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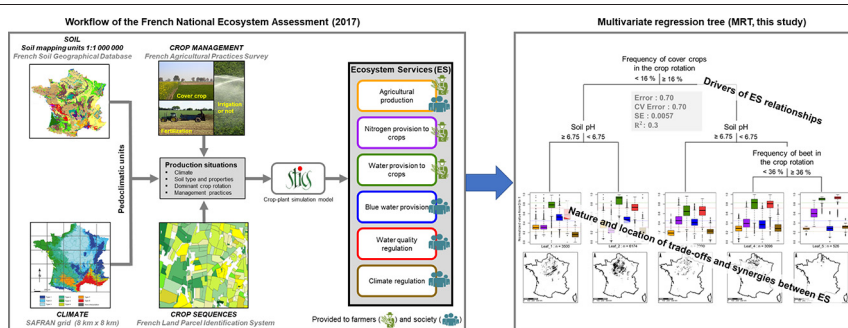
Using a multivariate regression tree to analyze trade-offs between ecosystem services: Application to the main cropping area in France

Gregory Obiang Ndong^{a,*}, Jean Villerd^b, Isabelle Cousin^a, Olivier Therond^c^a INRAE, URSOLS, F-45075 Orléans, France^b Université de Lorraine, INRAE, LAE, F-54000 Nancy, France^c Université de Lorraine, INRAE, LAE, F-68000 Colmar, France

HIGHLIGHTS

- We analyzed the relationships between ecosystem services (ES) in agroecosystems.
- We implemented a multivariate regression tree (MRT)-based approach.
- We show a synergy between regulating ES and trade-off with agricultural production.
- Cover crops and soil properties can drive a trade-off between two water-related ES.
- Our results provide key information to design ecosystem management strategies.

GRAPHICAL ABSTRACT



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ABSTRACT

Analysis of trade-offs and synergies between ecosystem services (ES) and their underlying drivers is a main issue in ES research. The analysis is complex and requires innovative analytical approaches. To address this complexity, we used an original approach that combines a multivariate regression tree (MRT), data analysis, and spatial mapping. We applied this approach to the main cropping region in France (mainly the Paris basin of production) using an existing dataset (i.e. soil, climate, crop sequences and management) from the French National Ecosystem Assessment to determine relationships between agricultural production, two services to farmers – nitrogen provision to crops and water provision to crops – and three services to society – blue water provision, water quality regulation, and climate regulation. To support land managers and decision-makers, we also analyzed the extent to which manageable soil properties and agricultural practices (crop rotation and management) are major drivers of trade-offs or synergies. We demonstrated that water quality regulation, nitrogen provision to crops, and climate regulation have synergistic relationships in production situations in the northeastern region of the study area due to the types of crop rotation, frequency of cover crops in the crop rotation, the soil pH, and the soil available water capacity. We also identified that cover crops, while promoting these three ES, can drive a trade-off between two key water-related services: water provision to crops and blue water provision (i.e. between a service to farmers and one to society). By capturing non-linear relationships and threshold effects, our MRT-based approach overcomes the main limitations of classic statistical approaches. The approach is also spatially explicit and simple and intuitive to interpret, especially for non-scientists; our results thus provide researchers and ecosystem managers (e.g. agricultural policy makers) with key information to design ecosystem management strategies that promote a balanced bundle of ES.

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* Corresponding author.

E-mail address: gregory.obiang-ndong@inrae.fr (G. Obiang Ndong).

1. Introduction

Ecosystem services (ES) are defined as the direct and indirect contributions that ecosystems (i.e. living systems) make to human well-being (Haines-Young and Potschin, 2010; TEEB Foundations, 2010). Since the work of the Millennium Ecosystem Assessment (MEA, 2005), initiated to assess consequences of changes in the ecosystems on which human well-being depends and the means to deal with them, this concept has grown within the scientific community (Fisher et al., 2009; Vihervaara et al., 2010; Seppelt et al., 2011; Chaudhary et al., 2015); thus, the scientific literature to date includes many studies that have quantified ES (see for example review studies by Seppelt et al., 2011; Egoh et al., 2012; Martínez-Harms and Balvanera, 2012; Malinga et al., 2015; Schroter et al., 2016; Englund et al., 2017; Rau et al., 2019). Furthermore, the concept of ES has been integrated into public policies both locally and internationally (Cardinale et al., 2012).

