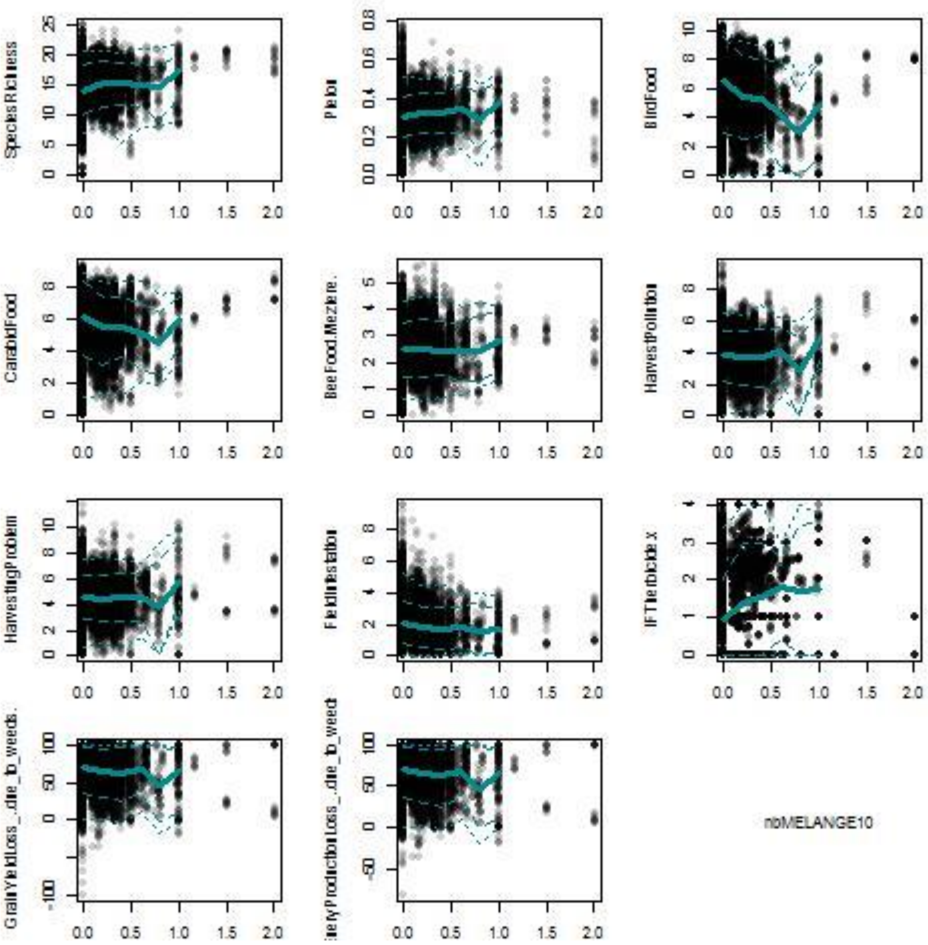
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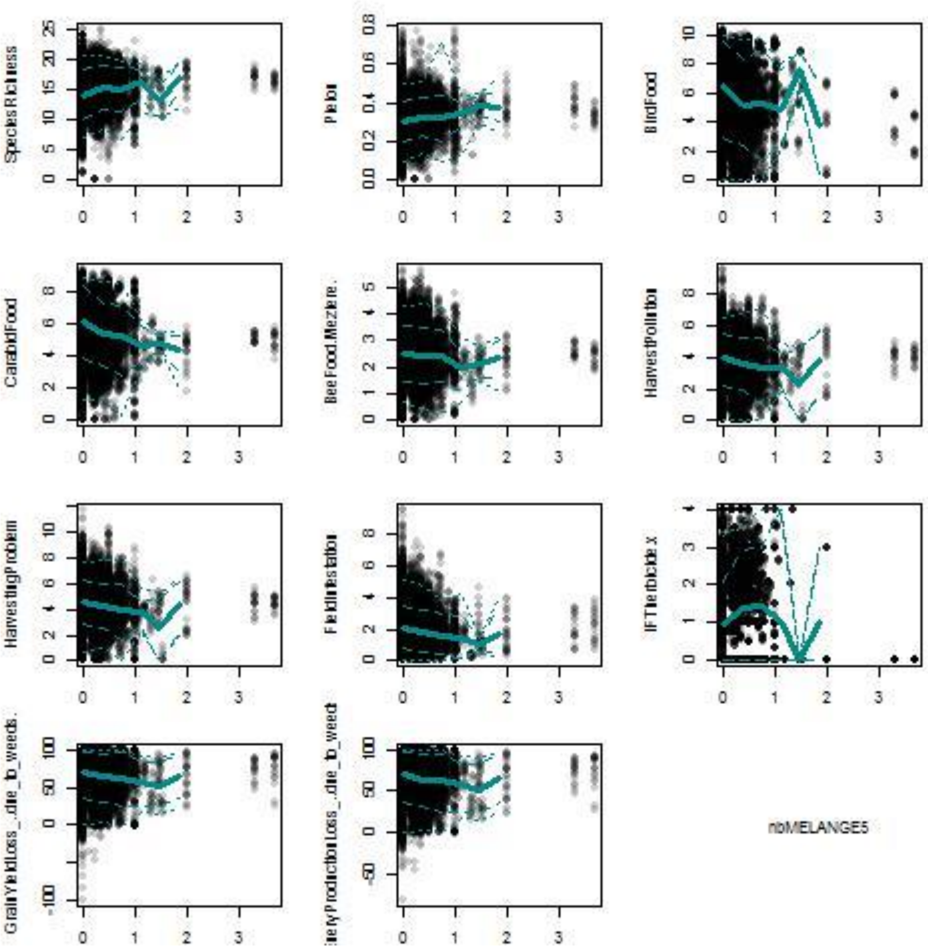
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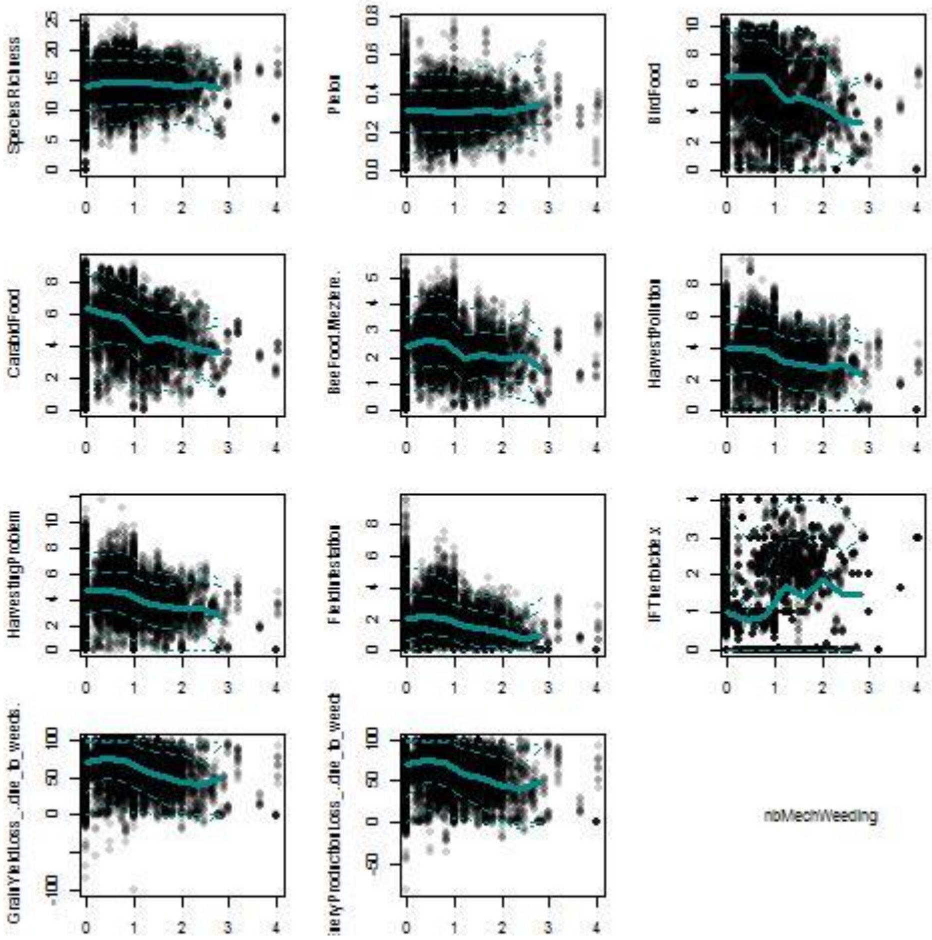
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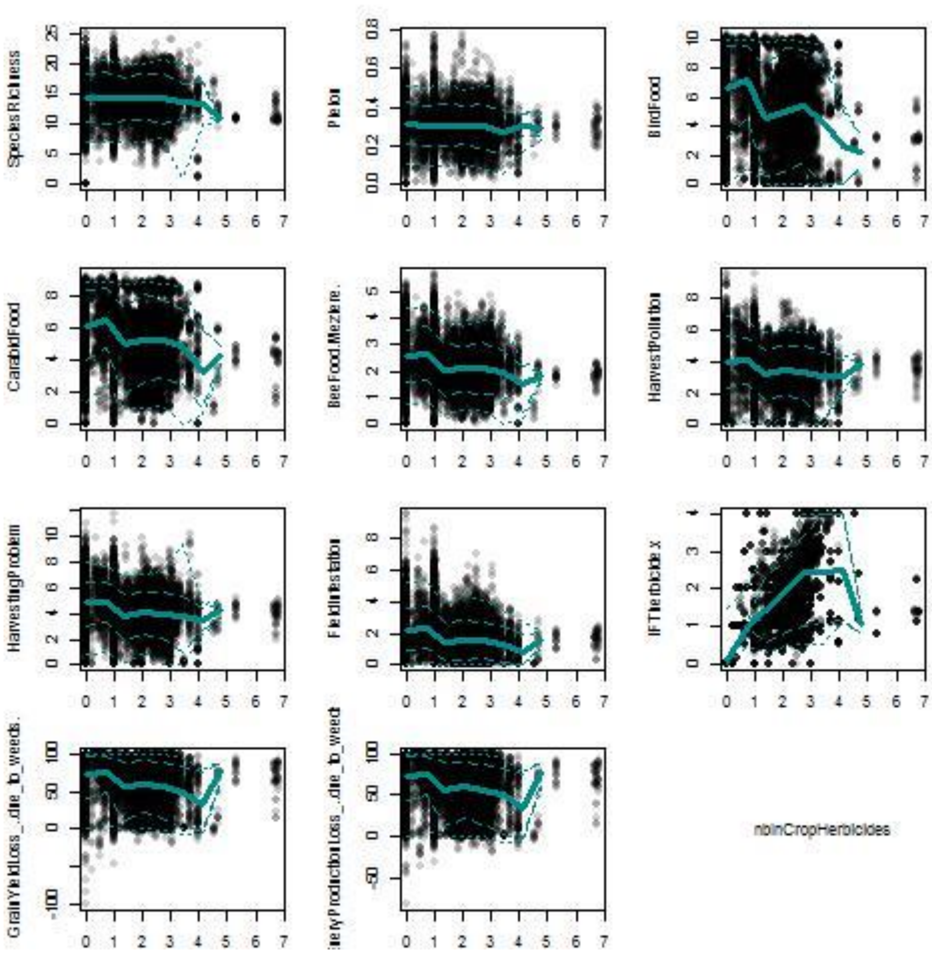
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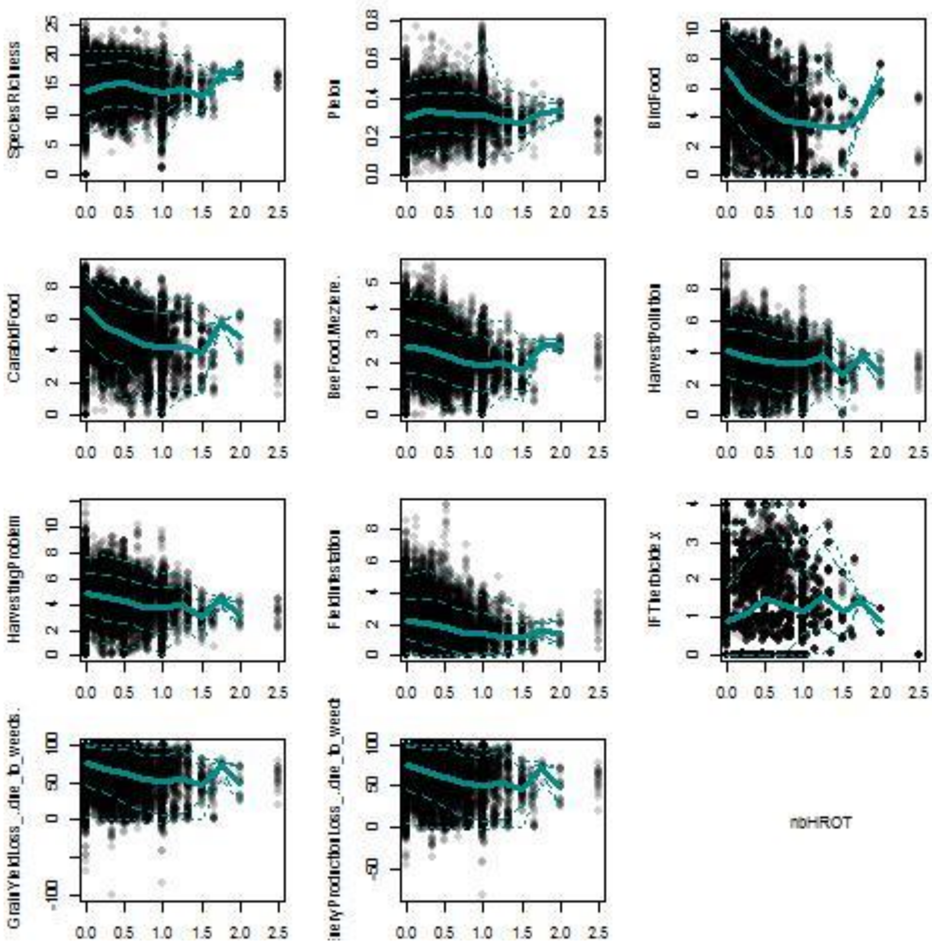
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CarabidFood
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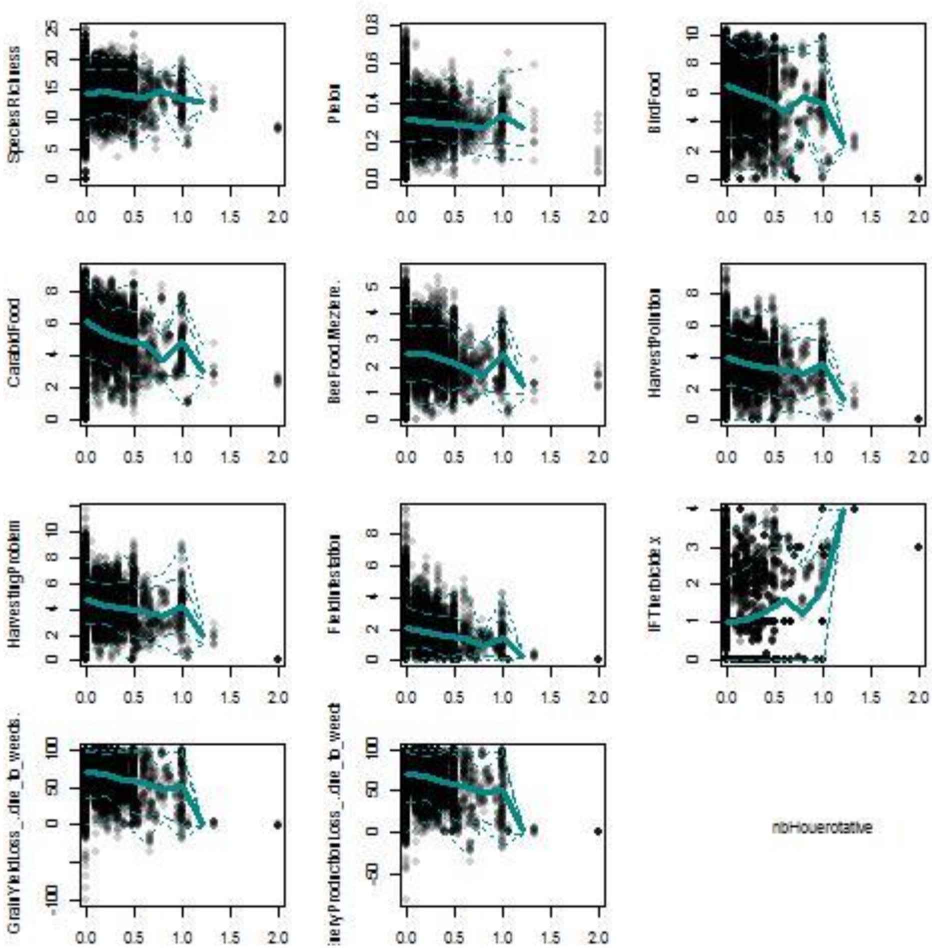
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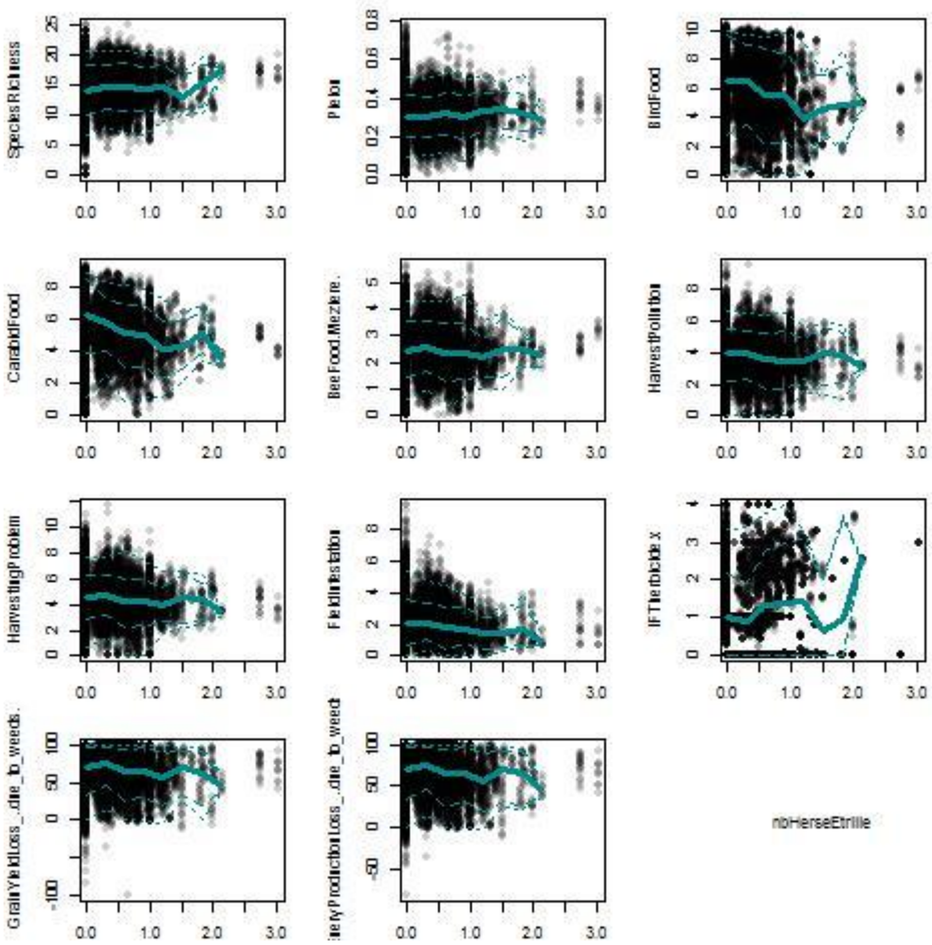
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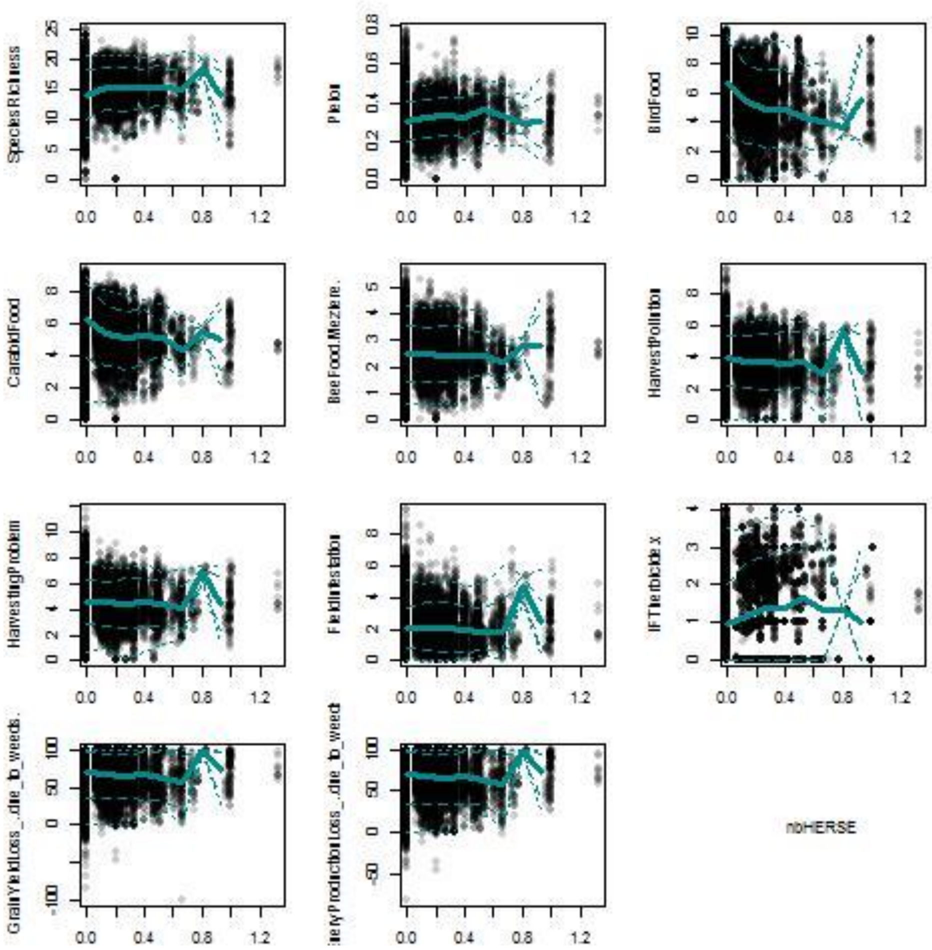
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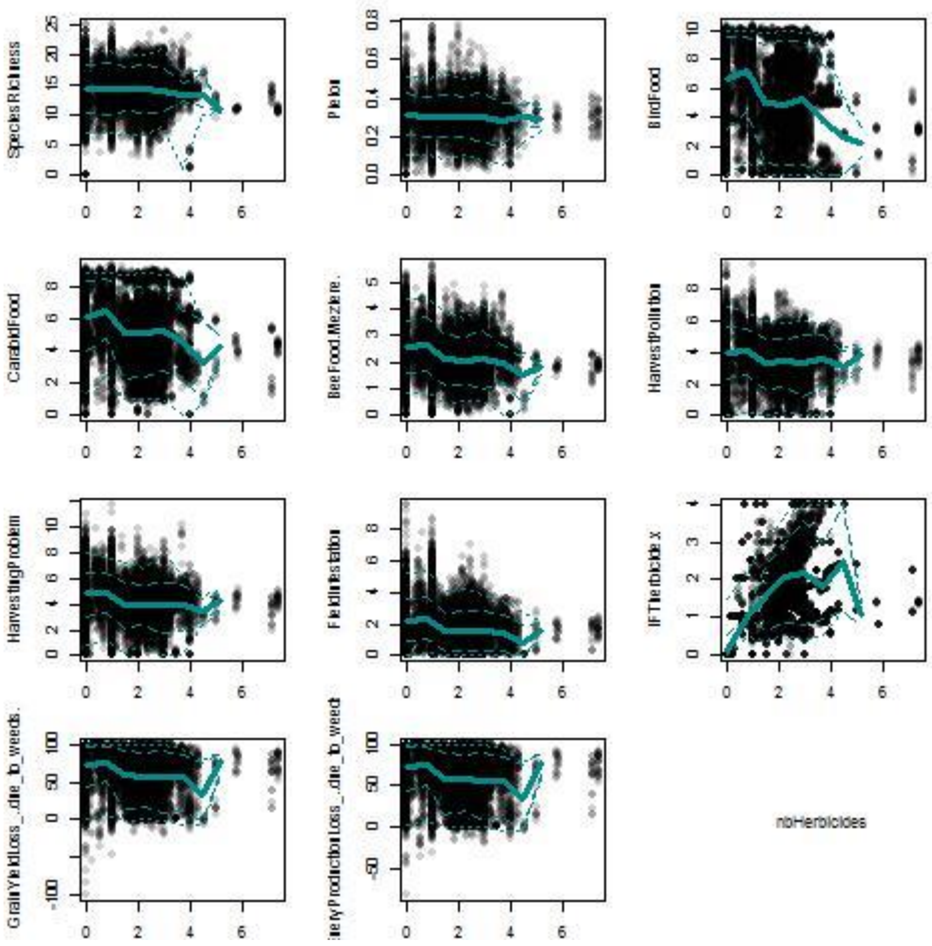
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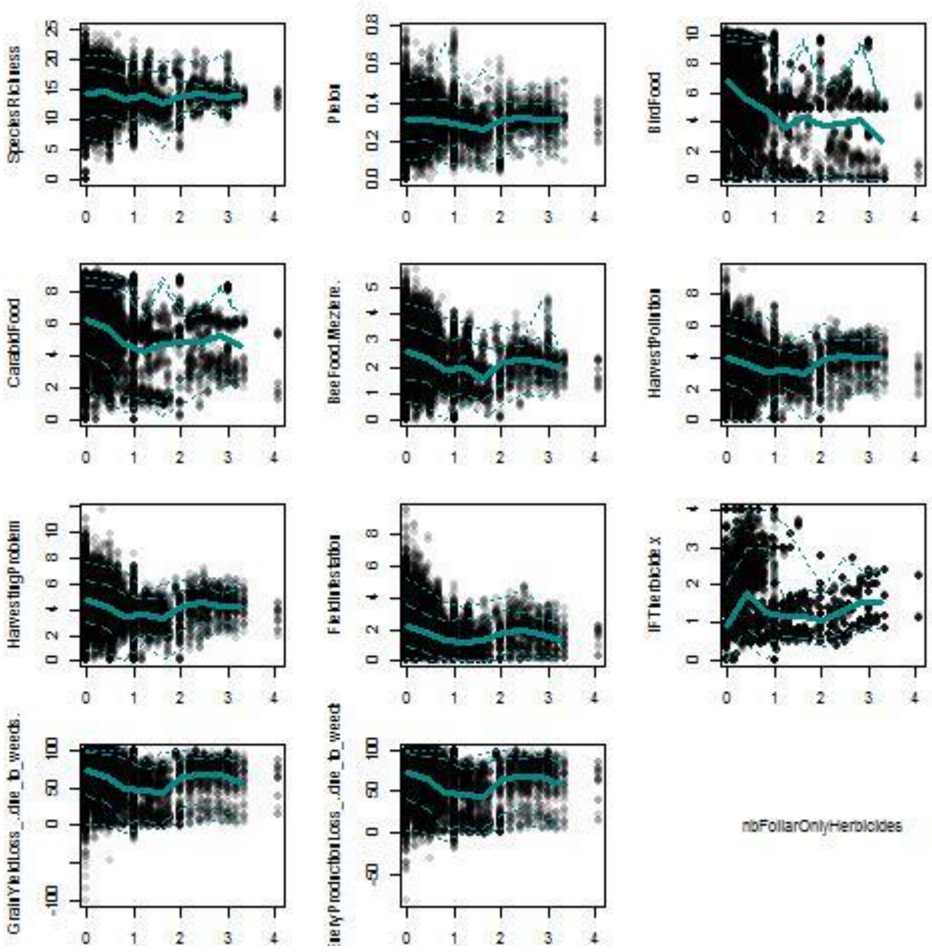
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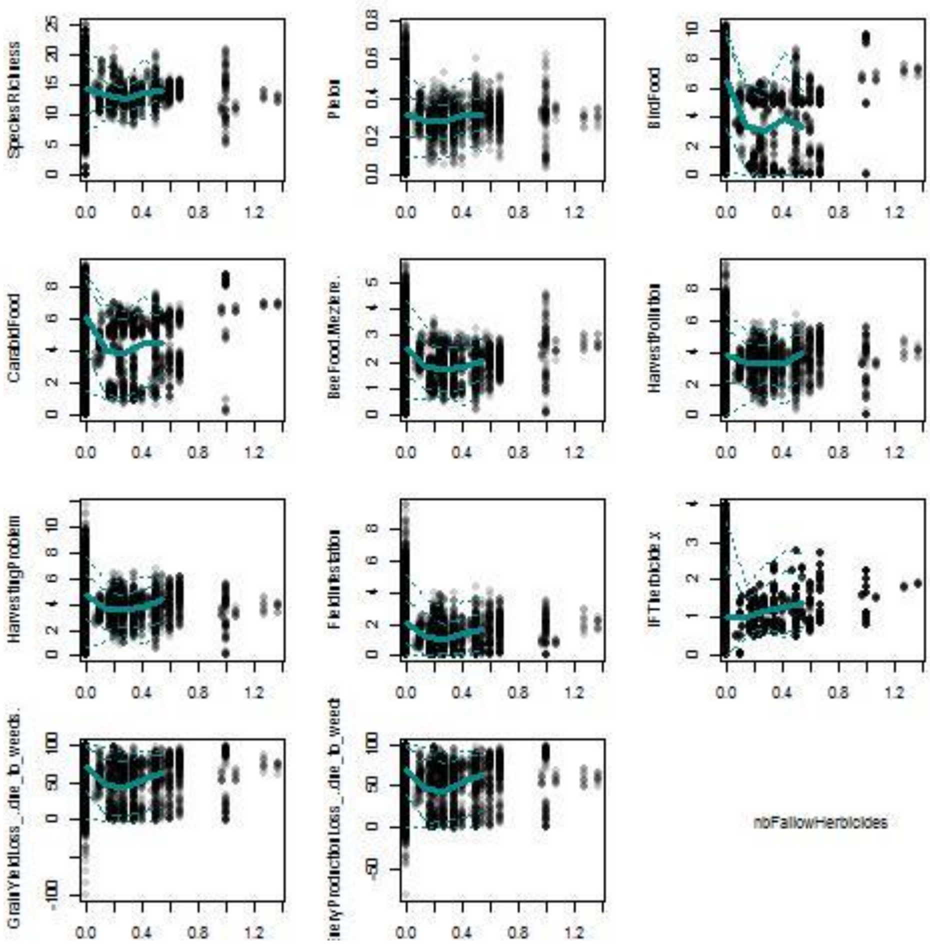
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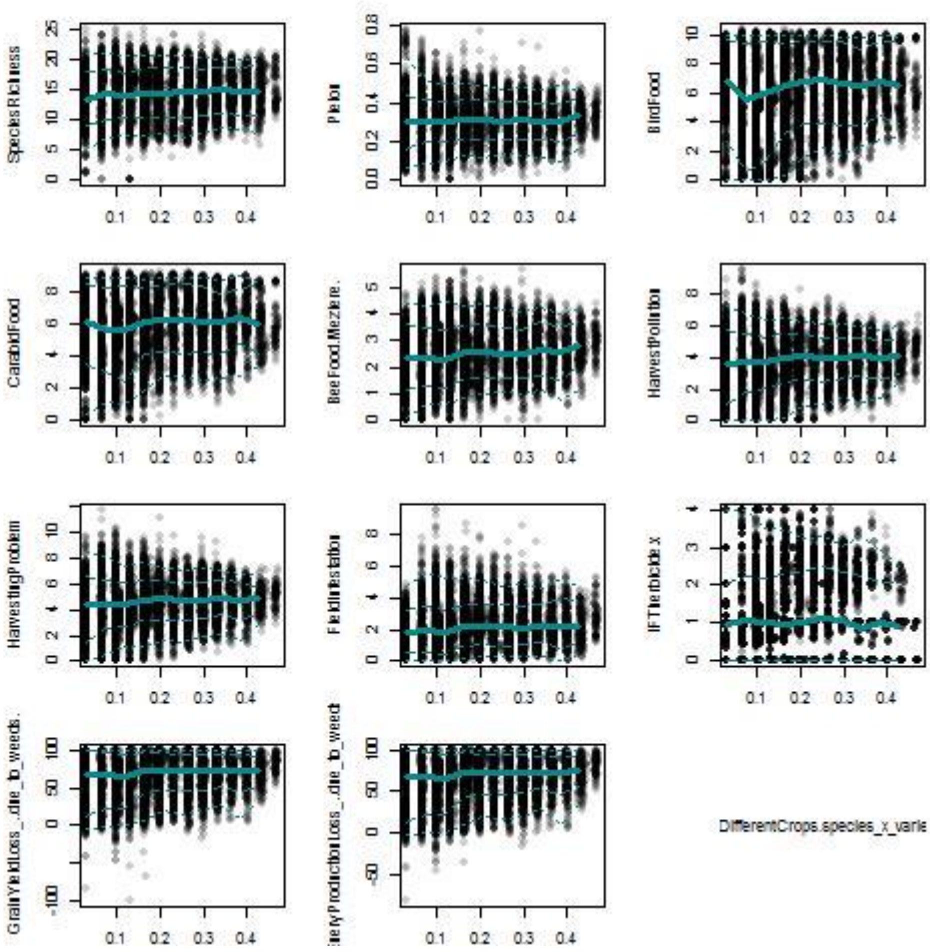
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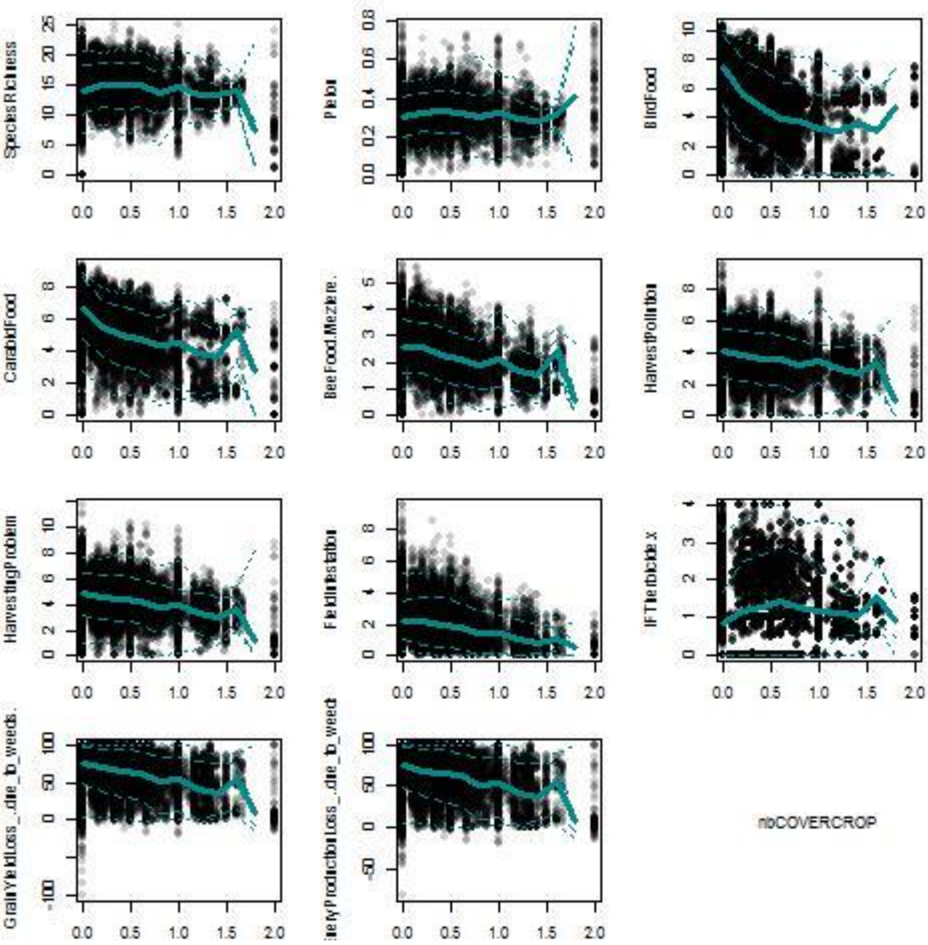