Among the scientific issues in ES research, analysis of trade-offs or synergies between services is a main challenge for decision-makers (Fu et al., 2015). Trade-offs occur when the provision of one ES increases while another decreases (Rodríguez et al., 2006; Howe et al., 2014; Tomscha and Gergel, 2016), while synergies occur when two or more ES change in the same direction (Bennett et al., 2009; Howe et al., 2014). This analysis provides decision makers with key information for land management or planning (Castro et al., 2014). However, the trade-offs and synergies between ES are complex due to their large natural variation in space and time and their potential non-linear relationships (Bennett et al., 2009; Koch et al., 2009; Power, 2010; Lester et al., 2013; Birkhofer et al., 2015).

Among the many quantitative methods used to quantify and analyze ES trade-offs and synergies, common statistical methods include analyzing correlations (e.g. Spearman or Pearson), manifold learning (e.g. principal components analysis), clustering-based visualization (e.g. k-means clustering), graphical methods (e.g. petal diagrams, star coordinate system), and overlay analysis (see Mouchet et al., 2014; Birkhofer et al., 2015; Martínez-Harms et al., 2015; Lee and Lautenbach, 2016; Li et al., 2017; Dade et al., 2018; Saidi and Spray, 2018; Vallet et al., 2018 for a review). Few studies to date have followed a more complex approach to analyze trade-offs between ES (Lautenbach et al., 2019). According to Mouchet et al. (2014), these methods are particularly appropriate for identifying positive or negative associations among ES and providing initial information to identify trends and compare the relative provision of multiple ES. Some of the methods (e.g. overlap analysis) are also simple and intuitive ways to identify spatially explicit ES associations (Mouchet et al., 2014). However, most of the methods have strong limitations (Mouchet et al., 2014; Lee and Lautenbach, 2016). For example, correlation analysis cannot adequately address potential non-linear trade-offs or synergies between ES and critical thresholds. The methods also cannot explore how multiple and complex external natural (e.g. solar radiation, precipitation) or anthropogenic (e.g. management practices) factors influence relationships between ES. Several authors (Bennett et al., 2009; Gos and Lavorel, 2012; Landuyt et al., 2016; Dade et al., 2018) indicate that understanding trade-offs and synergies between ES is insufficient without carefully examining the drivers and mechanisms that underlie the relationships.

To address these limitations, Cord et al. (2017) suggest that future studies use innovative analytical approaches to quantify expected trade-offs or synergies better, and improve the understanding of the drivers that support them. For the drivers considered, future studies should go beyond examining the large-scale and coarsely defined drivers of changes in land use/land cover and the climate, which are often considered in studies, and provide more detailed and useful information to land managers and decision-makers (see Dade et al., 2018; Obiang Ndong et al., 2020). To this end, several studies suggest that soil properties (e.g. Dominati et al., 2010; Dominati et al., 2014; Adhikari and Hartemink, 2016; Calzolari et al., 2016; Greiner et al.,

2017) and agricultural management practices (see Lee et al., 2019 review) are important for the supply of many ES (e.g. food production, water provision, climate regulation). However, according to reviews of Dade et al. (2018) and Obiang Ndong et al. (2020), only a few studies have considered these drivers when analyzing ES trade-offs or synergies.

The objective of this study was to present an innovative use of multivariate regression trees (MRT) to analyze trade-offs and synergies between ES and their drivers at a regional level. MRT is a method that originated in the field of ecology (Smith et al., 2019). To our knowledge, to date, MRT has not been used to investigate trade-offs and synergies between ES and their drivers. For example, a search performed in June 2020 with the keywords ("regression tree") AND ("ecosystem service") AND ("bund*" OR "relationship*" OR "trade*" OR "synerg*") in the Web of Science Core Collection (Topic; from 2000 to 2020) returned only 20 references. Only three of them explicitly relate to ES analysis. Rositano et al. (2018) used k-means clustering and classification trees to identify the dependence of ES supply on the variation in environmental and crop management factors in Pampean agroecosystems. Lutz et al. (2016) used regression trees to investigate trade-offs between three ES across the state of New Hampshire, USA. Zhang and Ouyang (2019) used boosted regression trees to explore relationships between key ecological indicators at different scales. Thus, these three studies used only univariate or boosted regression trees (vs. multiple regression trees) to determine the influence of multiple predictor variables on a single response variable.

We used an MRT-based approach (i.e. a combination of MRT, data analysis, and spatial mapping) to address two major research issues in the analysis of ES relationships: (i) Do trade-offs or synergies between ES exist, and if so, where are they located in the landscape? and (ii) What drivers influence spatial variation in trade-offs and synergies between them?

2. Materials and methods

We applied our MRT-based approach to part of the dataset produced by the French National Ecosystem Assessment (NEA) of agricultural ecosystems (see Therond and Tibi, 2018) to analyze trade-offs and synergies between agricultural production (goods) and ES related to soil functioning provided to farmers and society in the main cropping region in France.

2.1. Dataset of ecosystem service levels

The French NEA of agricultural ecosystems – part of the French version of the European MAES (Mapping and Assessment of Ecosystems and their Services) program (<https://biodiversity.europa.eu/maes>) – was performed from 2014 to 2017. Therond and Tibi (2018) provide a detailed description of the study that was performed within this program to assess ES in agricultural areas in France. The main objective of this study was to estimate the range of ES and goods that agricultural ecosystems provide by using the finest-scale and most current biophysical assessment approaches and databases.

The crop-plant simulation model STICS ("Simulateur multidisciplinaire pour les Cultures Standard") (Brisson et al., 1998, 2002, 2003, 2009) was used to predict agricultural production (goods) and five ES related to soil functioning: two services to farmers ((i) nitrogen (N) provision to crops and (ii) water provision to crops (i.e. crop transpiration, hereafter called green water) and three services to society (iii) blue water provision (i.e. water flowing from agricultural ecosystems to hydrosystems), (iv) water quality regulation, and (v) climate regulation through carbon (C) sequestration in the soil. Specific indicators were developed in the French NEA to assess the levels of ES (Table 1). STICS was chosen because it had been determined to simulate dynamics of agrosystems accurately for a wide range of agro-

environmental variables and conditions in France (Coucheney et al., 2015).

In the French NEA, STICS was run on a daily time step for a 30-year period (1983–2013) for the main cropping systems in pedoclimatic units (“PCUs”) in mainland France. PCUs correspond to the spatial intersection between soil mapping units of the 1:1,000,000 French Soil Geographical Database (Jamagne et al., 1995) and the 8 km × 8 km SAFRAN climate grid (Durand et al., 1993; Quintana-Seguí et al., 2008; Vidal et al., 2010). Only the 23,149 PCUs with more than 100 ha of agricultural area, as described in the French Land Parcel Identification System, were considered in the French NEA, because they represented 99.2% of the total agricultural area in France. They represented 27.29 Mha of annual and perennial crops, grasslands, market gardens, and fallow land.

Initial soil organic C (SOC) stocks in the first 0.3 m of the soil were estimated from data provided by Mulder et al. (2016) at a 90 m × 90 m resolution, considering only pixels with crops in each PCU. Soil organic N content (0–0.3 m) was then calculated using a constant C:N ratio of 11 and the bulk density of this layer for each soil type. The other soil characteristics used by STICS (clay content, water content at field capacity and at the permanent wilting point) were estimated using pedotransfer rules applied to the 1:1,000,000 French soil data (Jamagne et al., 1995).

A two-step approach was used to describe the dominant cropping systems (i.e. rotation and crop management practices) in each PCU. First, the crop rotation database developed by the French National Research Institute for Agriculture, Food and Environment (INRAE), (Leenhardt et al., 2012) was used to identify the main crop rotations in each PCU. For each PCU and by type of crop rotation (i.e. pure crop or ley/crop) one dominant rotation was selected if it represented more than 50% of the agricultural area. Otherwise, we selected the first two dominant rotations with an area greater than 10% of the PCU area. Based on these rotations and the crops calibrated in STICS, the crops simulated were maize (grain and forage maize), winter wheat, rapeseed, sugar beet, sunflower, and winter and spring pea. For maize, one cultivar with a precocity adapted to the number of growing degree days between sowing and harvest for at least 8 out of 10 years was selected per PCU. For the other crops, we selected the most common cultivar used in France for which STICS was calibrated.