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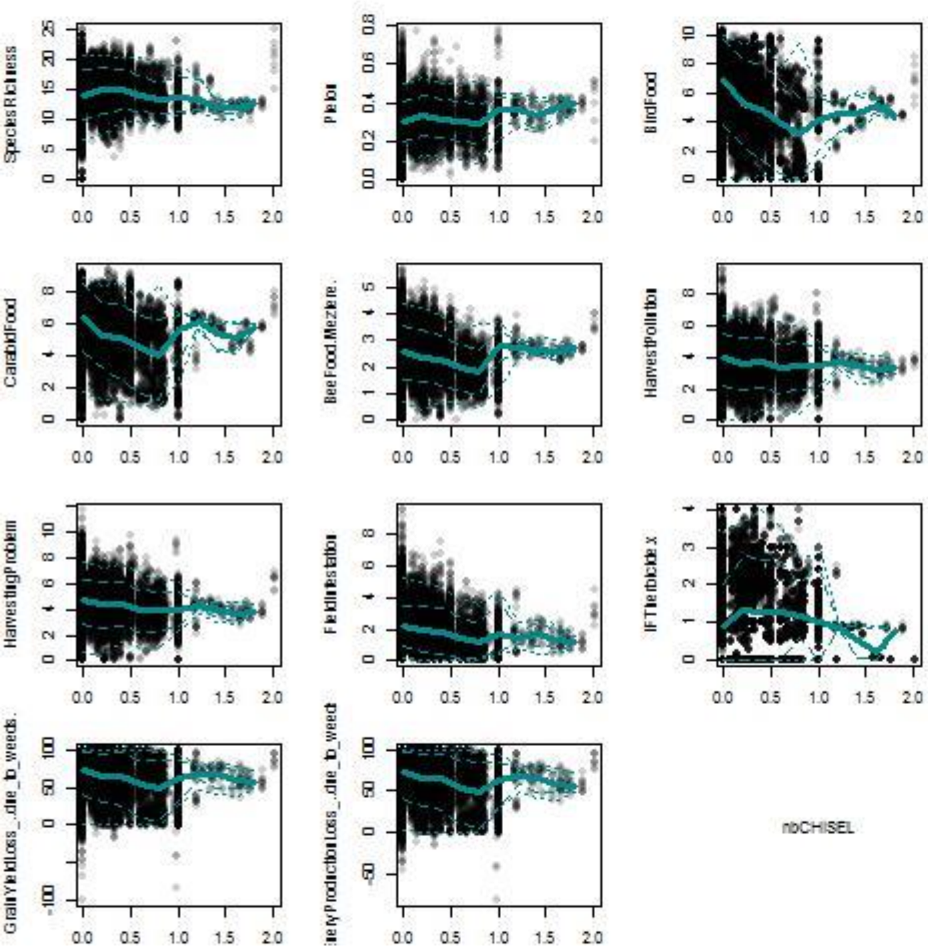
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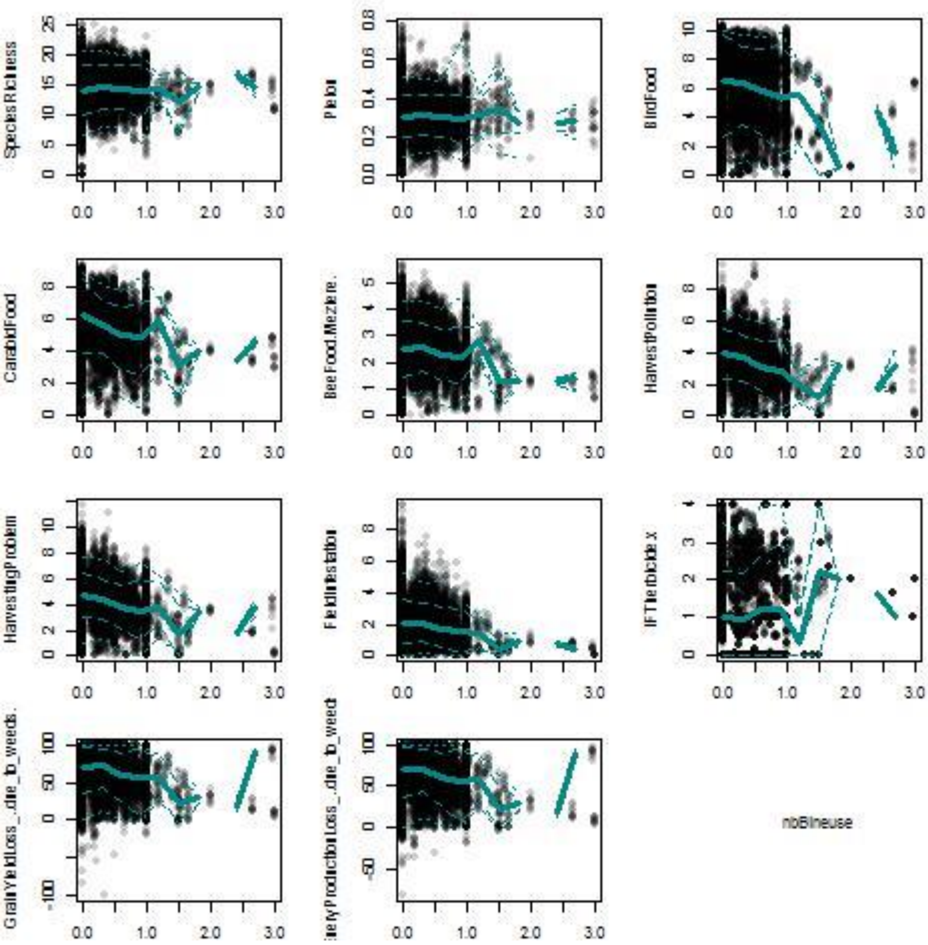
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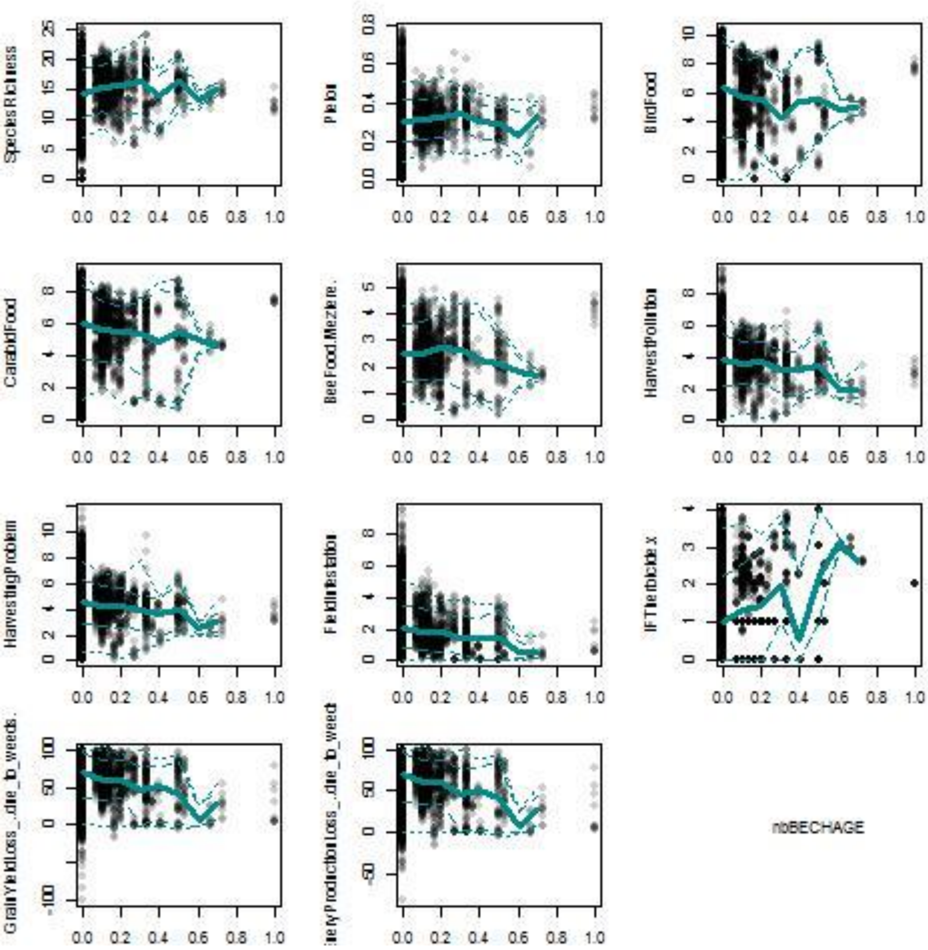
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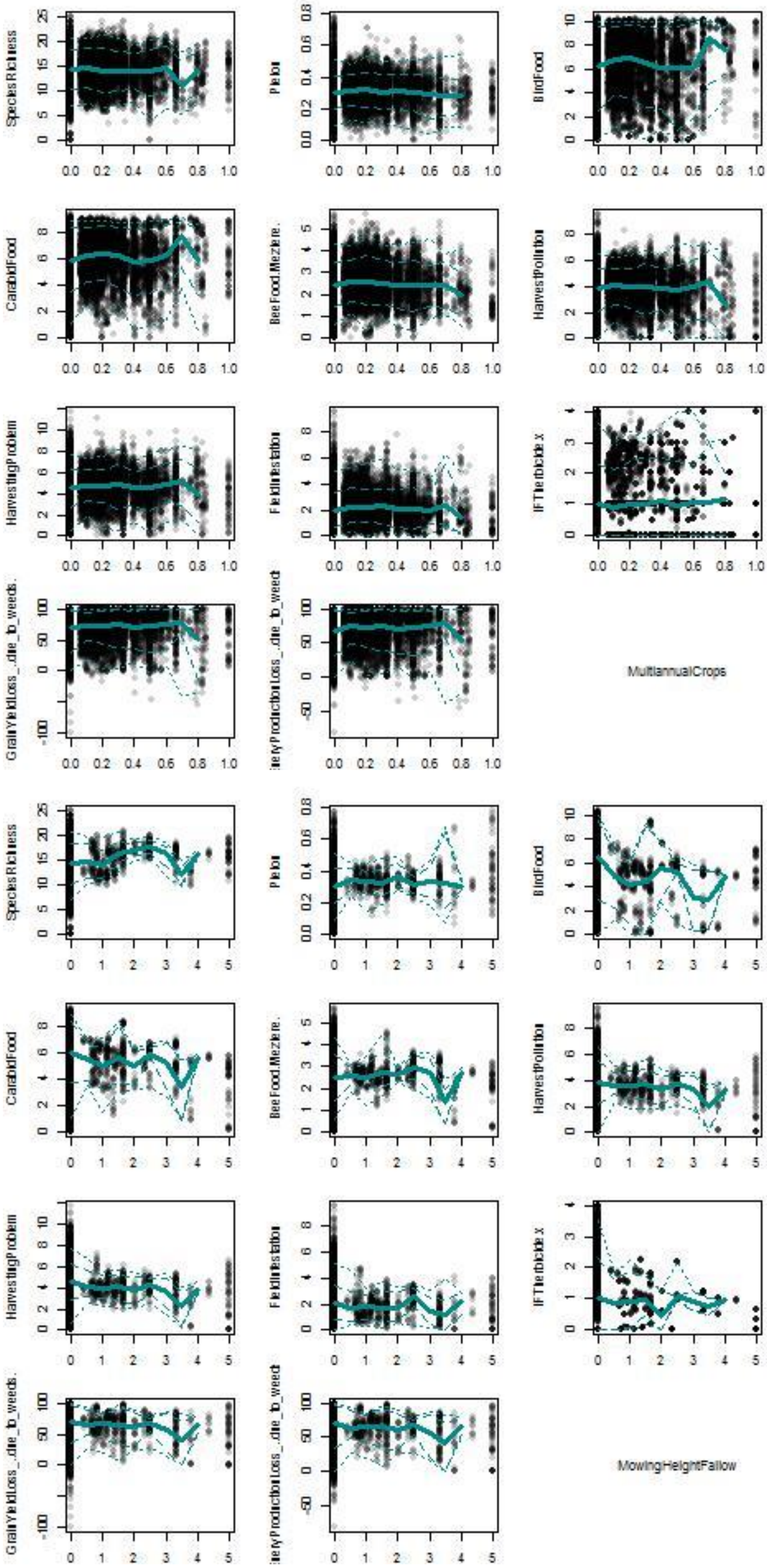
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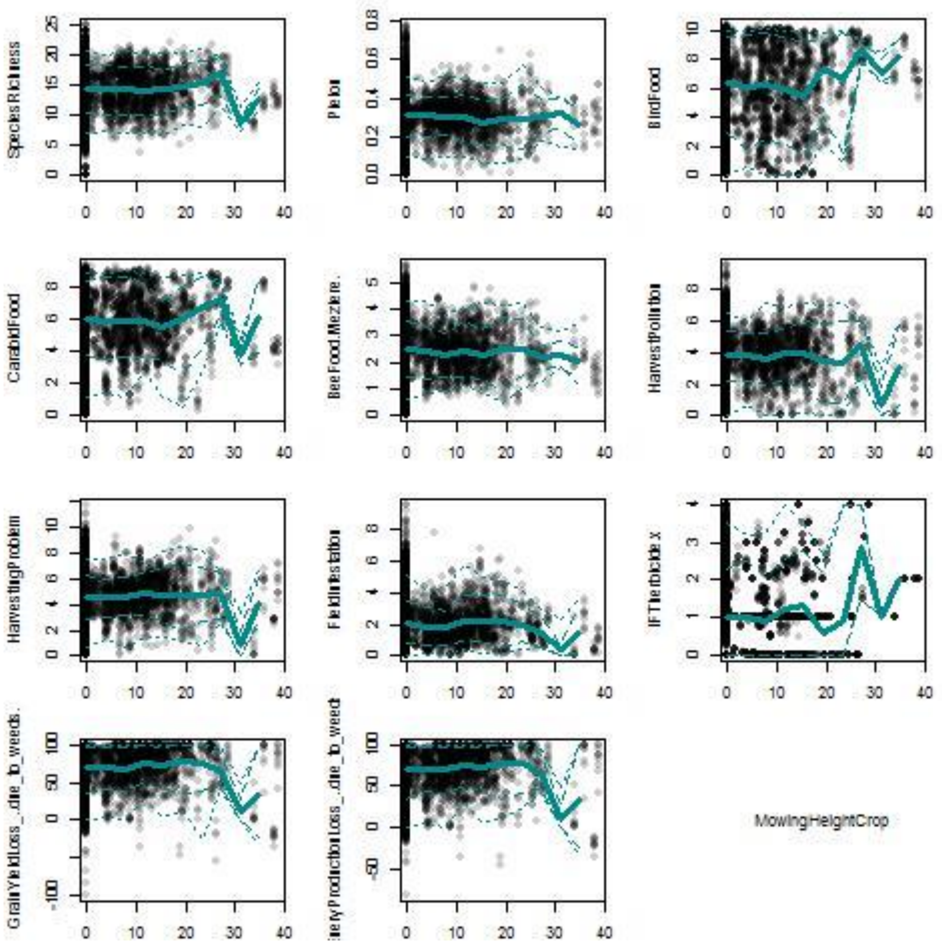
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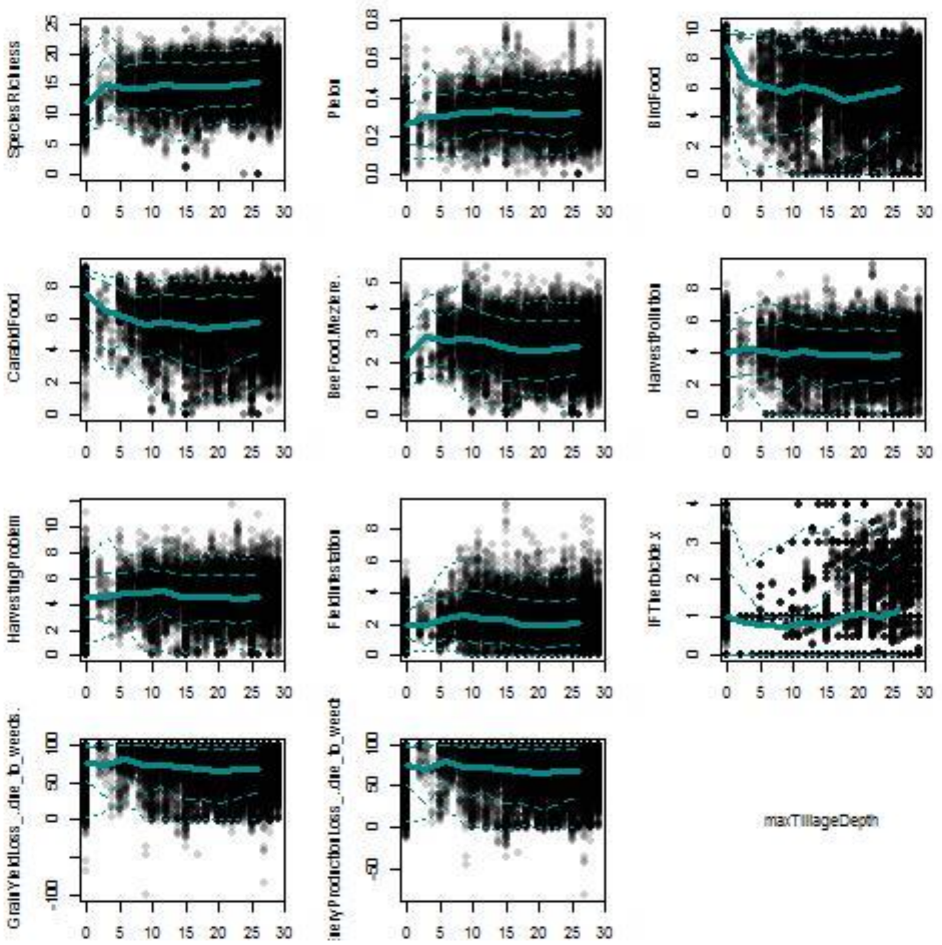
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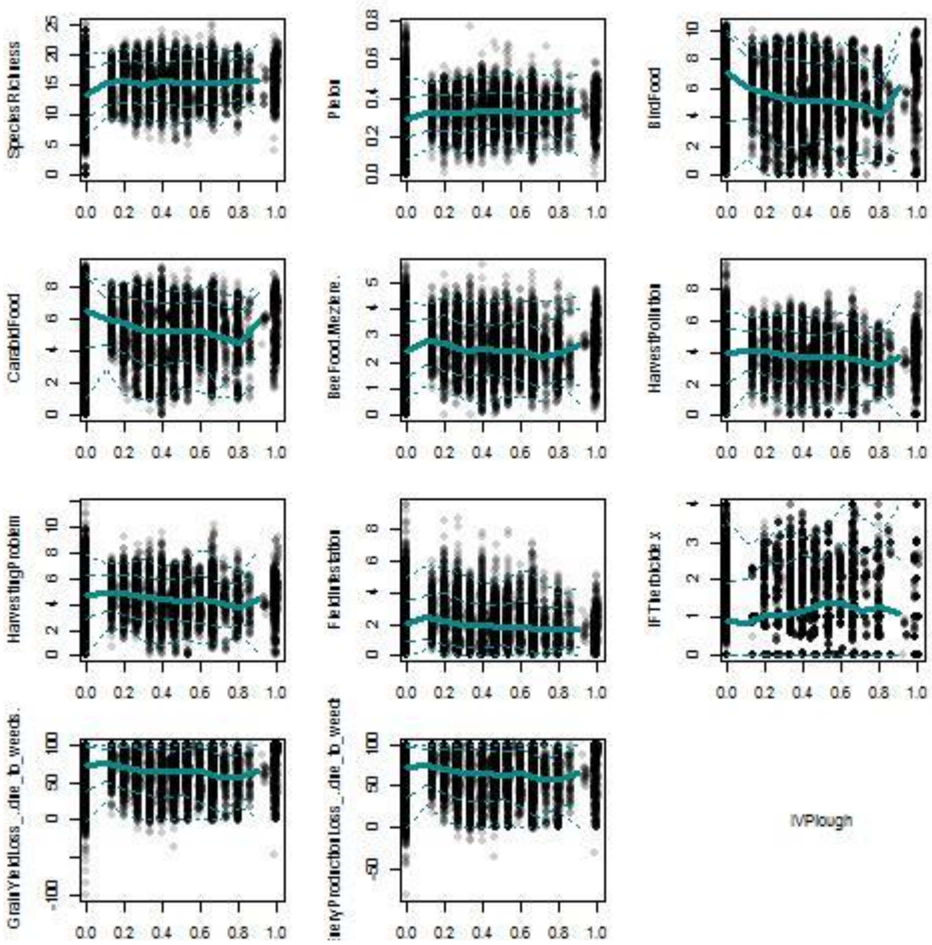
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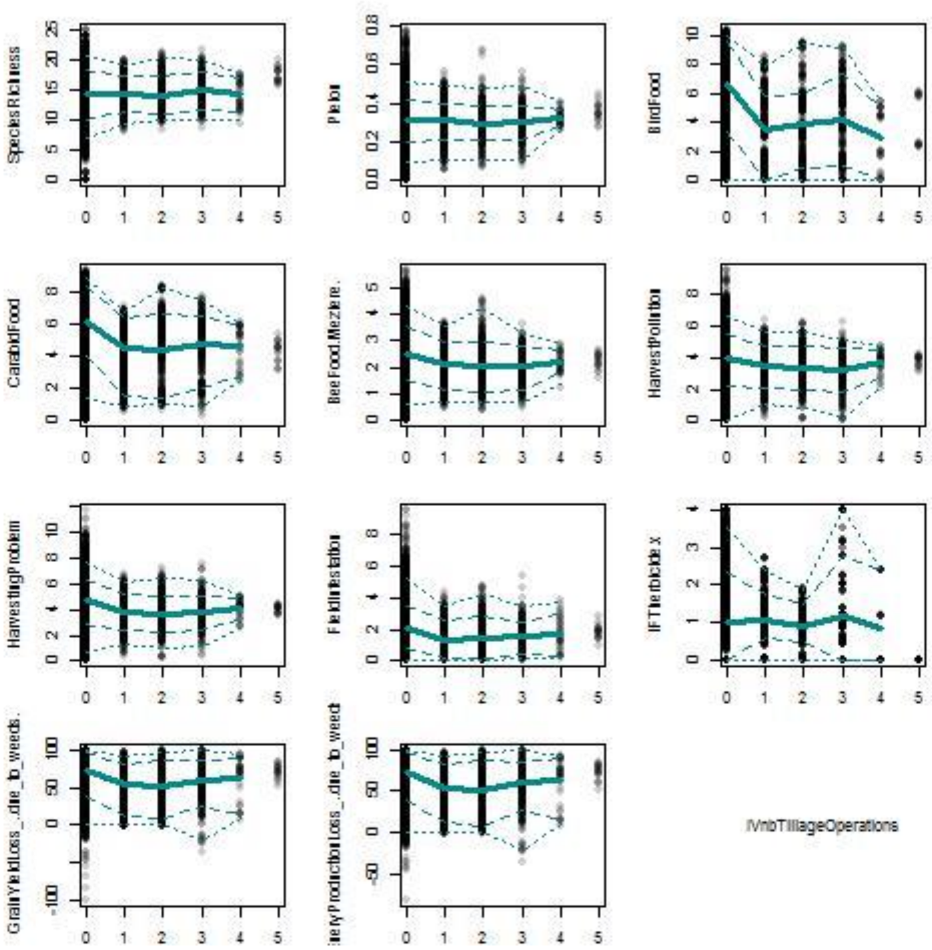
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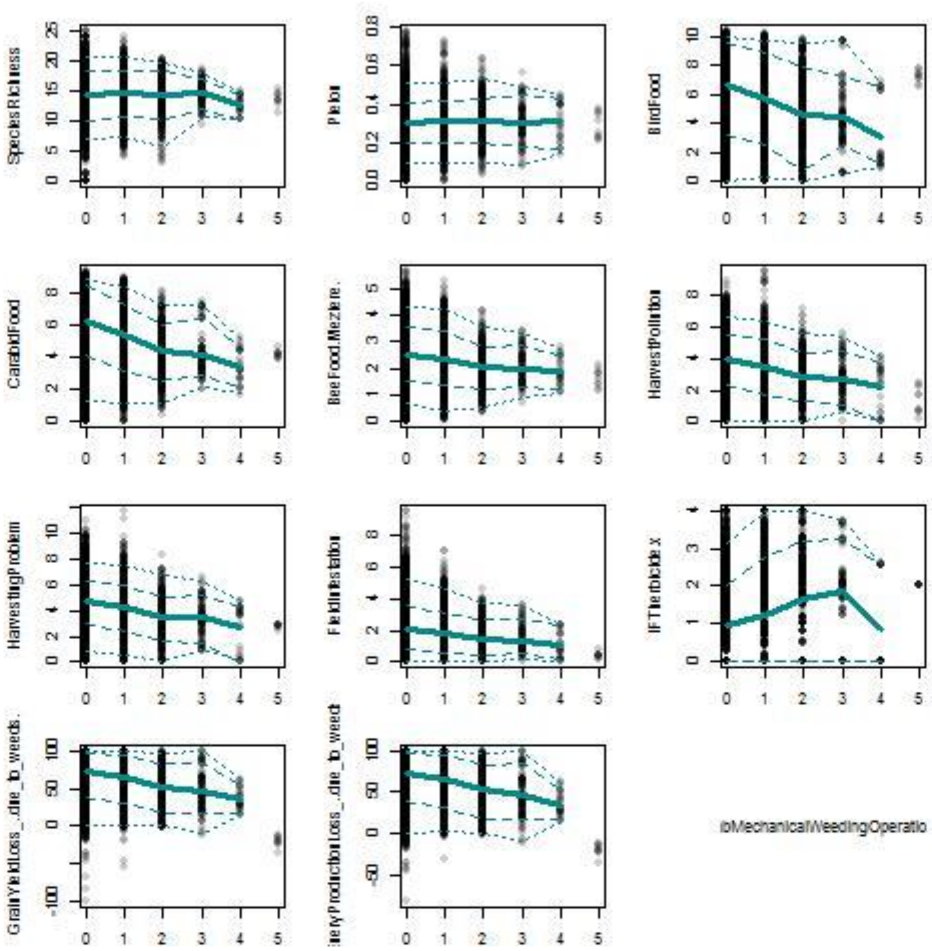
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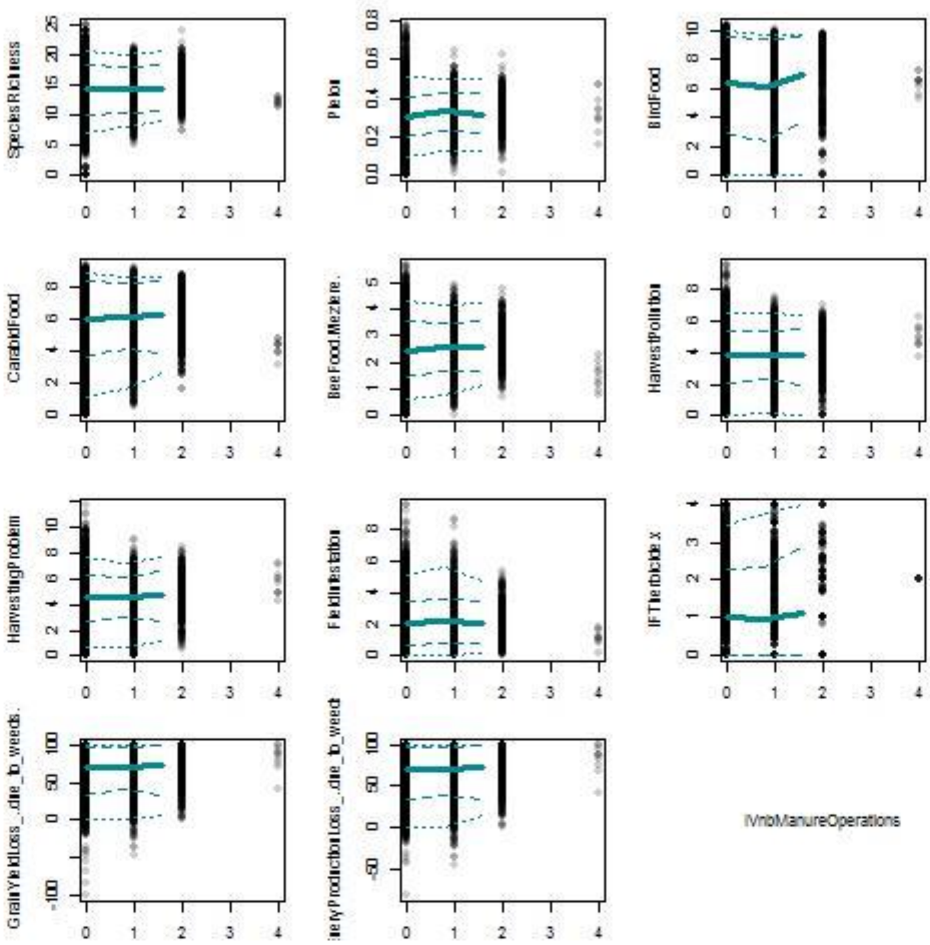
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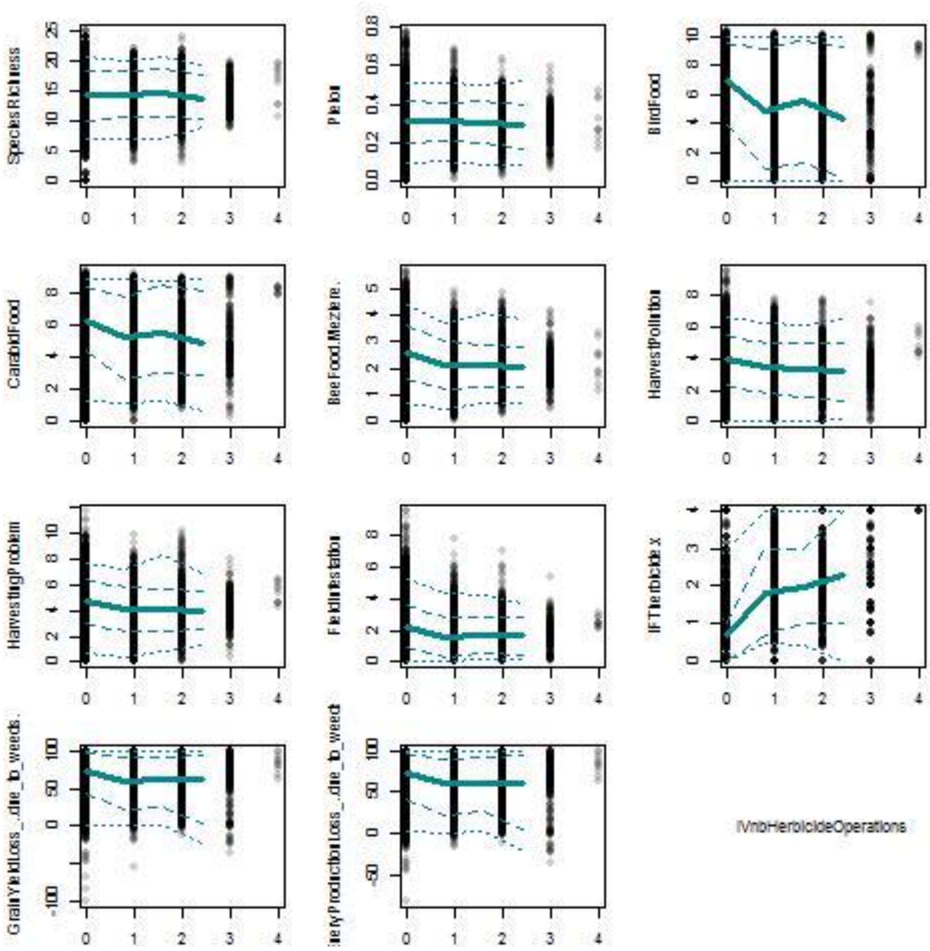
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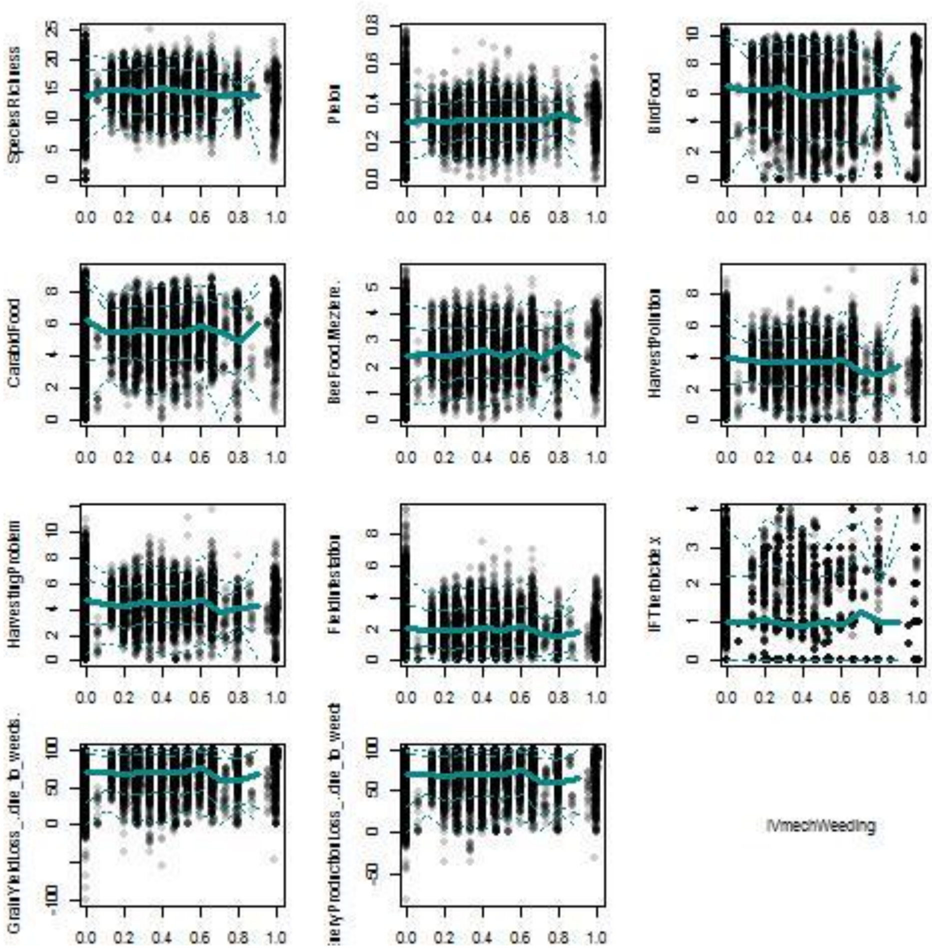
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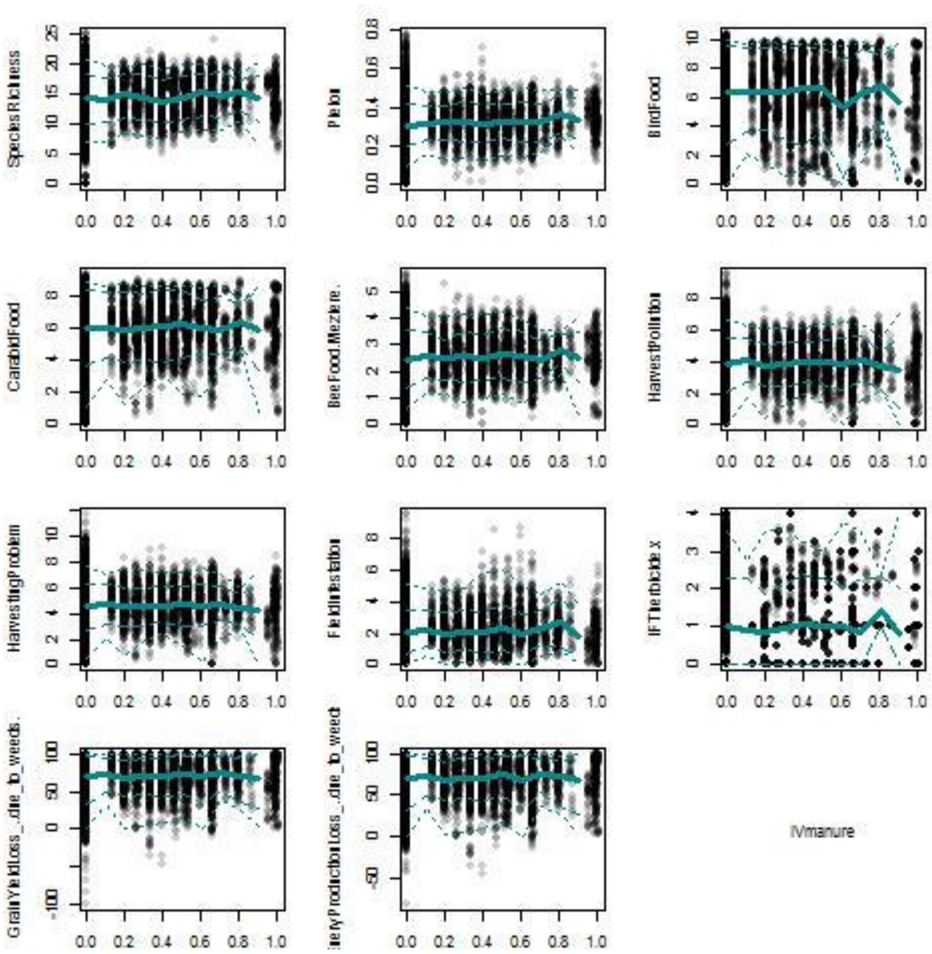