Second, management practices for each simulated crop were determined using results of the French Agricultural Practices Survey conducted in 2006 and 2011 (Agreste, 2014). Since these data are considered representative of administrative regions (geocode standard NUTS II) and are available only at this level, median observations per crop and region were used for sowing and harvest dates, mineral or organic fertilizer doses, splitting of mineral N fertilization, percentage of crops with organic N fertilization, type and frequency of organic N fertilization, and frequency of tillage.

Ultimately, STICS was run to simulate daily dynamics of 49,935 production situations in 10,263 PCU that covered all arable land in France, for annual crops only (since perennial crops, grasslands, market gardens, and fallow land were not simulated with STICS, we excluded them from this study). The production situations corresponded to a combination of soil type, climate, dominant rotation, and median crop management practices (see Willocquet et al. (2008)). STICS simulation outputs were used in calculations to estimate the indicators of agricultural production and the five ES selected (Table 1). Descriptive statistics of these indicators are shown in Table S1 in the Supplementary material. To ensure that the yield data were similar among crops, simulated biomass dry matter yields were transformed into energy yields using energy content coefficients like in Dittrich et al. (2017) and Xu and Liu (2019). The energy content coefficients of wheat, sugar beet, maize (grain and forage), sunflower, rapeseed, and pea were 379, 70, 384, 636, 641, and 381 kcal/100 g dry matter, respectively.

Because these indicators of agricultural production and ES had different units, they were normalized to range from 0 to 1, as follows:

$$X'_i = \frac{X_i - X_{\min}}{X_{\max} - X_{\min}} \quad (1)$$

where X'_i is the normalized value of the indicator, X_i is the value of the indicator for each production situation, and X_{\min} and X_{\max} are the minimum and maximum value of each considered indicator variable over the production situations, respectively.

According to Calzolari et al. (2016), this equation “gives high priority (i.e. values close to 1) to higher values of the considered indicator; the lowest value, 0, does not indicate that the function is not provided, but that it is the lowest in the considered area”. The normalization should provide a meaningful comparison of indicators to identify trade-offs and synergies.

2.2. Selecting potential drivers of trade-offs/synergies in ecosystem services

To analyze drivers of trade-offs or synergies between agricultural production and ES, we selected 16 potential driver variables (Table 2) that were either initial inputs used in STICS or certain outputs simulated by it. To support land managers and decision-makers, we considered only manageable drivers (i.e. manageable soil properties and agricultural practices (crop rotation and management)). For soil properties, we selected SOC content, pH, and calcium carbonate (CaCO_3) content. These soil characteristics are frequently included in ES studies that focus on soil functioning (see Adhikari and Hartemink (2016); Greiner et al. (2017)) and are included in the minimum dataset for representing soil quality (Garrigues et al., 2012).

For agricultural practices, we selected characteristics of crop rotations (i.e. number of crops simulated and the frequency of each, namely the percentage of the number of crops in rotation) and crop management practices. (i.e. mineral N added via mineral/organic fertilizers and SOC inputs to the soil profile).

2.3. Multivariate regression tree approach for analyzing trade-offs/synergies between ecosystem services

We used a MRT approach (i) to analyze trade-offs and synergies between agricultural production and the five ES selected (Table 1), and (ii) to identify potential drivers (Table 2) that influence the spatial variation and ES trade-offs and synergies in the study area.

MRT is a machine-learning technique developed by De'ath (2002). As an extension of univariate regression trees (Breiman et al., 1984), MRT can address more than one response variable (Questier et al., 2005) and “can be used to analyze complex ecological data, and especially to explore, describe, and predict relationships between multispecies data and environmental characteristics” (De'ath, 2002). According to Borcard et al. (2018), “MRT is a powerful and robust method that can handle a wide variety of situations, even those where some values are missing, and where the relationships between the response and explanatory variables are non-linear or high-order interactions among explanatory variables are present.”

MRT were fitted using R statistical software (R Core Team, 2018), specifically the archive version 1.6-2 of the R package “mvpart” (Therneau et al., 2014). MRT was used as an exploratory approach to identify dependence between the ES bundles i.e. “sets of ES that repeatedly appear together across space or time” (Raudsepp-Hearne et al., 2010) and their underlying drivers. Thus, the 16 potential drivers (Table 2) were considered exploratory variables, and the agricultural production and five ES indicators (Table 1) were considered response variables. To ensure equal contribution to the multivariate response, the normalized values of agricultural production and ES indicators were used (Eq. (1)). The potential driver variables were not normalized, to facilitate interpretation in their original units.

Table 1
Biophysical indicators of agricultural production and the five ecosystem services used in the study.

Ecosystem service	Indicator	Units	Calculation method	Variable	Definition	Units
Agricultural production	Biomass-based energy sources (EP)	$10^7 \text{ kcal ha}^{-1} \text{ yr}^{-1}$	$EP = \text{crop yield} \times \text{energy content coefficient}$	Mafruit (crop yield)	Biomass of harvested organs	$\text{t ha}^{-1} \text{ yr}^{-1}$
				DMexported (crop yield)	Cumulative amount of harvested biomass (for maize fodder)	t ha^{-1}
				Energy content coefficient (kcal per 100 g)	Wheat: 379; sugar beet: 70; maize (grain and forage maize): 384; sunflower (grain): 636; rapeseed: 641; and, winter and spring pea (grain): 381	kcal yr^{-1}
Nitrogen (N) provision to crops	Amount of mineral N supplied by the ecosystem during the cropping cycle (i.e. N mineralized from humus and residues, and N from fixation)	$\text{kg N ha}^{-1} \text{ yr}^{-1}$	$N_{\text{mineral_from_plt}} + Q_{\text{fix}}$	$N_{\text{mineral_from_plt}}$	Cumulative amount of N mineralized during the crop cycle (sowing to harvest)	$\text{kg N ha}^{-1} \text{ yr}^{-1}$
				Q_{fix}	Amount of N fixed symbiotically between two cuts	$\text{kg N ha}^{-1} \text{ yr}^{-1}$
Water provision to crops (called green water)	Amount of water restored to the soil during the cropping cycle based on maximum evapotranspiration crop needs	Dimensionless	$\frac{\text{cep_sirr}}{\text{cep_irr}}$	cep_sirr	Cumulative transpiration during the cropping season, without irrigation	mm yr^{-1}
				cep_irr	Cumulative transpiration during the cropping season with irrigation	mm yr^{-1}
Blue water provision	Mean annual water yield	Dimensionless	$\frac{\text{drat}}{\text{rr_mm}}$	drat	Cumulative amount of water drained at the base of the soil profile during the simulation period	mm yr^{-1}
				rr_mm	Precipitation (from Meteo France data)	mm yr^{-1}
Water quality regulation	The proportion of N not leached	Dimensionless	$\frac{\text{totapN} + \text{minN} - Q_{\text{les}}}{\text{totapN} + \text{minN}}$ With: $\text{minN} = Q_{\text{minh}} + Q_{\text{minr}}$	totapN	Cumulative amount of mineral N added via mineral and organic fertilizers	$\text{kg N ha}^{-1} \text{ yr}^{-1}$
				Q_{les}	Cumulative amount of $\text{NO}_3\text{-N}$ leached at the base of the soil profile	$\text{kg N ha}^{-1} \text{ yr}^{-1}$
				Q_{minh}	Cumulative amount of mineralized N derived from humus decomposition	$\text{kg N ha}^{-1} \text{ yr}^{-1}$
				Q_{minr}	Cumulative amount of mineralized N derived from organic residue decomposition	$\text{kg N ha}^{-1} \text{ yr}^{-1}$
Climate regulation	Relative annual change (%) in soil organic carbon (SOC) stock	Dimensionless	$\frac{\text{SOC_final} - \text{SOC_initial}}{\text{SOC_initial}}$	SOC_initial	Amount of C in humified organic matter (active + inert)	$\text{mg C ha}^{-1} \text{ yr}^{-1}$