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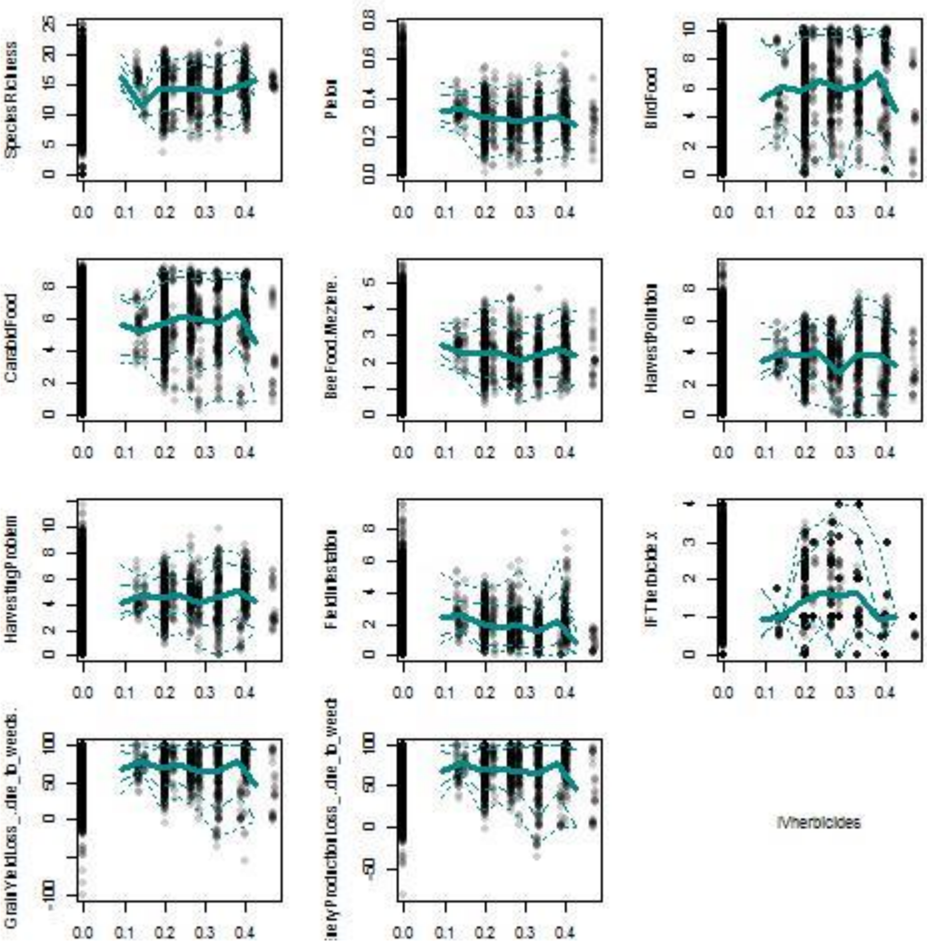
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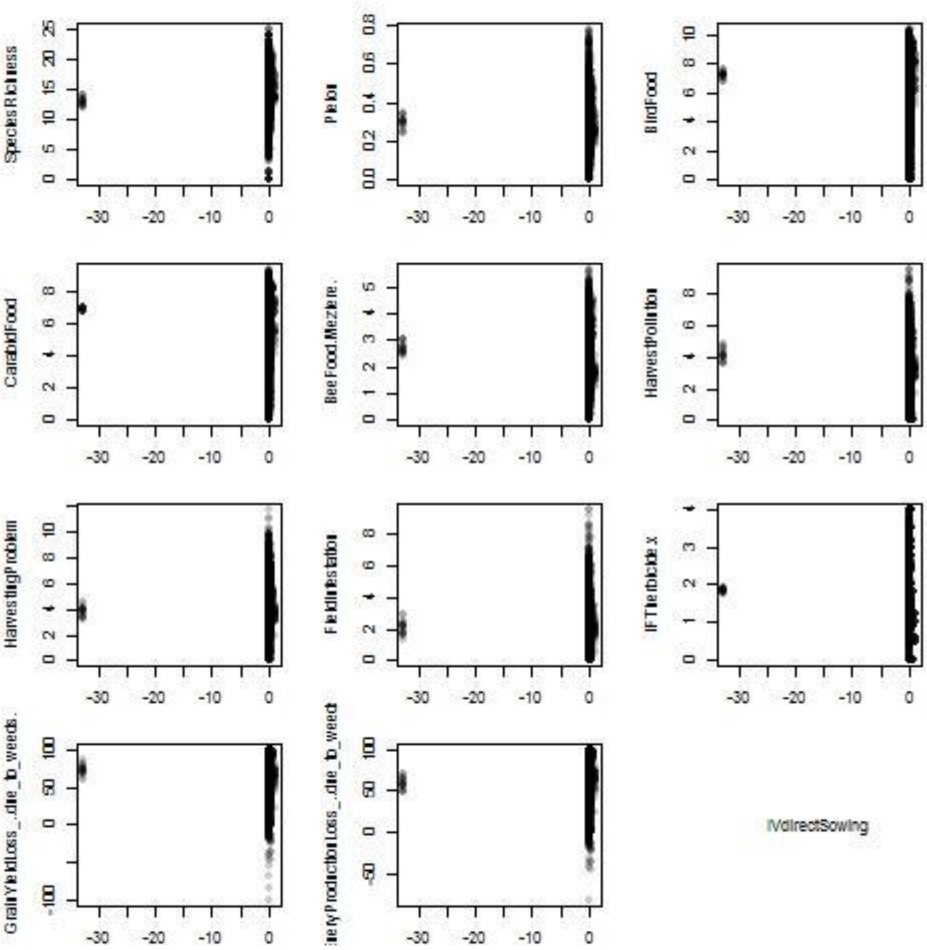
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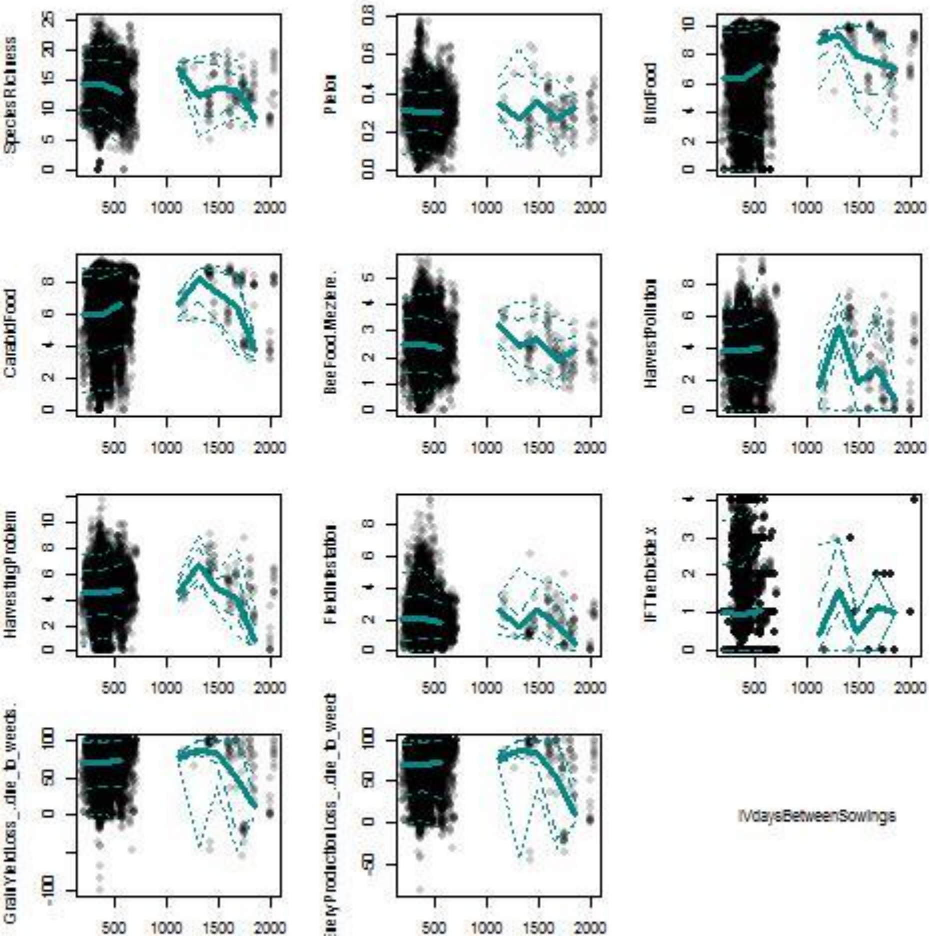
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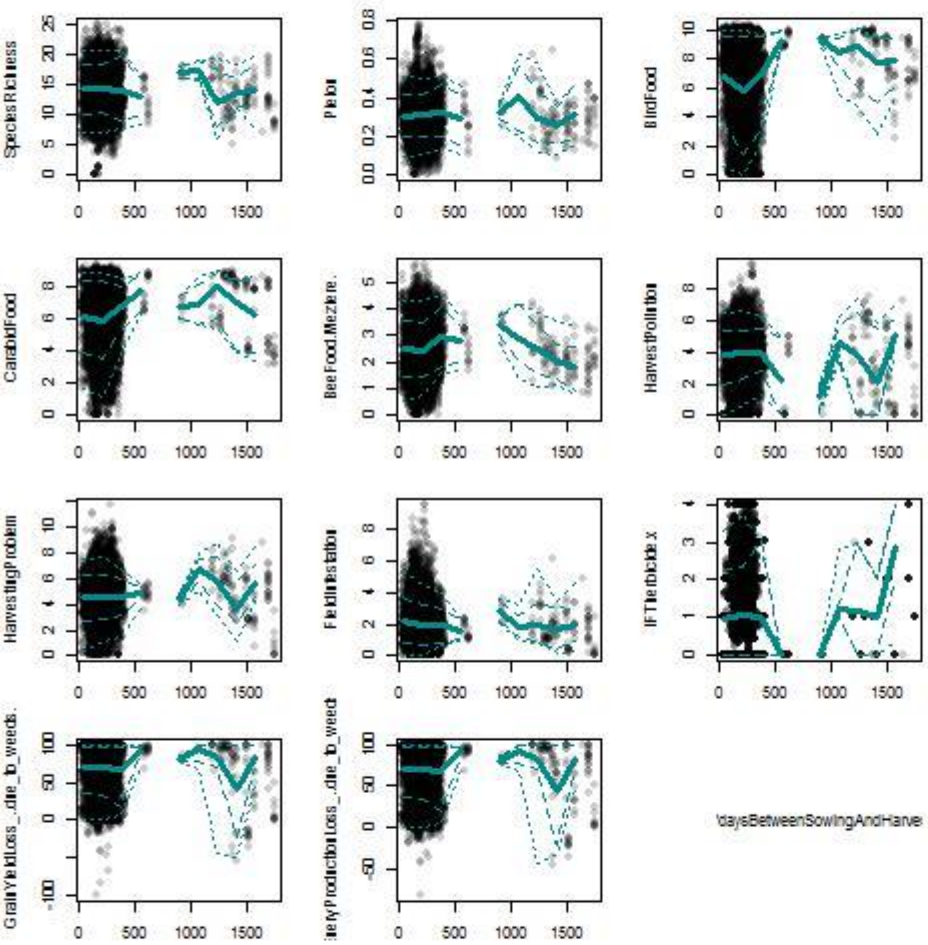
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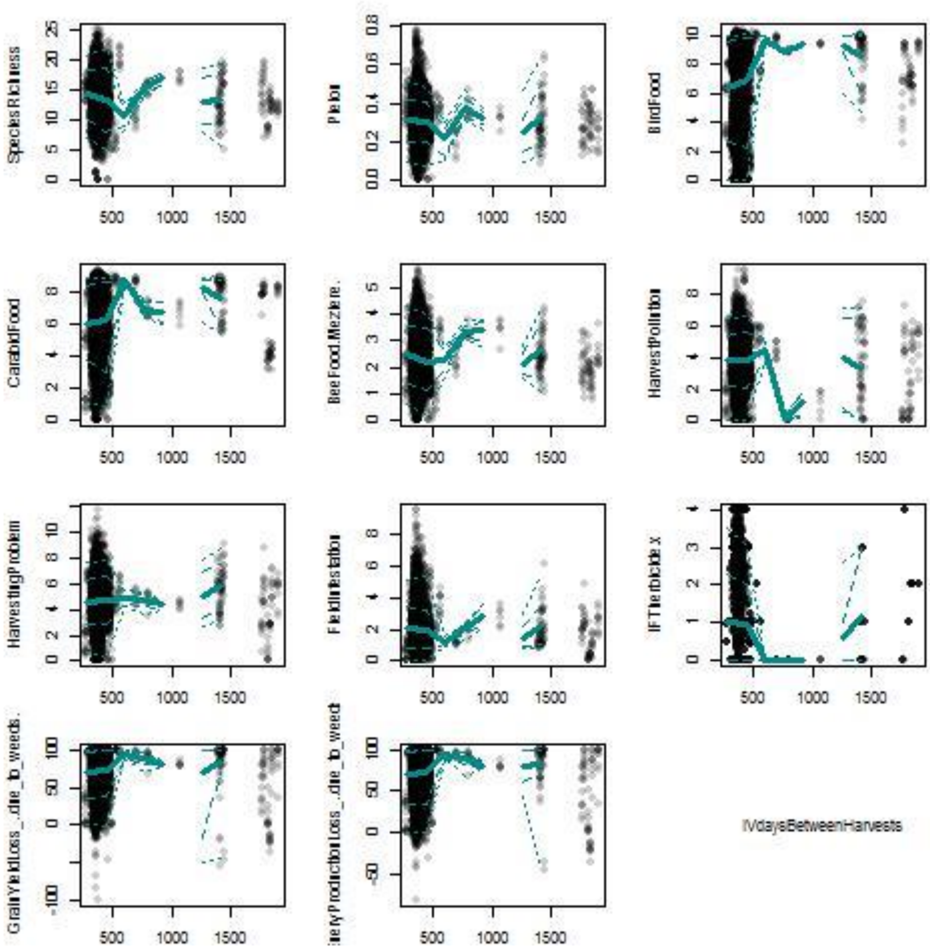
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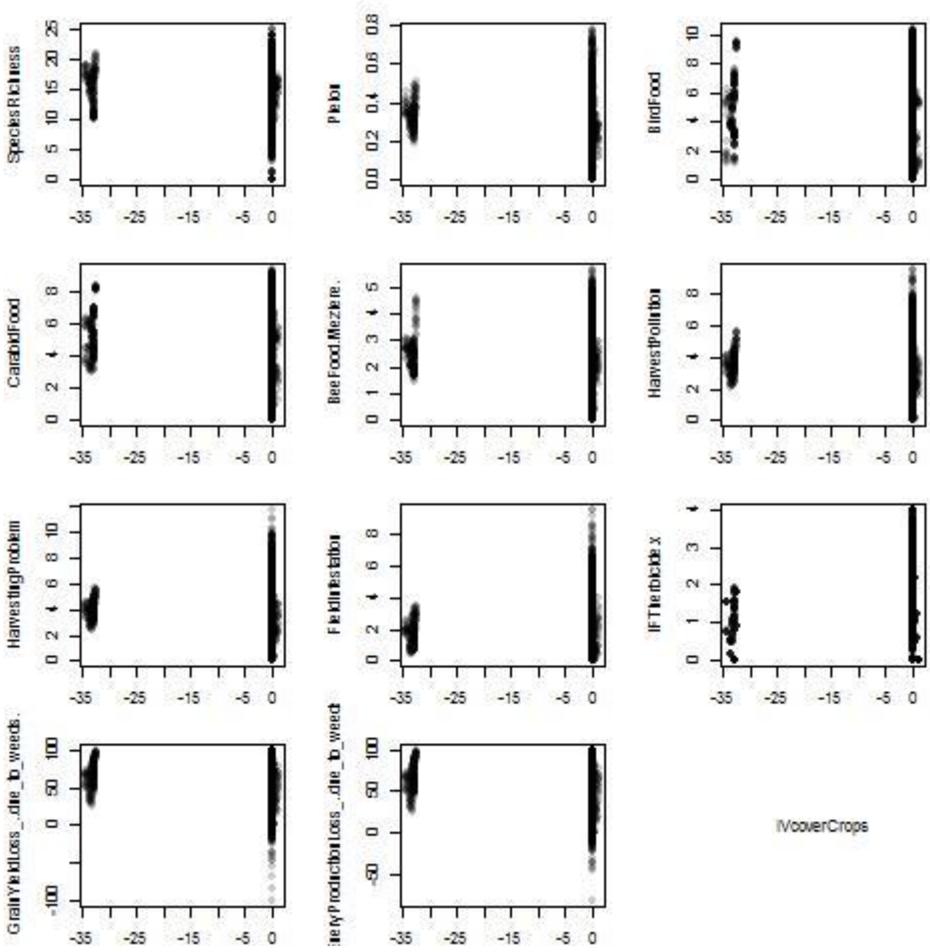
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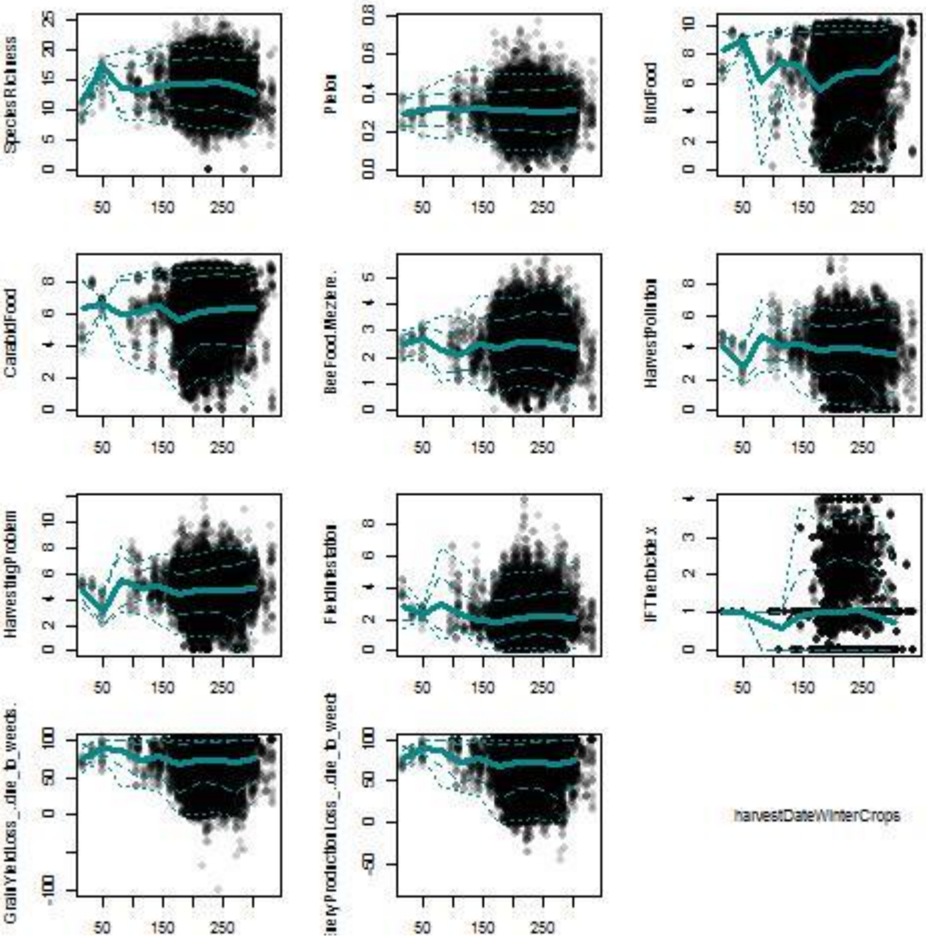
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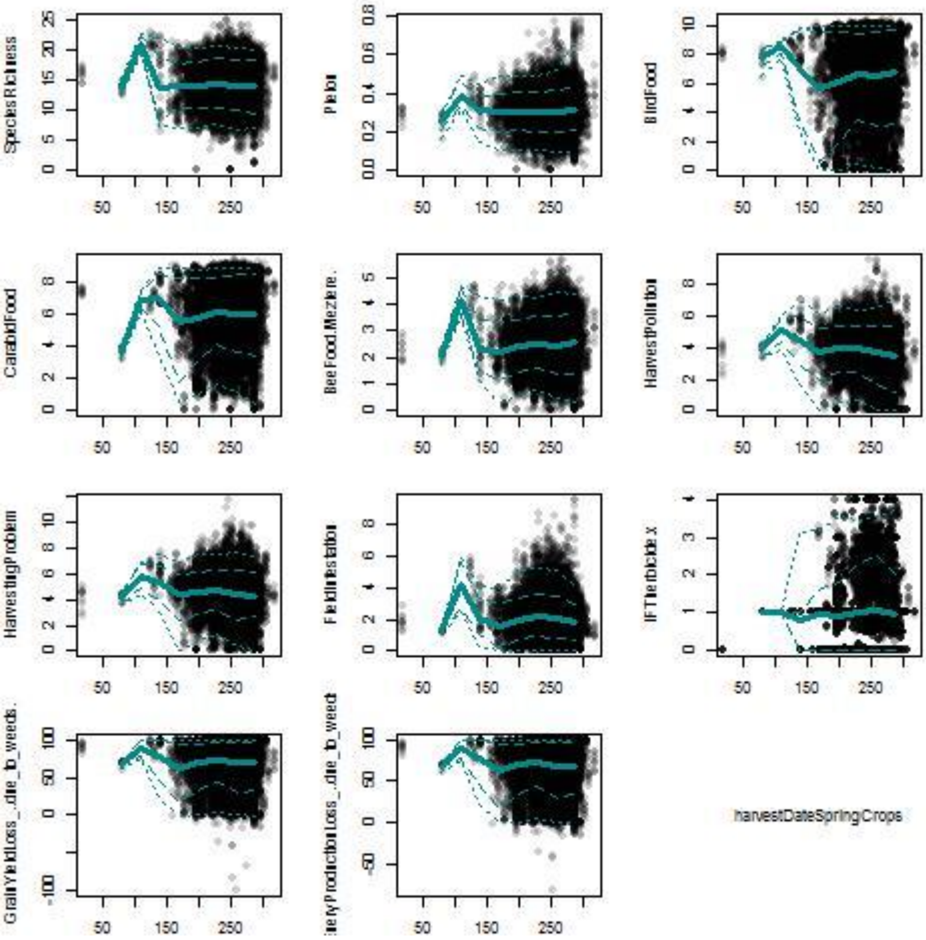
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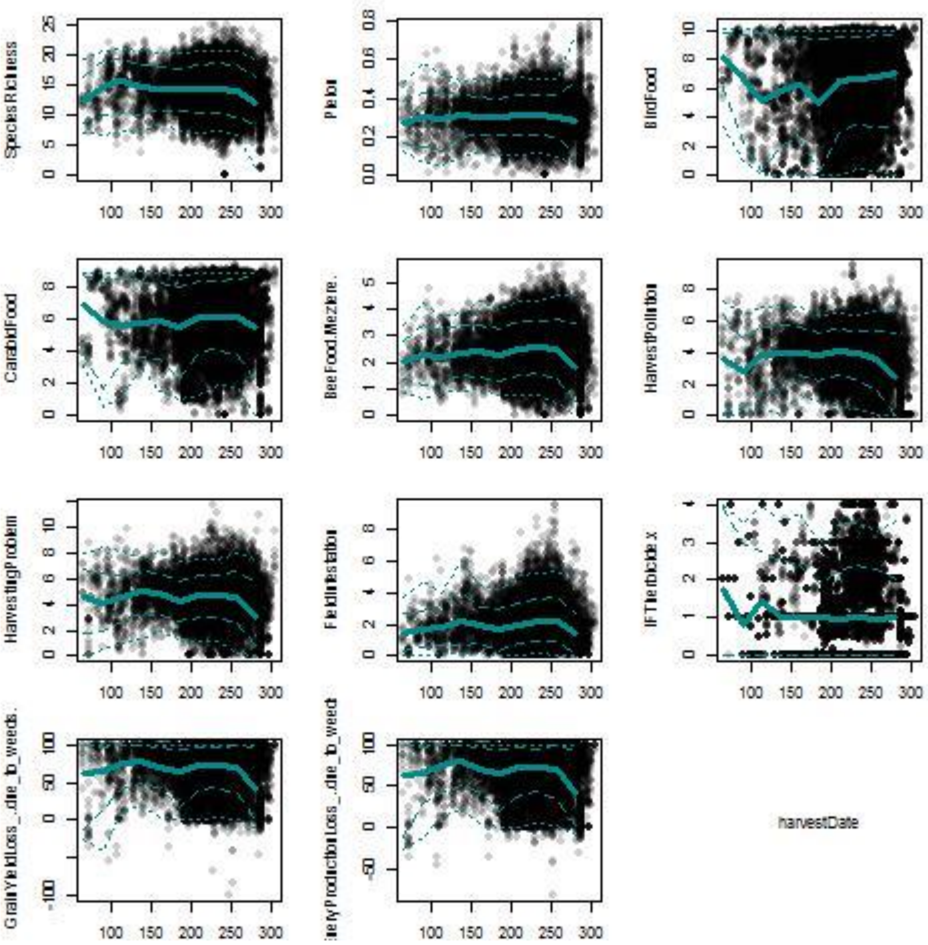
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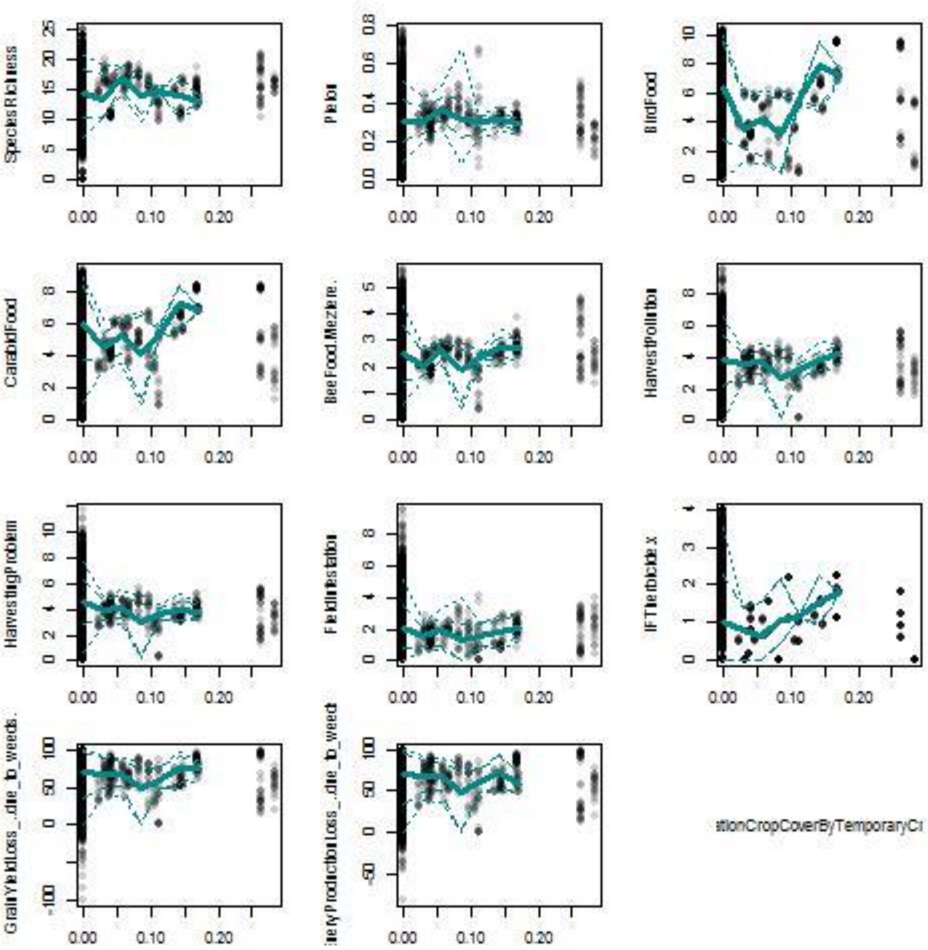
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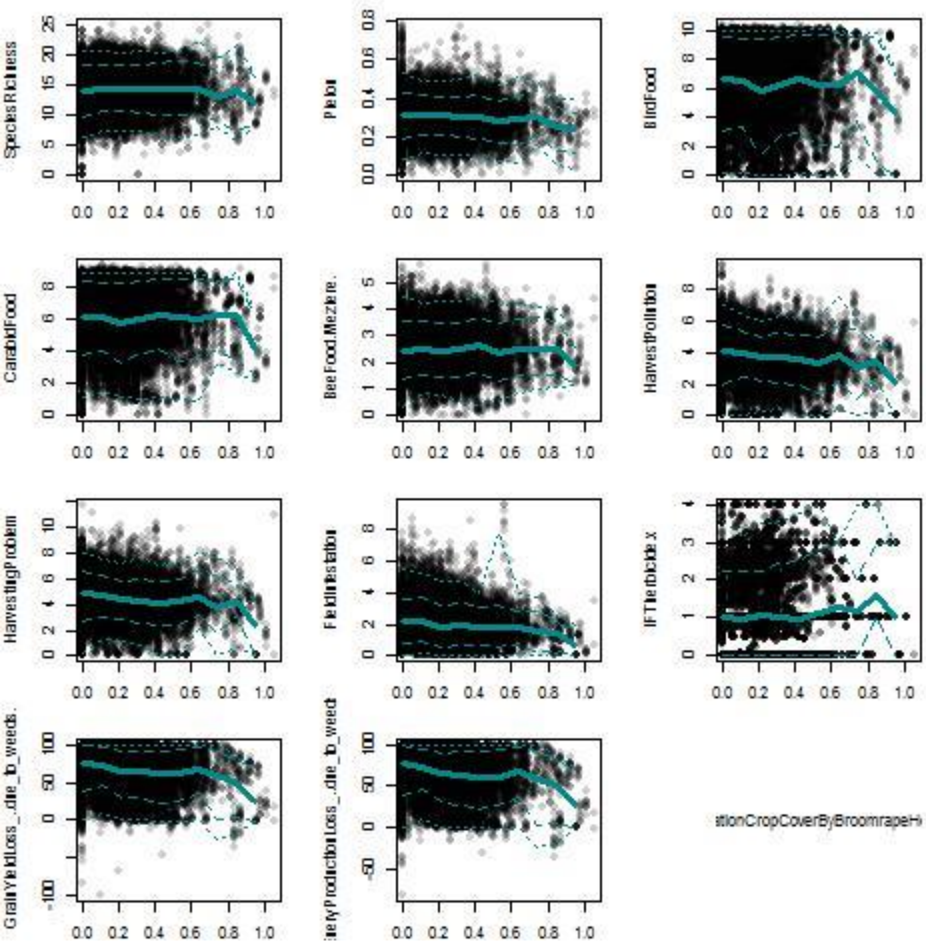
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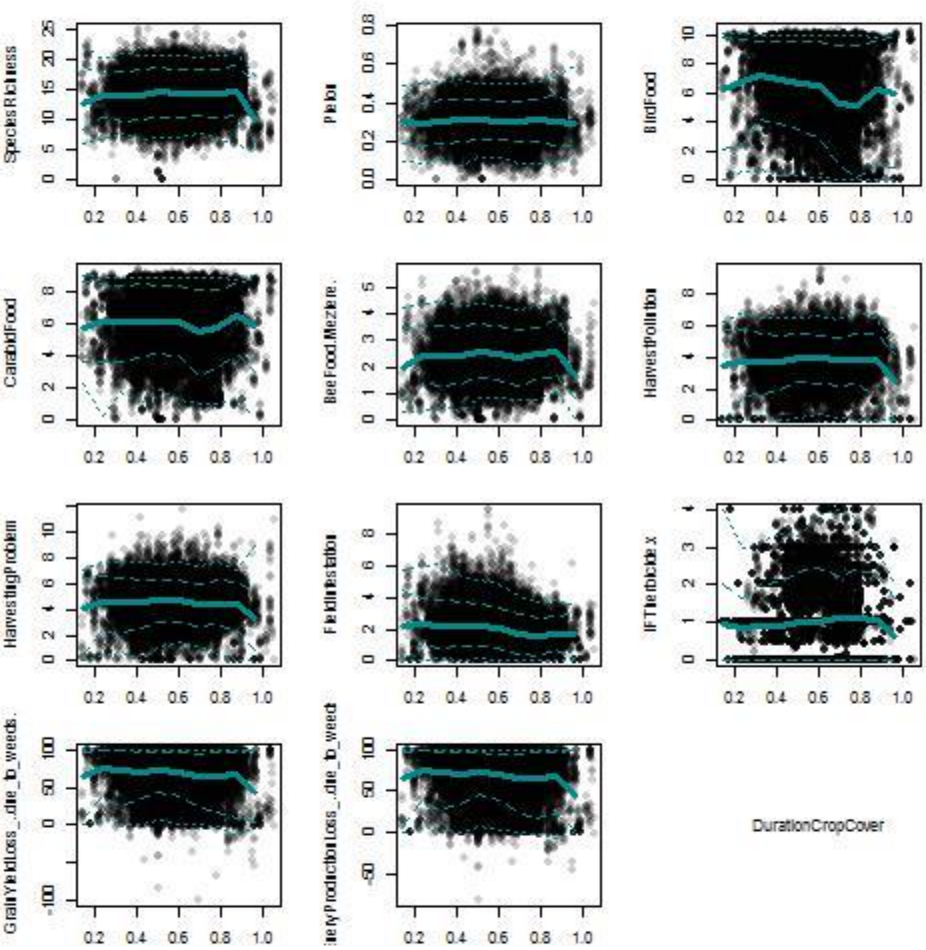
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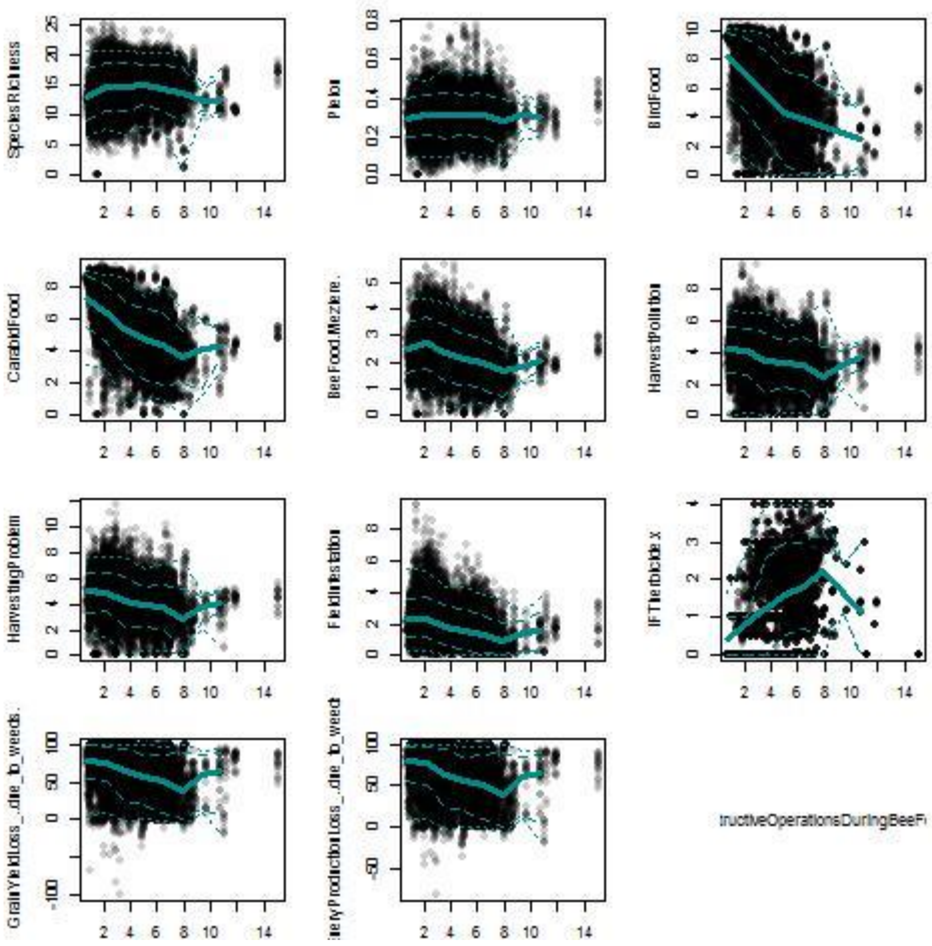