To avoid overfitting, we first identified the optimal tree size by following a 10-fold cross validation procedure and selecting the tree size that minimized the cross-validated error (as described by Breiman et al. (1984)). We then plotted the error vs. tree size (i.e. model complexity), which showed that the size selected lay on the plateau of the curve. These preliminary analyses led us to decide that a shorter tree with five “leaves” was the best compromise between prediction and interpretability, because it allowed us to focus on a few interactions, and thus hypotheses to be tested with confirmatory methods in future studies. Consequently, the tree was pruned to five “leaves” in this study to balance the descriptive power of the tree with the interpretability of its results. The predictive accuracy of the MRT was assessed using a k-fold cross-validation procedure, as follows. The dataset was divided into $k = 10$ equal-sized subsets according to a widely used rule of thumb (see Kuhn and Johnson, 2013). A five-leaf MRT was fitted using the union of $k-1$ subsets as a training set and evaluated with the remaining subset as test set. By permutating the test subset, k five-leaf MRT were fitted and evaluated, and thus the mean of the k pseudo R^2 was considered as the predictive accuracy on unseen data. This cross-validation procedure was performed internally using *mvpart*. Like Smith et al. (2019), we replaced the bar plot generated by *mvpart* for each leaf with a boxplot to provide more detailed information.

To strengthen analysis of the tree, we calculated the “importance” of each driver according to the definition of importance of Breiman et al. (1984). Doing so allowed us to distinguish, among the driver variables that did not appear in the tree, those that explained nothing (zero

importance) from those that were “masked” by another driver variable (i.e. “surrogate”). We also created boxplots of the initial drivers (Fig. S1 in the Supplementary material), as for the initial input dataset of the

Table 2

Sixteen variables used as proxies of potential drivers of trade-offs and synergies between agricultural production and ecosystem services; See Table S1 in the Supplementary material for descriptive statistics of the crop rotation and management practice drivers.

Driver type	Definition	Units
Crop rotations	Number of crops and cover crops in the rotation	Absolute
	Number of crops in the rotation (excluding cover crops)	Absolute
	Frequency of cover crops in the crop rotation	%
	Frequency of wheat in the crop rotation	%
	Frequency of rapeseed in the crop rotation	%
	Frequency of beet in the crop rotation	%
	Frequency of forage maize in the crop rotation	%
	Frequency of grain maize in the crop rotation	%
	Frequency of sunflower in the crop rotation	%
	Frequency of spring pea in the crop rotation	%
Management practices	Frequency of winter pea in the rotation	%
	Cumulative amount of mineral N added via mineral and organic fertilizers	kg N ha^{-1}
Soil properties	Soil organic carbon (C) inputs to the soil profile	kg C ha^{-1}
	Initial soil organic C stock	mg C ha^{-1}
	Soil pH	Unitless
	Calcium carbonate content	%

MRT (Table 2), according to each leaf of the final tree. We also included drivers not initially present, such as yield, soil clay content, and available water capacity. Although the latter two are not manageable (i.e. do not depend on short- or medium-term human actions or cannot be changed without prohibitive costs (Dominati et al., 2010)), they provided crucial information about the soil (Dominati et al., 2010) that was relevant for analyzing the MRT results. In these boxplots, to understand whether the drivers differed significantly between the leaves of the final tree (i.e. significant differences of the production situations between leaves), the non-parametric Kruskal-Wallis ANOVA test (KW) was performed (Fig. S1 in the Supplementary material), using the R package *pgirmess* (Giraudoux, 2018). If significant differences were observed at $p < 0.05$, a multiple comparison rank test was performed to identify the differences.

2.4. Case study: the main non-irrigated arable agricultural systems in France

To illustrate the potential of the MRT approach, we applied it to identify relationships between agricultural production and the five ES in the PCUs located in the modified oceanic climate of the central and northern plains, as described in Joly et al. (2010). In this French sub-area, the mean annual temperature is about 11 °C, and the dominant soil classes (based on the World Reference Base for Soil Resources classification) are cambisols, luvisols, umbrisols, and fluvisols. This sub-area represents 3748 PCUs and 15,296 sampled non-irrigated production situations.

We applied the MRT approach to only one climate region to mitigate effects of strong climatic drivers that could hide effects of manageable drivers. For the same reason, we focused only on non-irrigated arable systems. We chose this climatic region because the central and northern plains of France correspond to “the most important agricultural production region of France and one of the biggest cereal producing regions in Europe” (de Frutos et al., 2017). It also covers the most important aquifers in France - the Beauce groundwater area (nearly 10,000 km²) - with important water-deficit and associated water inflow issues (Verley, 2020).