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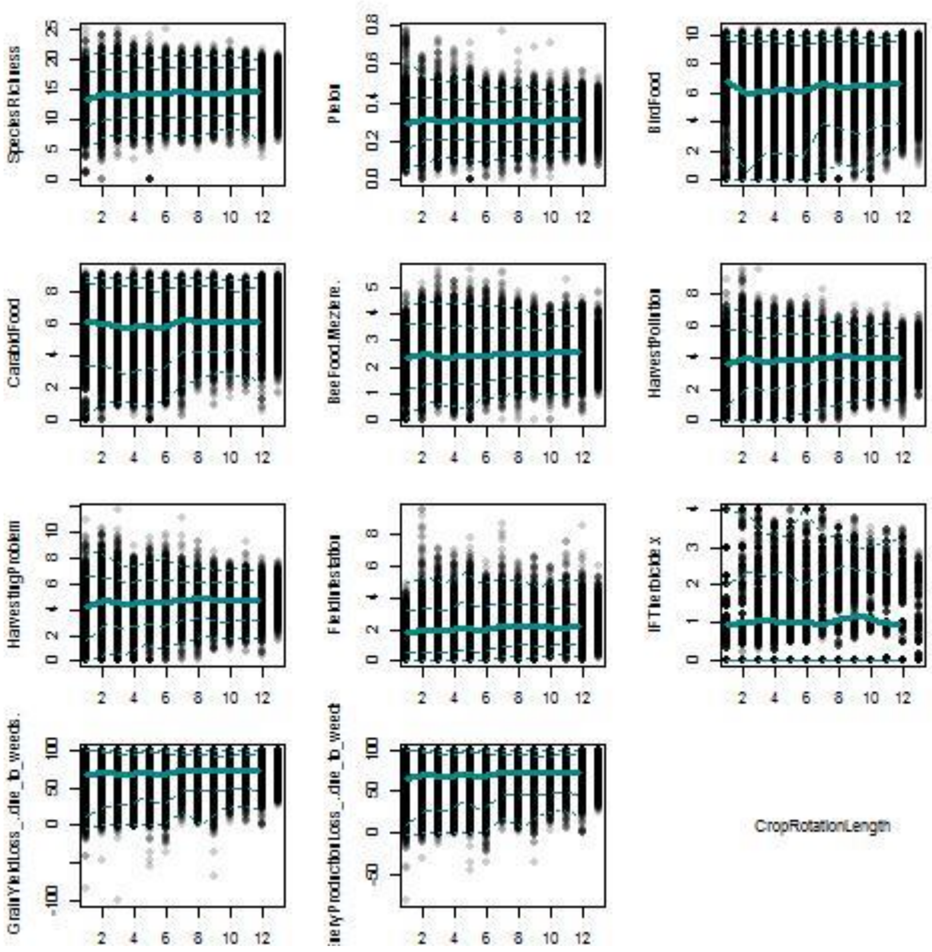

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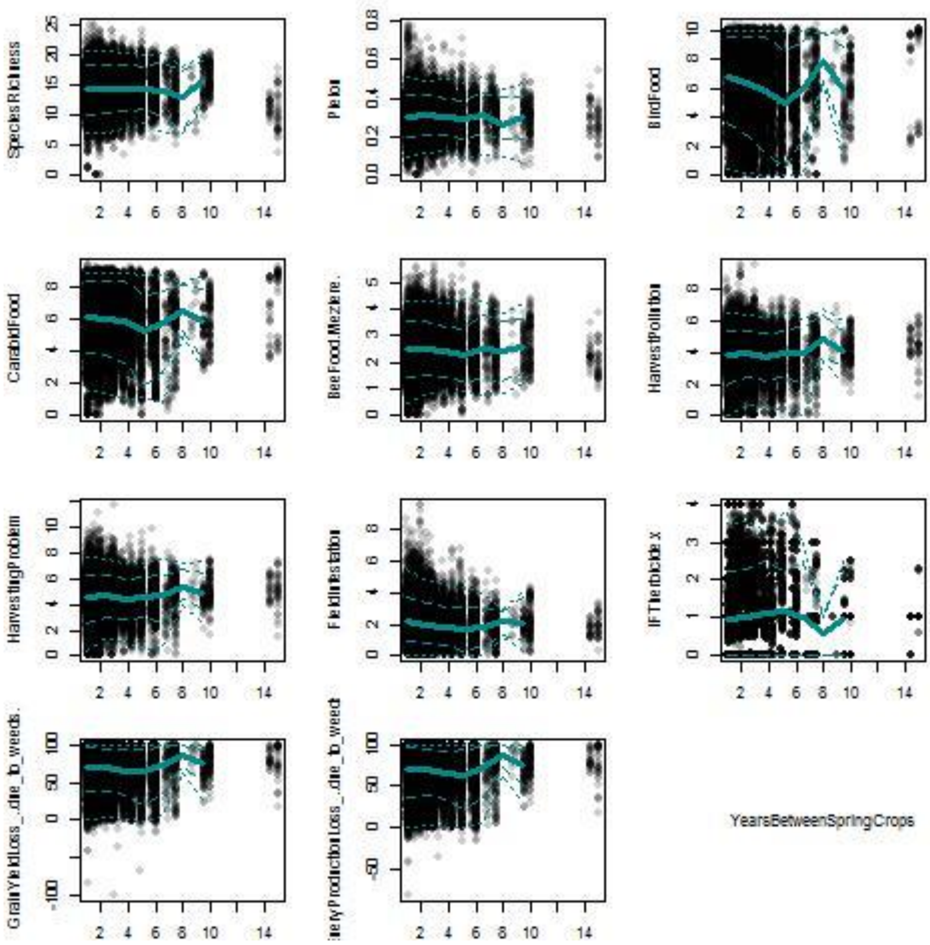


Figure S. 4 Weed impact indicator values depending on the cropping system descriptors. Dots are indicator value averaged over all simulated years of a cropping system x weather repetition. In blue, moving mean and quantiles, for 10 points (or 5 for (*) marked figures), mean in bold, 0.01 and 0.99 quantiles in dotted line and 0.1 and 0.9 quantiles in dashed line.

6 Production situation

Table 4 : Description of all production situation descriptors. Weather variable values are averaged over simulation length for a given cropping system x weather repetition.

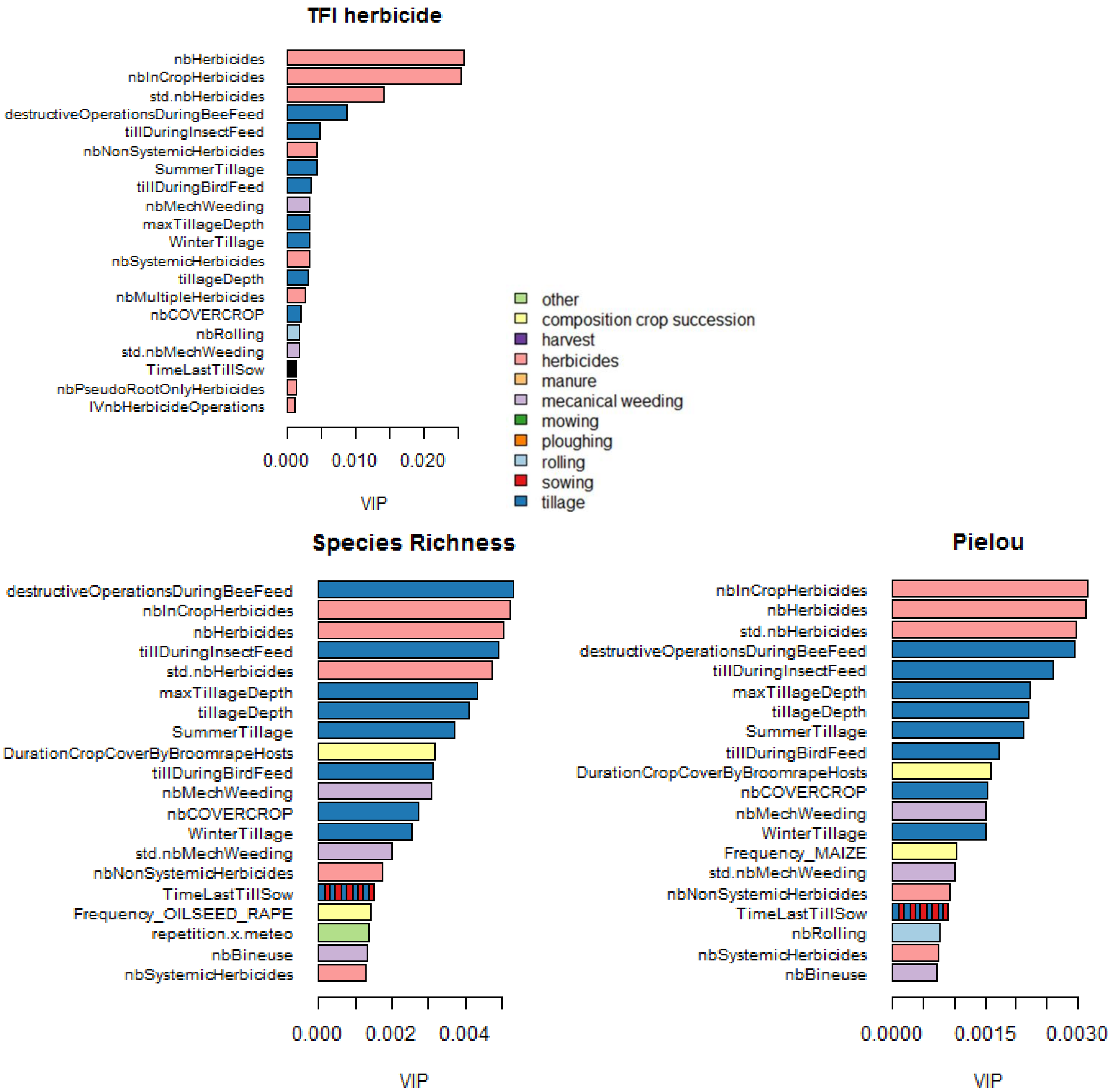
Short name	Units	Description
stones	%	Gravel content
soil_depth	cm	Soil depth
N_org	[0.05%-0.3%]	Mass content of organic nitrogen in the humification soil horizon (from the surface to below to 60 cm)
lime	%	Lime content of the uppermost soil horizon
pH	no unit	Soil pH
average_temp	°C	Average daily temperature
average_temp_SS	°C	Average daily temperature for Spring and Summer
average_temp_FW	°C	Average daily temperature for Fall and Winter

average_temp_Winter	°C	Average daily temperature for Winter
average_temp_Spring	°C	Average daily temperature for Spring
average_temp_Fall	°C	Average daily temperature for Fall
average_temp_Summer	°C	Average daily temperature for Summer
min_temp	°C	Average minimum daily temperature
min_temp_SS	°C	Average minimum daily temperature for Spring and Summer
min_temp_FW	°C	Average minimum daily temperature for Fall and Winter
min_temp_Winter	°C	Average minimum daily temperature for Winter
min_temp_Spring	°C	Average minimum daily temperature for Spring
min_temp_Fall	°C	Average minimum daily temperature for Fall
min_temp_Summer	°C	Average minimum daily temperature for Summer
max_temp	°C	Average maximum daily temperature
max_temp_SS	°C	Average maximum daily temperature for Spring and Summer
max_temp_FW	°C	Average maximum daily temperature for Fall and Winter
max_temp_Winter	°C	Average maximum daily temperature for Winter
max_temp_Spring	°C	Average maximum daily temperature for Spring
max_temp_Fall	°C	Average maximum daily temperature for Fall
max_temp_Summer	°C	Average maximum daily temperature for Summer
frost_frequency	Days	Average number of frost (below 0°C) days per year
heat_frequency	Days	Averaged number of hot (over 30°C) days per year
cold_intensity_P1	°C	Cold severity, 1st percentile of annual daily temperatures
cold_intensity_P5	°C	Cold severity, 5th percentile of annual daily temperatures
cold_intensity_P10	°C	Cold severity, 10th percentile of annual daily temperatures
heat_intensity_P90	°C	Heat severity, 90th percentile of annual daily temperatures
heat_intensity_P95	°C	Heat severity, 95th percentile of annual daily temperatures
heat_intensity_P99	°C	Heat severity, 99th percentile of annual daily temperatures
drough_intensity	Days number	Drought intensity, maximum number of consecutive days without rain per year
average_rain	mm	Average annual sum of daily precipitation
average_rain_SS	mm	Average sum of daily precipitation during Spring and Summer
average_rain_FW	mm	Average sum of daily precipitation during Fall and Winter
average_rain_Winter	mm	Average sum of daily precipitation during Winter
average_rain_Spring	mm	Average sum of daily precipitation during Spring
average_rain_Fall	mm	Average sum of daily precipitation during Fall
average_rain_Summer	mm	Average sum of daily precipitation during Summer
rain_frequency	Days number	Annual number of days with precipitation ≥ 1mm per year
rain_frequency_SS	Days number	Annual number of days with rainfall ≥ 1mm for Spring and Summer
rain_frequency_FW	Days number	Annual number of days with rainfall ≥ 1mm for Fall and Winter

rain_frequency_Winter	Days number	Annual number of days with rainfall ≥ 1mm for Winter
rain_frequency_Spring	Days number	Annual number of days with rainfall ≥ 1mm for Spring
rain_frequency_Fall	Days number	Annual number of days with rainfall ≥ 1mm for Fall
rain_frequency_Summer	Days number	Annual number of days with rainfall ≥ 1mm for Summer
average_radiation	$J.cm^{-2}$	Annual sum of daily solar radiation
average_radiation_SS	$J.cm^{-2}$	Sum of daily solar radiation for Spring and Summer
average_radiation_FW	$J.cm^{-2}$	Sum of daily solar radiation for Fall and Winter
average_radiation_Winter	$J.cm^{-2}$	Sum of daily solar radiation for Winter
average_radiation_Spring	$J.cm^{-2}$	Sum of daily solar radiation for Spring
average_radiation_Fall	$J.cm^{-2}$	Sum of daily solar radiation for Fall
average_radiation_Summer	$J.cm^{-2}$	Sum of daily solar radiation for Summer
average_PET	mm	Annual sum of daily potential evapotranspiration
average_PET_SS	mm	Sum of daily potential evapotranspiration for Spring and Summer
average_PET_FW	mm	Sum of daily potential evapotranspiration for Fall and Winter
average_PET_Winter	mm	Sum of daily potential evapotranspiration for Winter
average_PET_Spring	mm	Sum of daily potential evapotranspiration for
average_PET_Fall	mm	Sum of daily potential evapotranspiration for Fall
average_PET_Summer	mm	Sum of daily potential evapotranspiration ngth for Summer
field_capacity	$g(water).g^{-1}(soil)$	Mean field capacity of all soil horizons

7 Variable importance for individual indicators

Following figures: Key cropping system descriptors driving overall weed impact (mean of variable importance values of all indicators) averaged over simulation in the learning data set. Random forest VIP values for the first 20 most important cropping system descriptors for for each indicators. Colours represent types of cropping system descriptors, hatched bars are for descriptors concerning two different types. For the meaning of the cropping system descriptors, see Appendix (§ III.2.7). Variance explained for whole learning data set 83.78 %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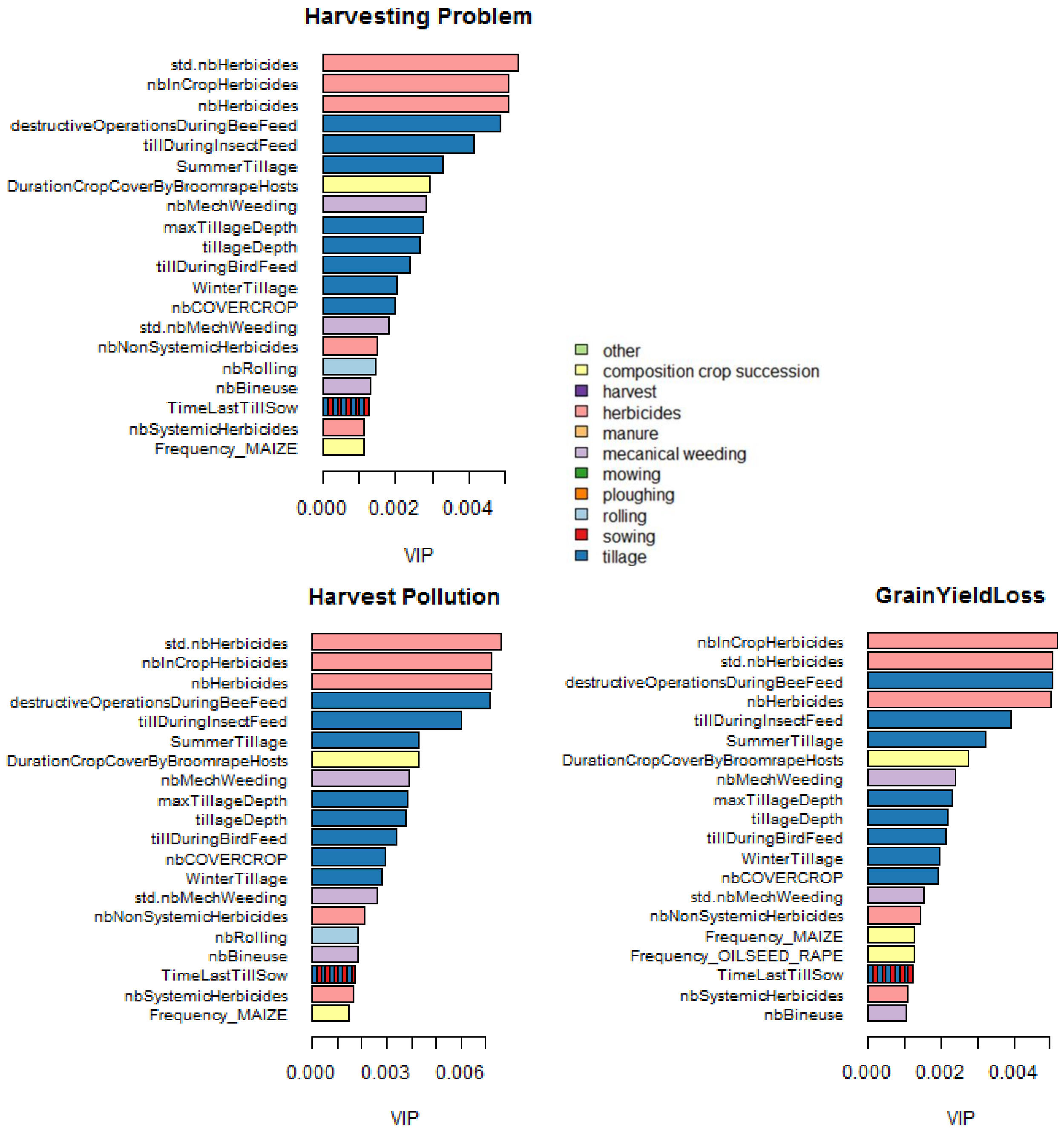
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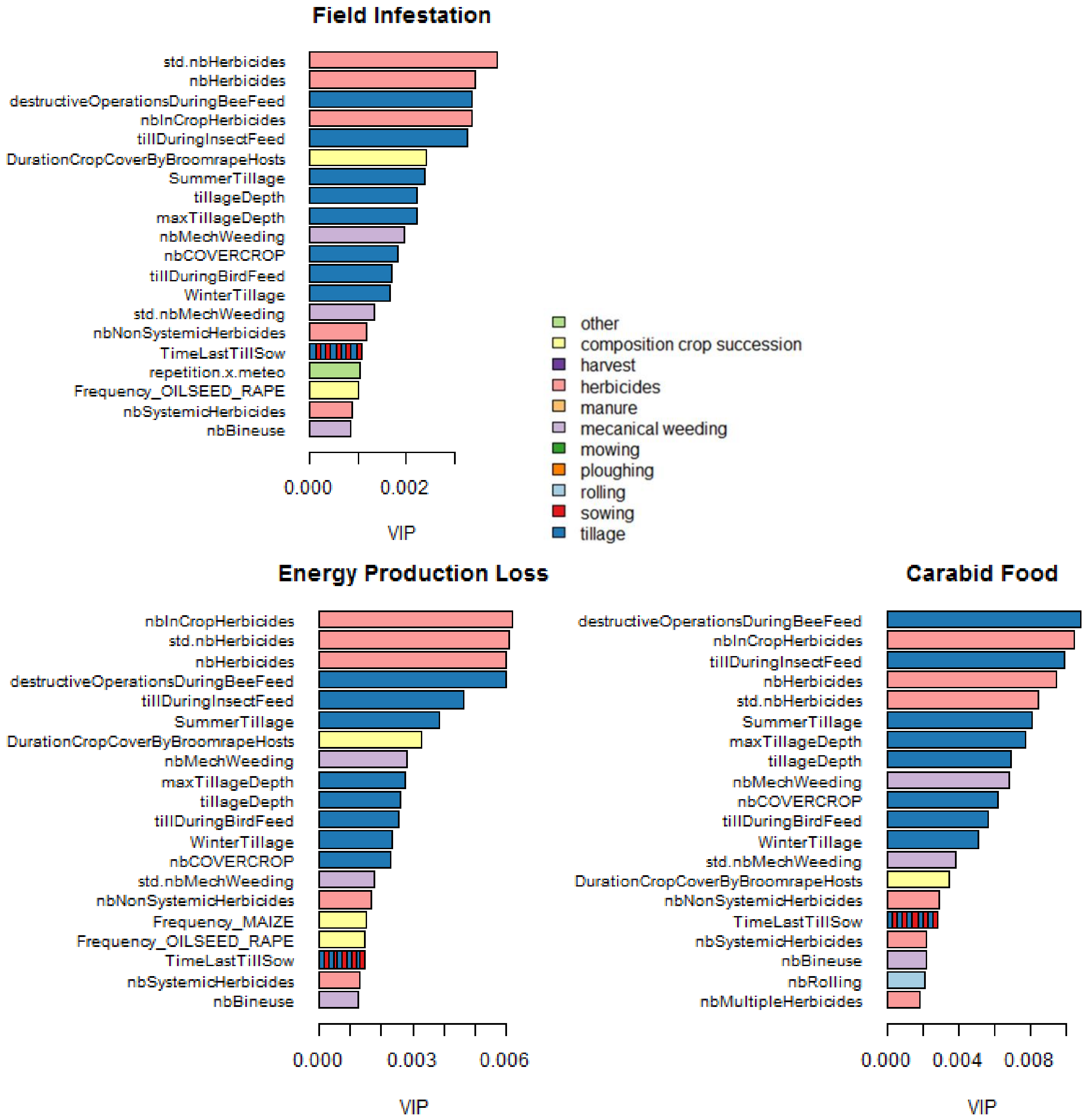
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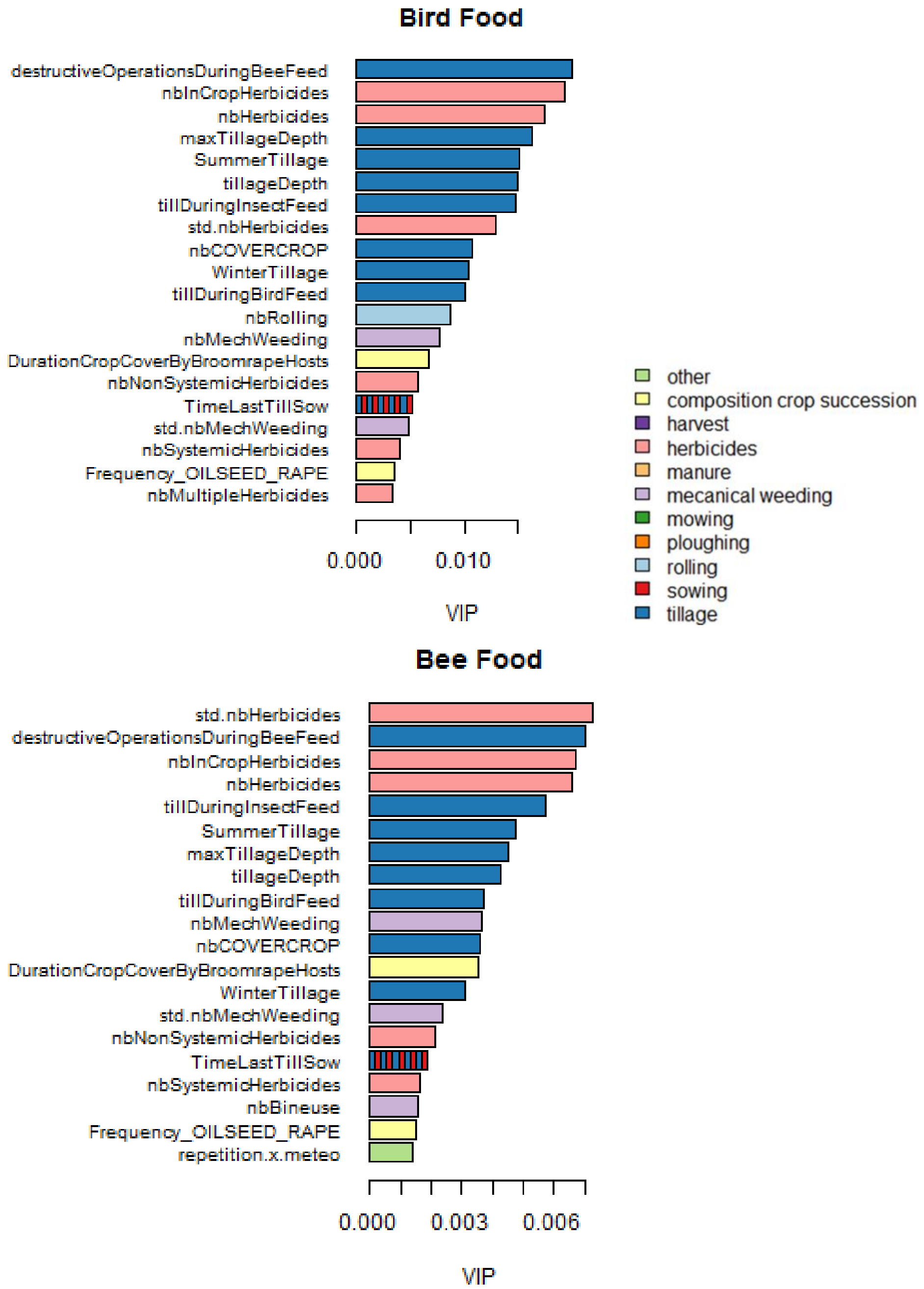
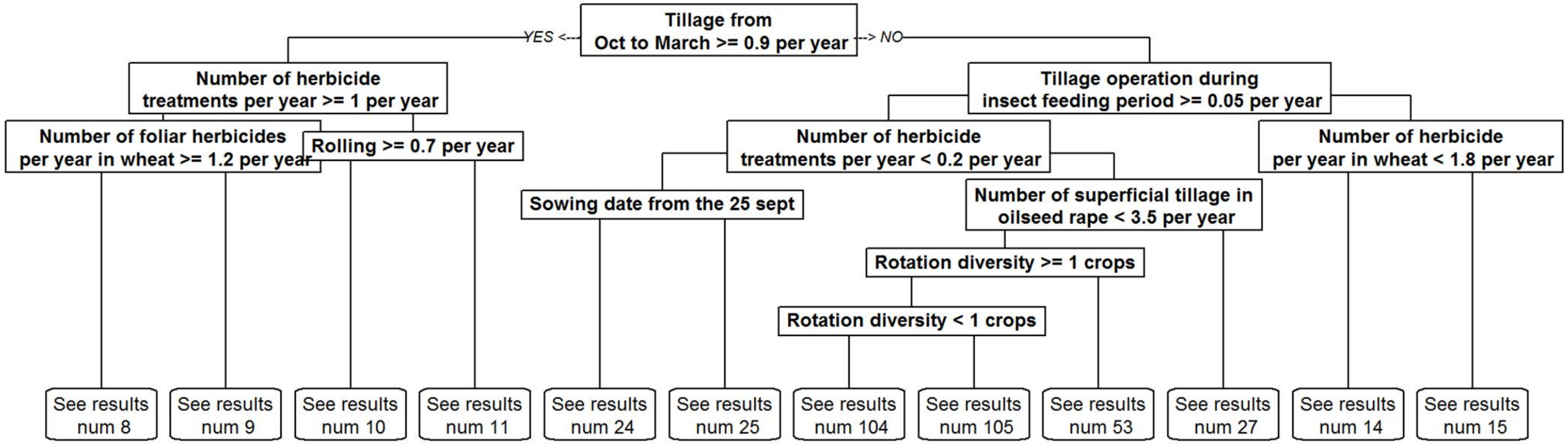


Figure 5 : Key cropping system descriptors driving overall weed impact (mean of variable importance values of all indicators) averaged over simulation in the learning data set. Random forest VIP values for the first 20 most important cropping system descriptors for for each indicators. Colours represent types of cropping system descriptors, hatched bars are for descriptors concerning two different types. For the meaning of the cropping system descriptors, see Appendix (§ III.2.7). Variance explained for whole learning data set 83.78 % .

8 Regression tree for productivity profile



	num 8	num 9	num 10	num 11	num 24	num 25	num 104	num 105	num 53	num 27	num 14	num 15
Harvest pollution	2.44 +/- 0.74	3.02 +/- 1.37	2.71 +/- 2.17	3.57 +/- 0.94	3.87 +/- 1.3	3.95 +/- 0.47	1.72 +/- 1.86	1.58 +/- 1.23	3.86 +/- 1.26	4.15 +/- 0.44	3.8 +/- 1.57	4.16 +/- 0.27
Harvesting problem	2.75 +/- 0.74	3.67 +/- 1.51	3.7 +/- 2.95	4.06 +/- 1.05	4.62 +/- 1.26	4.62 +/- 0.51	2.68 +/- 2.22	2.27 +/- 1.41	4.68 +/- 1.38	4.71 +/- 0.47	4.61 +/- 1.58	4.42 +/- 0.28
Field infestation	0.32 +/- 0.47	1.64 +/- 0.93	0.81 +/- 0.72	1.4 +/- 0.7	2.3 +/- 0.77	1.94 +/- 0.48	1.93 +/- 0.91	1.08 +/- 0.49	2.3 +/- 0.89	1.59 +/- 0.49	2.32 +/- 0.92	1.31 +/- 0.24
Grain yield loss	13.82 +/- 13.7	53.74 -/- 25.57	20.76 -/- 19.66	59.82 -/- 17.12	72.15 -/- 18.61	74.8 +/- 9.09	41.52 -/- 39.06	26.48 +/- 21.2	73.75 -/- 19.43	82.32 +/- 5.9	72.23 -/- 23.83	80 +/- 5.03

Figure 6 : Multivariate regression tree identifying combinations of cropping techniques to achieve contrasting profiles of weed impact on crop production for the PS.C production situation (with more cropping systems from Burgundy) from main paper, (Chapitre IV), sorted on the 4 weed impact indicators for the production profile. All branch on the right: NO, branch on the left: YES. Cells were coloured from white (nil) to green (maximum) for biodiversity, from white to red (maximum) for harmfulness for crop production averaged over years and weather repetitions. Uncoloured cells show standard-error including weather effects and variability among systems in a branch. Cross-validation error = 0.022, for indicator range of variation rescaled to [0,1].

Annexe 8
Supplementary material for co-development of a decision support system for integrated weed management: contribution from future users

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(2) UMR Agronomie, INRA, AgroParisTech, Université Paris Saclay, 78 850 Thiverval-Grignon, France

(3) Acta, 31450, Baziège, France

(4) LAE, INRA, Univ. Lorraine, F-54500 Vandœuvre-lès-Nancy, France

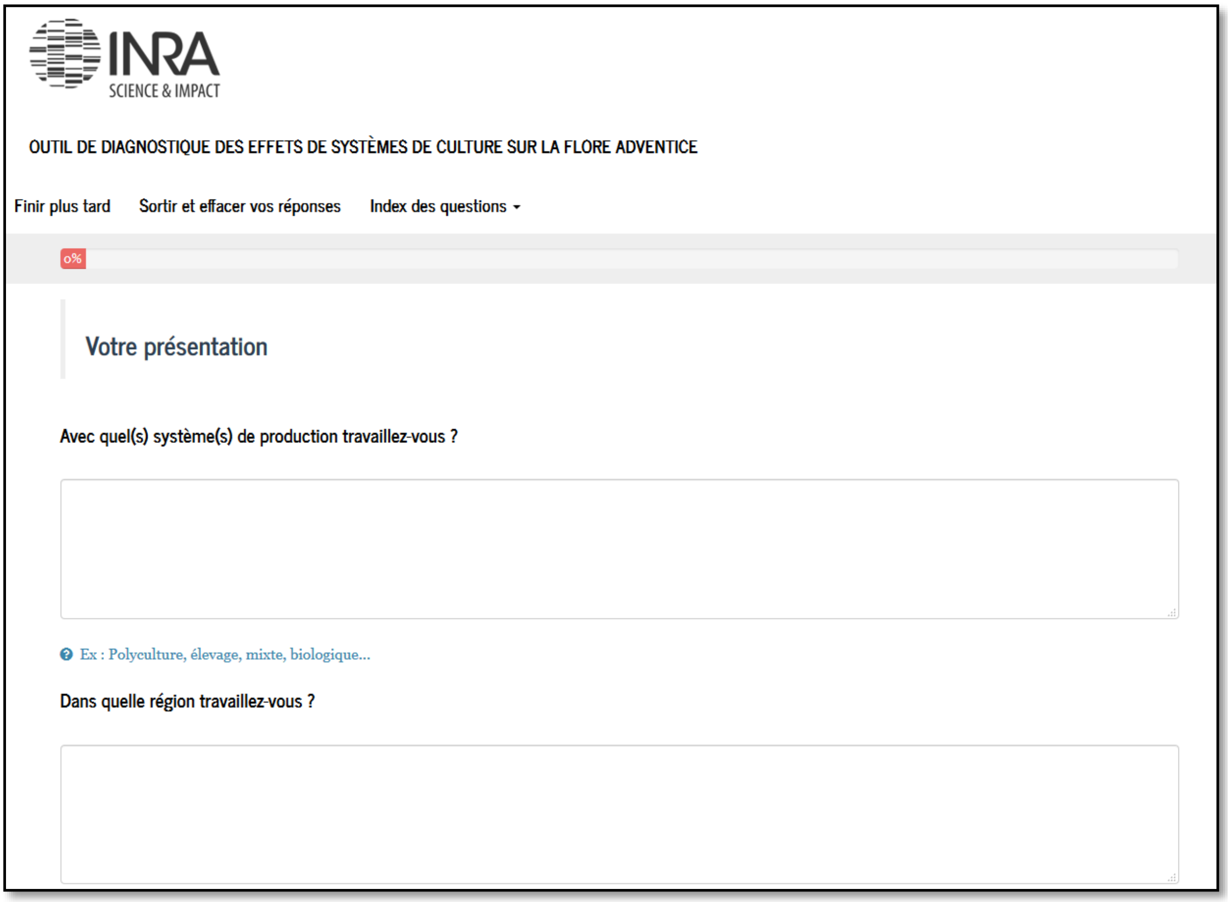
1 Short presentation of FLORSYS

Voir annexe A2 de la these.

2 Online surveys

2.1 Overview of the online survey

In the following images are print screen of the first pages of the online survey:



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SCIENCE & IMPACT

OUTIL DE DIAGNOSTIQUE DES EFFETS DE SYSTÈMES DE CULTURE SUR LA FLORE ADVENTICE

Finir plus tard   Sortir et effacer vos réponses   Index des questions

Outils d'aide à la décision

Voici quelques questions sur les outils d'aide à la décision et vos besoins les concernant.

Avez-vous déjà utilisé ou utilisez-vous un outil d'aide à la décision ?

Oui   Non   Sans réponse

Selon vous, un outil permettant de gérer au mieux les adventices à l'échelle des systèmes de culture doit vous aider à prendre quelles décisions ?

Exemples : Quelles rotations pratiquer ? Ou quel type de travail du sol ? Quelles dates de semis ?

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Données à renseigner

Afin d'analyser les systèmes de cultures (existants, mais aussi innovants), il est essentiel de renseigner certaines données. Les questions qui suivent vont nous aider à préciser les entrées potentielles à fournir dans l'outil.

Un modèle de recherche complexe ("parcelle virtuelle") existe déjà pour prédire la dynamique de la flore adventice en fonction des systèmes de culture testés (FLORSYS). L'outil en cours de développement sera tiré de ce modèle et dans celui-ci, il faut renseigner différentes variables. Dans le premier tableau vous retrouverez les types de variables correspondant aux pratiques et dans le suivant vous trouverez le détail de ces variables.

Pouvez-vous noter ces variables sur une échelle du moins contraignant à obtenir (1) au plus contraignant (16).

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	Non concerné
Succession culturale																	
Cultures intermédiaires																	
Travail du sol																	
Semis																	

2.2 Additional results from crop advisors

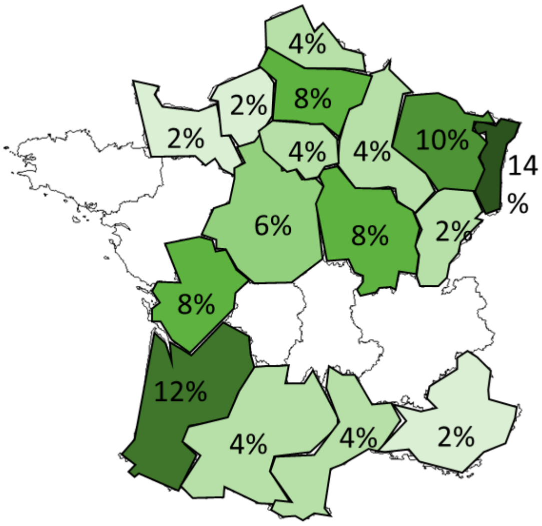


Figure A.8. 1: Regions from which crop advisors responded to the online survey. Some advisors worked in several regions.

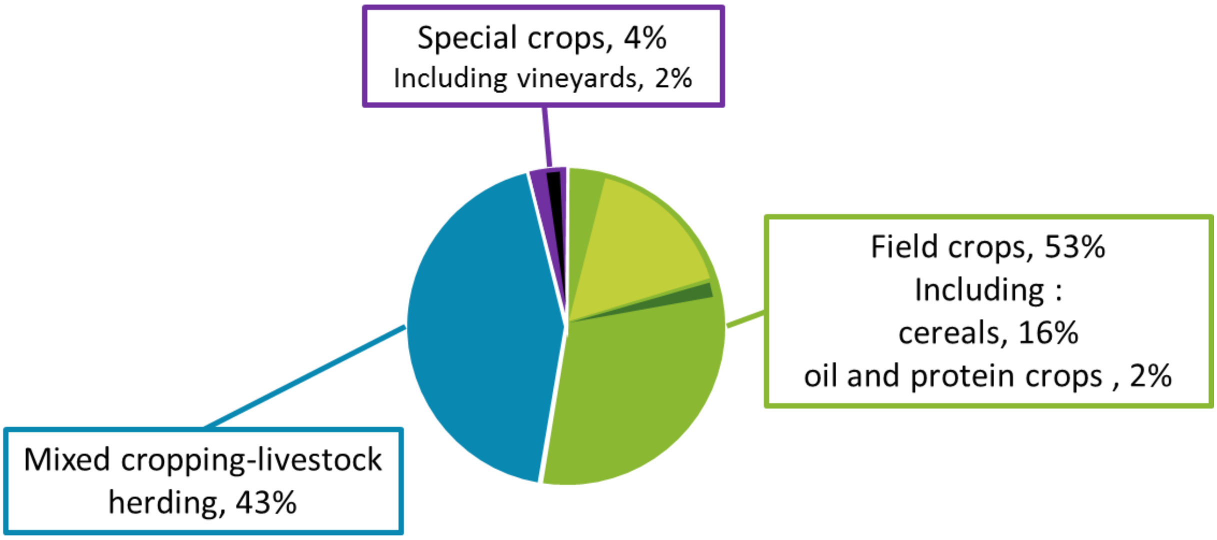


Figure A.8. 2 : The different crops managed by the crop advisors that answered the online survey.

Table A.8. 1: What is the use of decision support systems (DSS) by the crop advisors who answered the online survey? From the 37 responses at this stage of the survey.

Are you using a decision support system?	
Yes	70.3%
No	29.7%

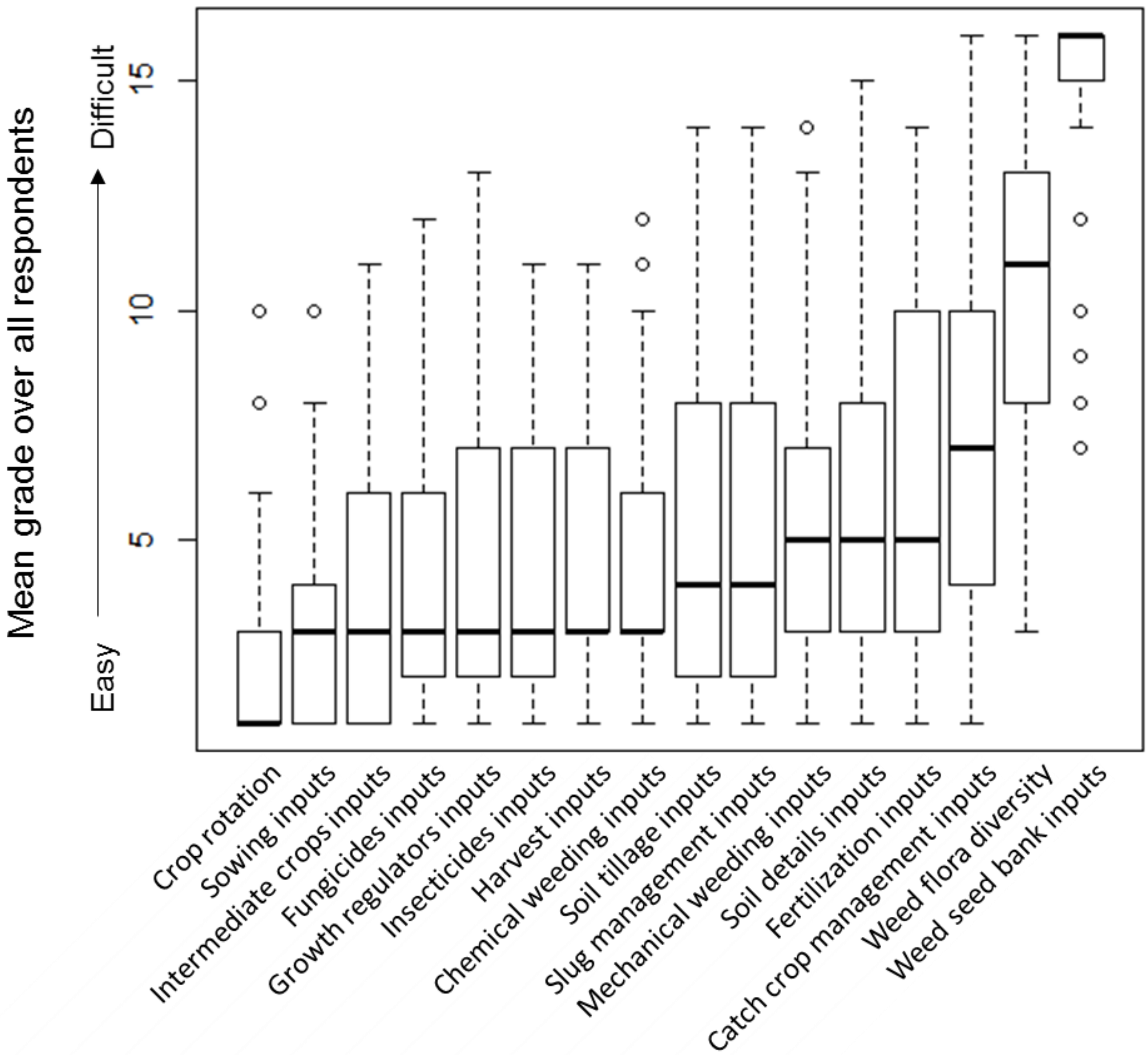


Figure A.8. 3 : Level of difficulty to find different types of cropping system information to feed the FLORSYS model. Crop advisors in the online survey were asked to rank the different types from 1 easy, to 16 hard, giving a mean grade.

Table A.8. 2: How much data are the users ready to provide for a decision-support system depending on their difficulties for managing weeds. Percentage (%) of answers

		How detailed should cropping systems be described?		
		Detailed (list of operations)	Synthetic (meta decision rules)	Both
Why are weeds difficult to manage?	Lack of efficiency of practices	12.2	1.4	2.0
	Lack of knowledge on weed biology	10.8	2.7	0.7
	Constraining species	8.8	1.4	0.0
	Generated costs	5.4	0.0	0.0
	Weeds competition with crops	2.7	0.0	0.0
	Dependence on the weather	2.7	0.0	0.0
	Weed diversity	2.7	0.0	2.0
	Poor image the weeds give of farmer because of the field infestation	2.0	0.7	0.0
	Too many techniques to choose and combine	0.0	0.0	3.4
	Multiannual scale	0.0	0.0	10.1
	The need to diversify crop rotation	8.1	8.1	6.1
	Weed resistance to herbicides	1.4	4.7	0.0

2.3 Additional results from farmers

Figure A.8. 4 : Origin of the 4 farmers having fully responded to the online survey

3 Additional results from the second meeting with farmers

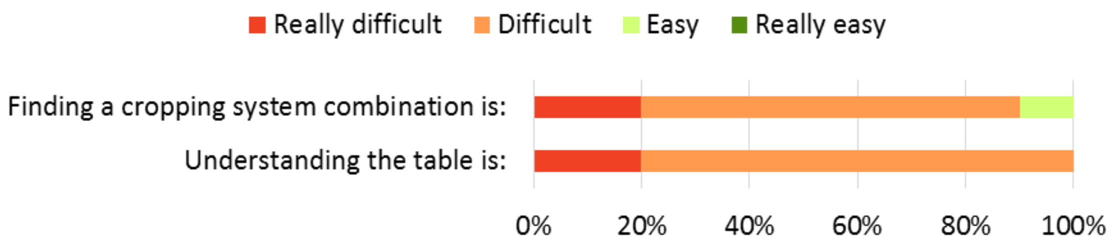


Figure 5: Ratings (from the 10 filled questionnaires) that farmers from the group meeting gave to the understanding of the table proposed as a possible format for the future Decision Support System.

4 Additional results from workshops with crop advisors

4.1 Example of cropping systems built the first day

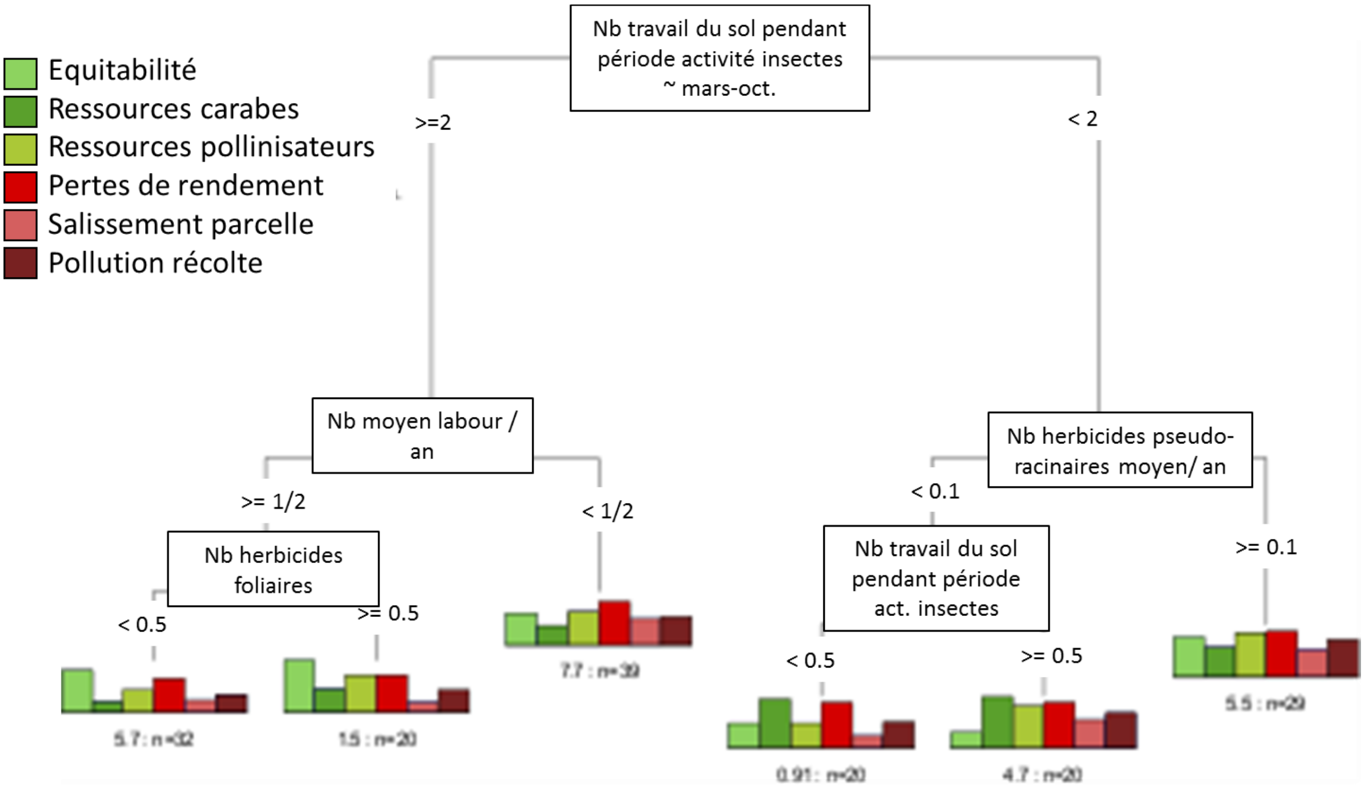
Figure A.8. 5 : Example of cards used during the workshop to combine management practices into a novel cropping system

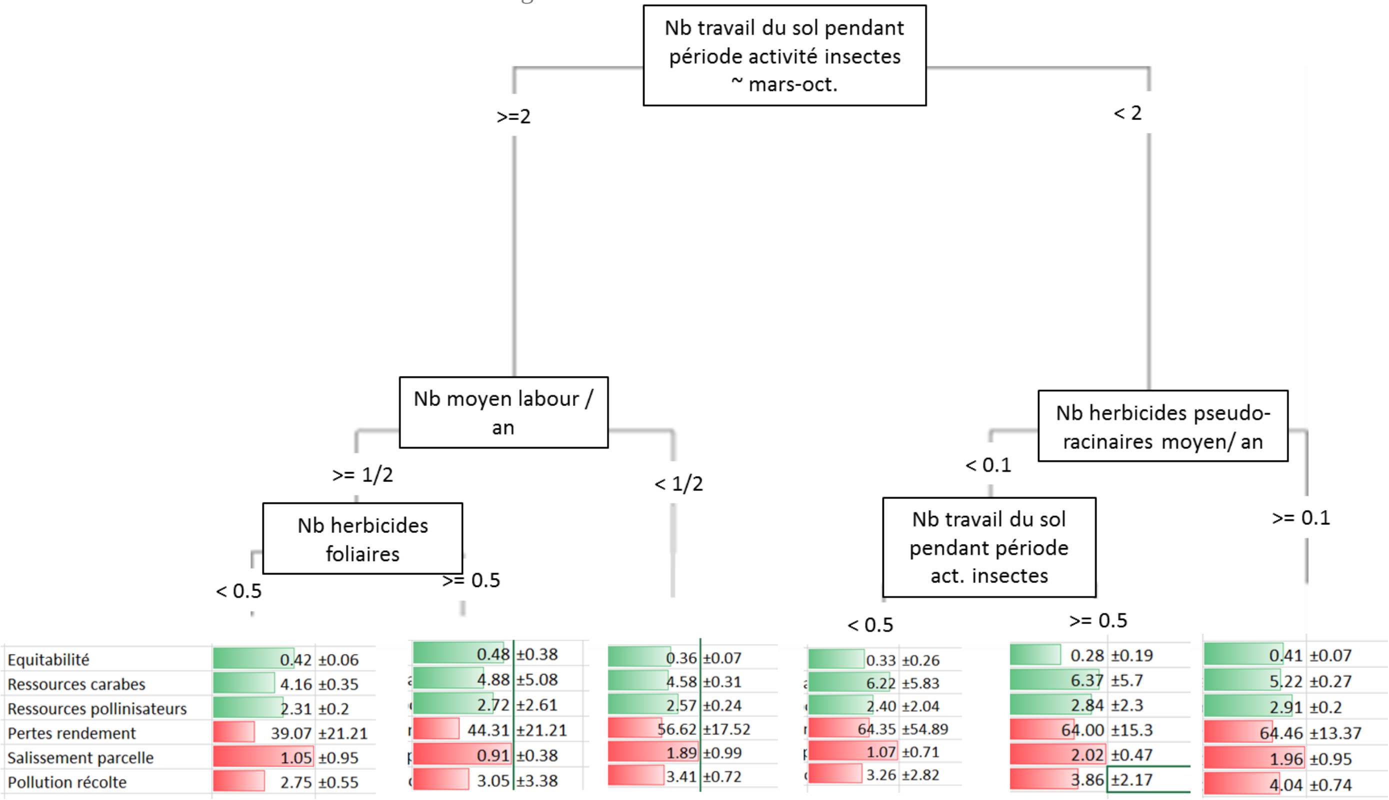
Oilseed rape	Wheat	Spring barley	Winter peas	Wheat	Winter barley
Early sowing	Early sowing	Catch crop: Spring peas Mustard Sunflower Feverole	3 stale seedbed	Late sowing	2 stubble breaking
Organic fertilizer	1 stubble breaking	1 rolling	HERBICIDES : KERBFLO Nirvanas	3 stale seedbed	HERBICIDES : Fosburi Tomigan
2 stubble breaking	HERBICIDES : Glyphosate Fosburi Defi	1 stubble breaking		HERBICIDES : Fosburi	
HERBICIDES : KERBFLO Napro Alabama (ButisanS)		HERBICIDES : Glypho Bofix			

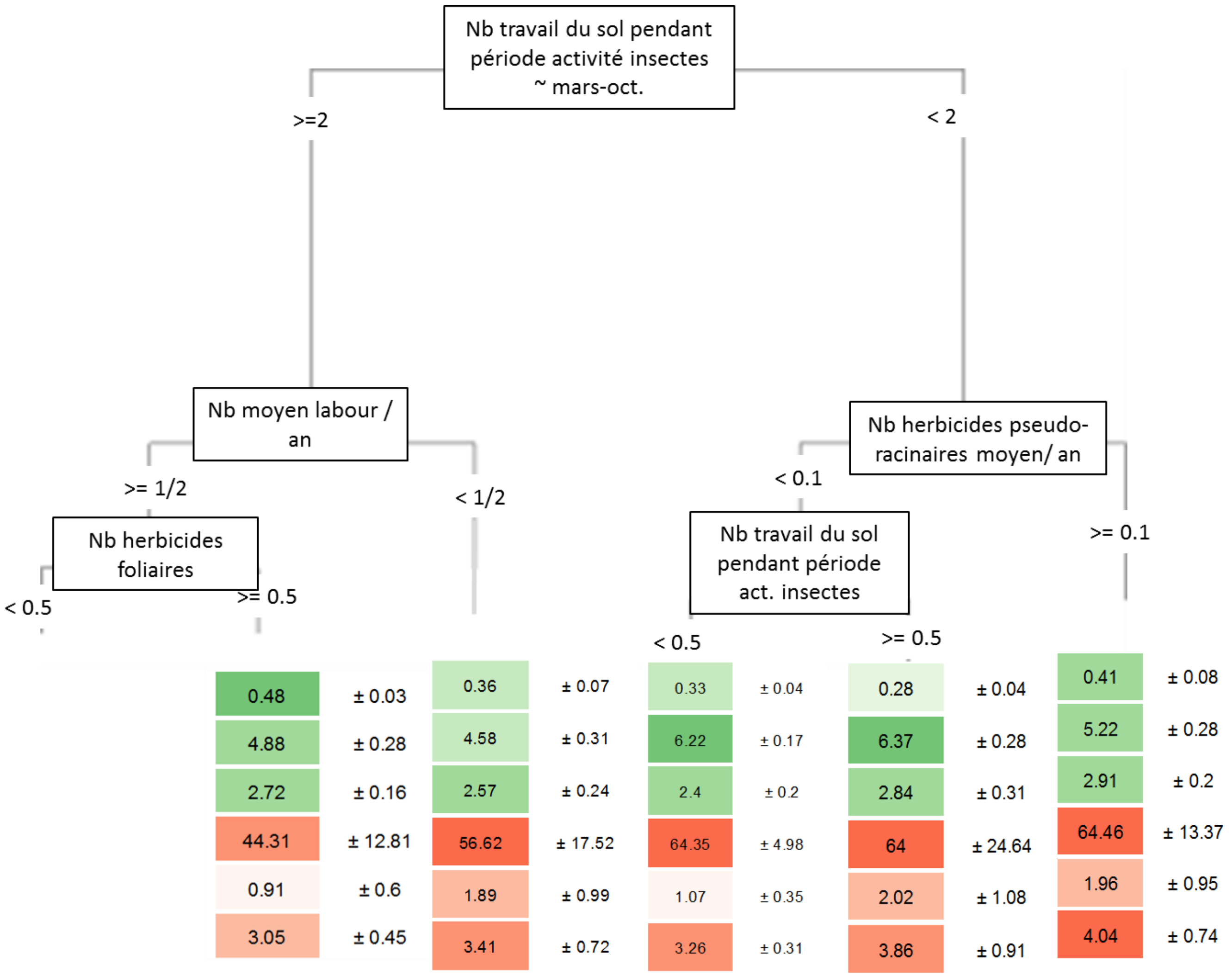
Figure A.8. 6 : Synthesis of the cropping system shown in Figure A.8. 5

4.2 Outputs shown on the second day

The following trees were shown to the crop advisors in the workshop (second day), they were asked to rank the different proposition to point out their favourite one.




Nb travail du sol pendant période activité insectes ~ mars-oct.
>=2
< 2
Nb moyen labour / an
>= 1/2
< 1/2
Nb herbicides pseudo-racinaires moyen/ an
< 0.1
>= 0.1
Nb herbicides foliaires
< 0.5
>= 0.5
Nb travail du sol pendant période act. insectes
< 0.5
>= 0.5
Equitabilité 0.42 ±0.06
Ressources carabes 4.16 ±0.35
Ressources pollinisateurs 2.31 ±0.2
Pertes rendement 39.07 ±21.21
Salissement parcelle 1.05 ±0.95
Pollution récolte 2.75 ±0.55
0.48 ±0.38
4.88 ±5.08
2.72 ±2.61
44.31 ±21.21
0.91 ±0.38
3.05 ±3.38
0.36 ±0.07
4.58 ±0.31
2.57 ±0.24
56.62 ±17.52
1.89 ±0.99
3.41 ±0.72
0.33 ±0.26
6.22 ±5.83
2.40 ±2.04
64.35 ±54.89
1.07 ±0.71
3.26 ±2.82
0.28 ±0.19
6.37 ±5.7
2.84 ±2.3
64.00 ±15.3
2.02 ±0.47
3.86 ±2.17
0.41 ±0.07
5.22 ±0.27
2.91 ±0.2
64.46 ±13.37
1.96 ±0.95
4.04 ±0.74


Nb travail du sol pendant période activité insectes ~ mars-oct.
>=2
< 2
Nb moyen labour / an
>= 1/2
< 1/2
Nb herbicides pseudo-racinaires moyen/ an
< 0.1
>= 0.1
Nb herbicides foliaires
< 0.5
>= 0.5
Nb travail du sol pendant période act. insectes
< 0.5
>= 0.5
0.48 ± 0.03
4.88 ± 0.28
2.72 ± 0.16
44.31 ± 12.81
0.91 ± 0.6
3.05 ± 0.45
0.36 ± 0.07
4.58 ± 0.31
2.57 ± 0.24
56.62 ± 17.52
1.89 ± 0.99
3.41 ± 0.72
0.33 ± 0.04
6.22 ± 0.17
2.4 ± 0.2
64.35 ± 4.98
1.07 ± 0.35
3.26 ± 0.31
0.28 ± 0.04
6.37 ± 0.28
2.84 ± 0.31
64 ± 24.64
2.02 ± 1.08
3.86 ± 0.91
0.41 ± 0.08
5.22 ± 0.28
2.91 ± 0.2
64.46 ± 13.37
1.96 ± 0.95
4.04 ± 0.74

5 Overview of the R-shiny app

In the following images are print screen of the R-shiny web app that was sent to the crop advisors having followed the workshop.

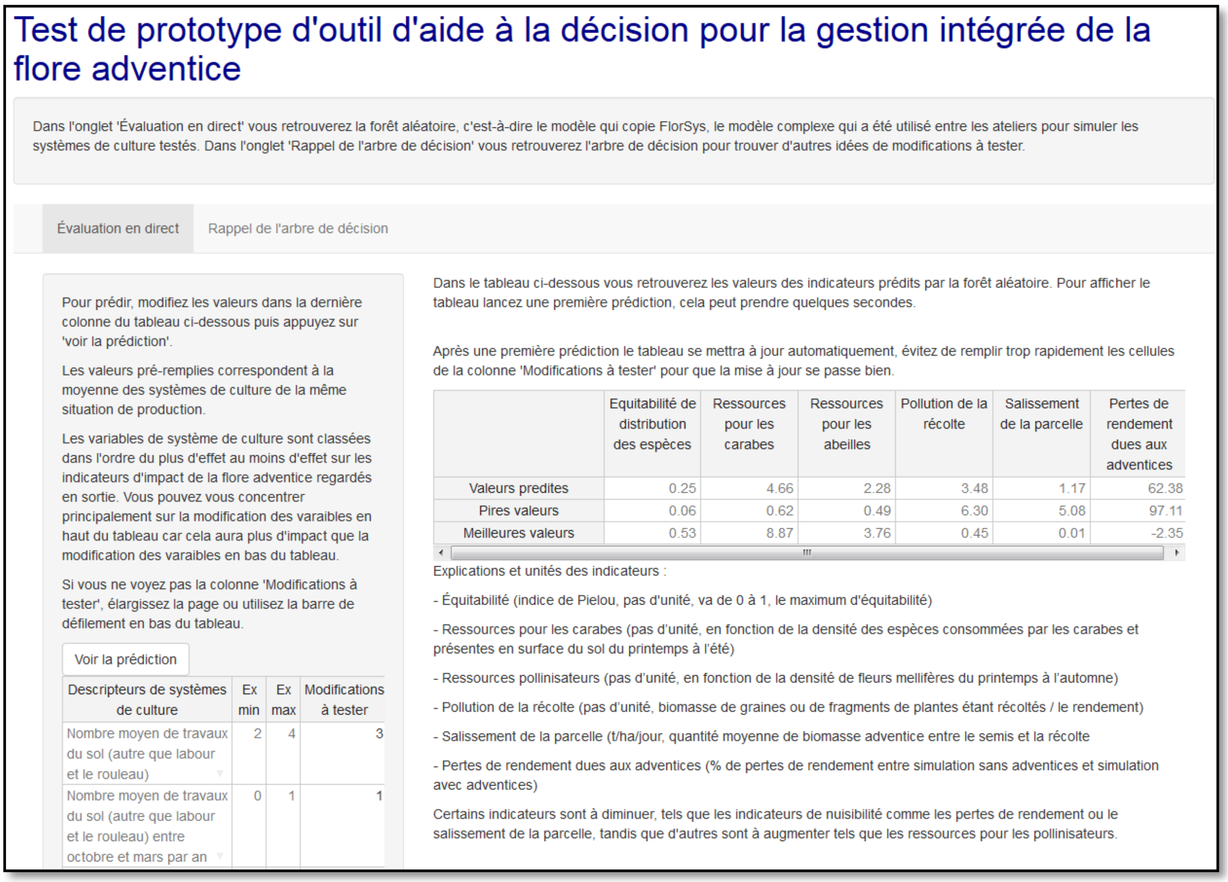
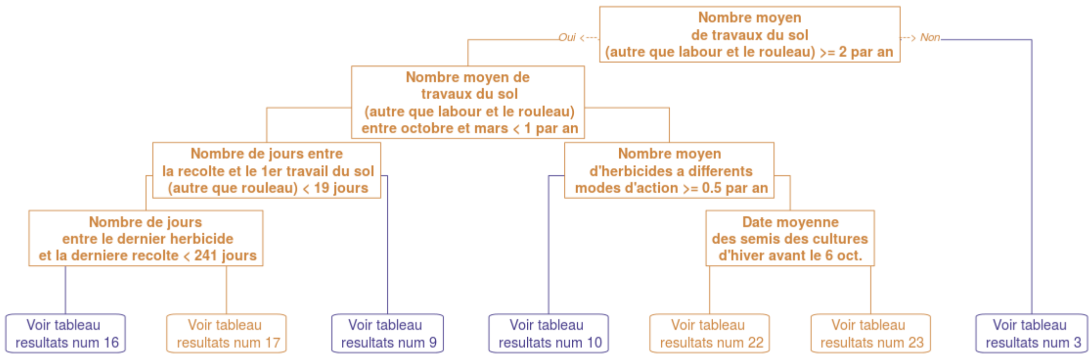


Figure A.8. 7 : First page of the application, with the random forest, on the left input entering area, on the right output showing area.



Légende de l'arbre : En orange, les chemins (ou combinaisons de pratiques) où se retrouvent les systèmes de culture testés lors des ateliers. Seuls les systèmes de cultures appartenant à la même situation de production ont été comparés.

Numéros des résultats	Equitabilité de distribution des espèces	Ressources pour les carabes	Ressources pour les abeilles	Pollution de la récolte	Salissement de la parcelle	Pertes de rendement
16	0.20	1.50	1.10	2.40	0.30	14.30
17	0.30	2.10	1.40	3.30	1.20	38.20
9	0.30	3.80	2.30	3.20	1.90	51.80
10	0.30	2.90	1.60	2.90	1.40	42.70
22	0.30	3.50	2.10	3.80	1.90	60.20
23	0.30	4.20	2.40	3.90	2.10	65.90
3	0.30	8.40	2.60	4.20	1.40	80.70

Légende du tableau : Valeurs des indicateurs d'impacts de la flore adventice pour les différentes feuilles de l'arbre. Ce sont des indicateurs d'impact, par exemple les pertes de rendement correspondent aux pertes de rendement causées par les adventices.

Figure A.8. 8 : Second page of the application, with the decision tree of the second day of workshop as a reminder. Orange branches include the cropping systems proposals

Annexe 9
Fiche de présentation pour les ateliers réalisés avec l'Expérimentarium

La fiche a été réalisée avec l'aide précieuse de l'équipe de l'Expérimentarium de Dijon : Coralie Biguzzi, Juliette Brey-Xambeu, Sophie Fallot et Lionel Maillot.

De l'aide pour gérer les mauvaises herbes

✚ AGRONOMIE

Floriane COLAS est jeune chercheuse en agronomie à l'INRA*. Les chercheurs de son équipe étudient comment préserver l'environnement en contrôlant la présence de mauvaises herbes dans les champs. Les agriculteurs cherchent à éliminer ces mauvaises herbes, mais, comme elles sont utiles pour la faune sauvage et l'environnement, il faut en laisser quelques-unes.

Floriane créé des champs virtuels sur ordinateur en essayant de limiter la présence de mauvaises herbes. Si cela pouvait être reproduit dans de vrais champs, cela aiderait les agriculteurs à faire de meilleurs choix.

* Institut National de la Recherche Agronomique

« J'essaye de préserver la biodiversité en aidant les agriculteurs à prendre des bonnes décisions pour les mauvaises herbes, le tout en jouant avec un champ virtuel sur mon ordinateur ! »

Floriane Colas

Les mauvaises herbes causent de nombreux problèmes aux agriculteurs, car elles volent la nourriture des plantes qui poussent dans leurs champs. Cependant, les mauvaises herbes sont utiles pour l'environnement et la biodiversité : elles peuvent notamment servir de nourriture et d'habitat pour les oiseaux et les insectes.

Pour cultiver un champ, les agriculteurs doivent prendre beaucoup de décisions : Quelles plantes cultiver une année après l'autre dans un même champ ? Quand semer ? Comment bien préparer le sol ? Comment limiter les mauvaises herbes ? Floriane souhaite apporter de l'aide aux agriculteurs pour qu'ils réussissent à limiter les mauvaises herbes en gardant leurs effets positifs.

Pour cela, Floriane utilise un programme informatique créé dans son laboratoire et basé sur des données réelles. Ce programme reproduit un champ virtuel sur son ordinateur et Floriane l'utilise comme si elle était agricultrice : elle peut choisir les cultures qu'elle souhaite faire pousser pendant plusieurs années, et décider quand utiliser des engins agricoles pour labourer le sol ou faire ses récoltes. Ensuite, elle regarde s'il y a eu beaucoup de mauvaises herbes dans ses cultures.

Or pour le moment, ce programme est trop compliqué et trop long. Il ne peut pas encore être utilisé pour conseiller des agriculteurs. Floriane est chargée de simplifier certaines parties du programme grâce à des calculs mathématiques, pour qu'il fonctionne plus vite mais toujours aussi bien. Puis elle va chercher les bonnes combinaisons de cultures et de pratiques à conseiller aux agriculteurs. Pour y parvenir, elle doit tester beaucoup de possibilités.

Les objectifs

- Simplifier une partie des calculs dans le programme qui crée les champs virtuels
- Faire des simulations de successions de cultures sur plusieurs années dans un champ pour étudier la présence de mauvaises herbes dans ce champ
- Trouver les meilleures combinaisons de cultures et de pratiques à conseiller aux agriculteurs

ÉCOLE DOCTORALE
Environnements - Santé
Bourgogne | Franche-Comté

Titre : Co-développement d'un modèle d'aide à la décision pour la gestion intégrée de la flore adventice. Méta-modélisation et analyse de sensibilité d'un modèle mécaniste complexe (FLORSYS) des effets des systèmes de culture sur les services et disservices écosystémiques de la flore adventice.

Mots clés : agroécologie, fouille de donnée, simplification, ateliers, conseiller agricole, conception multi critères

Résumé : Afin de réduire l'utilisation d'herbicides, nous avons besoin d'outils pour concevoir des stratégies de gestion des adventices économes en herbicides. La gestion complexe des adventices, la nécessité de la raisonner sur le long terme et la multiplicité des impacts du système de culture font que les outils de modélisation sont d'une grande aide pour concevoir des systèmes de culture innovants. L'objectif de la thèse est de développer un outil d'aide à la reconception de systèmes de culture réconciliant protection des cultures et des écosystèmes. Notre approche consiste à déterminer la structure de ce nouvel OAD en interaction avec les futurs utilisateurs et son contenu biophysique à partir du fonctionnement de l'agroécosystème du modèle de recherche FLORSYS. Cette « parcelle virtuelle » simule la dynamique des adventices en fonction des systèmes de culture et du pédoclimat et en déduit des indicateurs d'impact de la flore adventice sur la production agricole et les services écosystémiques. FLORSYS a été méta-modélisé par polynômes du chaos, puis utilisé pour simuler de nombreux systèmes de culture analysés ensuite par fouille de données. L'outil d'aide à la décision résultant est composé : (1) de grilles synthétisant les techniques culturales les plus influentes, (2) d'arbres de décision et (3) d'un simulateur rapide.

Title: Co-design of a decision support system for integrated weed management. Meta-modelling and sensitivity analysis of a complex mechanistic model (FLORSYS) of cropping system effects on ecosystem services and disservices of weeds.

Keywords: agroecology, data mining, simplification, workshops, crop advisor, multicriteria design

Abstract: In order to reduce our use of herbicides, we need a tool to design weed management strategies relying on fewer herbicides. Weed management is complicated and, together with necessity of scheduling operations at long-term and the multiplicity of cropping system impacts, it explains why models are so useful for designing innovative cropping systems. The aim of this thesis is to develop a decision support system, intended for crop advisors, reconciling crop protection and ecosystem services Our approach consisted in identifying the structure of the DSS in interaction with future users while using an existing research model, FLORSYS, for the biophysical content of the tool. FLORSYS is a "virtual field" simulating the weed flora dynamics depending on cropping systems and pedoclimatic conditions. As output, it provides weed impact indicators, both for crop production and ecosystem services. FLORSYS was metamodelled by polynomial chaos expansion to increase its simulation speed. Subsequently, it was used to simulate numerous cropping systems which were analyzed via data mining. The resulting decision support system is composed of: (1) charts of the most important cropping systems practices, (2) decision trees and (1) an emulator of FLORSYS based on random forests.

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