3. Results

3.1. Spatial distribution of ecosystem services

Agricultural production and climate regulation levels had similar spatial distributions, especially in the center of the study area, where they mainly had moderate values (Fig. 1). The spatial distribution of N provision to crops and blue water provision clearly shows strong opposite distributions in the northeastern areas: the blue water provision ES is lower than the median value, whereas N provision to crops is higher. The spatial distribution of water quality regulation and water provision to crops is also similar across the study area, and is mainly characterized by high values in the center. N provision to crops had the highest values in the western area of the study, whereas water provision to crops had the lowest values. See Fig. S2 in the Supplementary material for the spatial distribution of agricultural production and ES in their original units.

3.2. Multivariate regression tree

The final MRT consisted of three split levels and five leaves (Fig. 2). The accuracy (R^2) of MRT was 0.30 (1 – cross-validated residual error) (i.e. the tree explained 30% of the variance).

3.2.1. Regression tree description

Three of the 16 potential drivers were selected to split the five leaves: the frequency of cover crops in the crop rotation (level 1 of the split), soil pH (level 2 of the split), and the frequency of beet in the crop rotation (level 3 of the split). Other drivers, such as CaCO₃ content,

number of crops in the crop rotation, and mineral and organic N fertilization, were surrogates (Fig. S3 in the Supplementary material).

At level 1 of the split, the tree distinguished production situations with a low frequency (<16%) from those with a high frequency (≥16%) of cover crops in the crop rotation. The former branch was then split (level 2) into two branches, that distinguished high soil pH (≥6.75, leaf 1) from low pH (<6.75, leaf 2). The branch for cover crop frequency > 16% also split into two branches that distinguished high pH (≥6.75, leaf 3) from low pH (<6.75). The latter branch was then split (level 3) into two branches that distinguished low frequency (<36%, leaf 4) from high frequency (≥36% for leaf 5) of beet in the crop rotation. Although PCUs of certain leaves were located throughout the entire study area, leaves tended to cluster by region of the study area: leaf 1 mainly in the southeast, east, and in the south of the Paris basin; leaf 2 mainly in the Paris basin; leaf 3 in the northeast; leaf 4 in the center; and leaf 5 in the northeast.

3.2.2. Regression tree analysis

Each leaf was analyzed based on the tree results (Fig. 2 and Table 3) and the boxplots of the initial drivers (Fig. S1 in the Supplementary material).

- Leaf 1: low frequency of cover crops in the southeastern and eastern regions of the study area.

In leaf 1 production situations ($n = 3500$), levels of agricultural production and N provision to crops lay at the median of all situations investigated. Water quality regulation, climate regulation, and water provision to crops were below median, while blue water provision was above the median and thus had a trade-off relationship. Production situations in this leaf were characterized mainly by a short crop rotation that included a monoculture of wheat and a wheat-rapeseed rotation, which were associated with high mean mineral/organic fertilization (>175 kg/ha) (Fig. S1). They were located over slightly alkaline and calcareous soils (pH > 7 and CaCO₃ content about 10%, respectively) and had a lower available water capacity (<100 mm) than those of the other leaves.

- Leaf 2: low frequency of cover crops around the Paris basin of production

In leaf 2 production situations ($n = 6174$), water quality regulation, climate regulation, and blue water provision lay at median levels. Agricultural production and water provision to crops were particularly high, while N provision to crops was moderately low. Thus, these production situations had a synergistic relationship between agricultural production and water provision to crops, but a trade-off relationship between these two ES and N provision to crops. As for leaf 1, production situations in this leaf were characterized mainly by a short crop rotation that included a monoculture of wheat and a wheat-rapeseed rotation which were associated with high mean mineral/organic fertilization (>175 kg/ha) (Fig. S1). However, the soil was slightly acidic (pH < 7), without CaCO₃, and had a moderately low available water capacity (<150 mm).

- Leaf 3: medium frequency of cover crops in the northeastern region of the study area

In leaf 3 production situations ($n = 2000$), the climate regulation lay at the median level, while agricultural production, water quality regulation, water provision to crops, and blue water provision levels were low to very low. Since N provision to crops was particularly high, it had a trade-off relationship with agricultural production and the other regulating ES, except climate regulation. Unlike leaves 1 and 2, leaf 3 was characterized mainly by a long crop succession that included a wheat-beet-rapeseed-sunflower rotation associated with a medium frequency of cover crops and medium mean mineral/organic fertilization

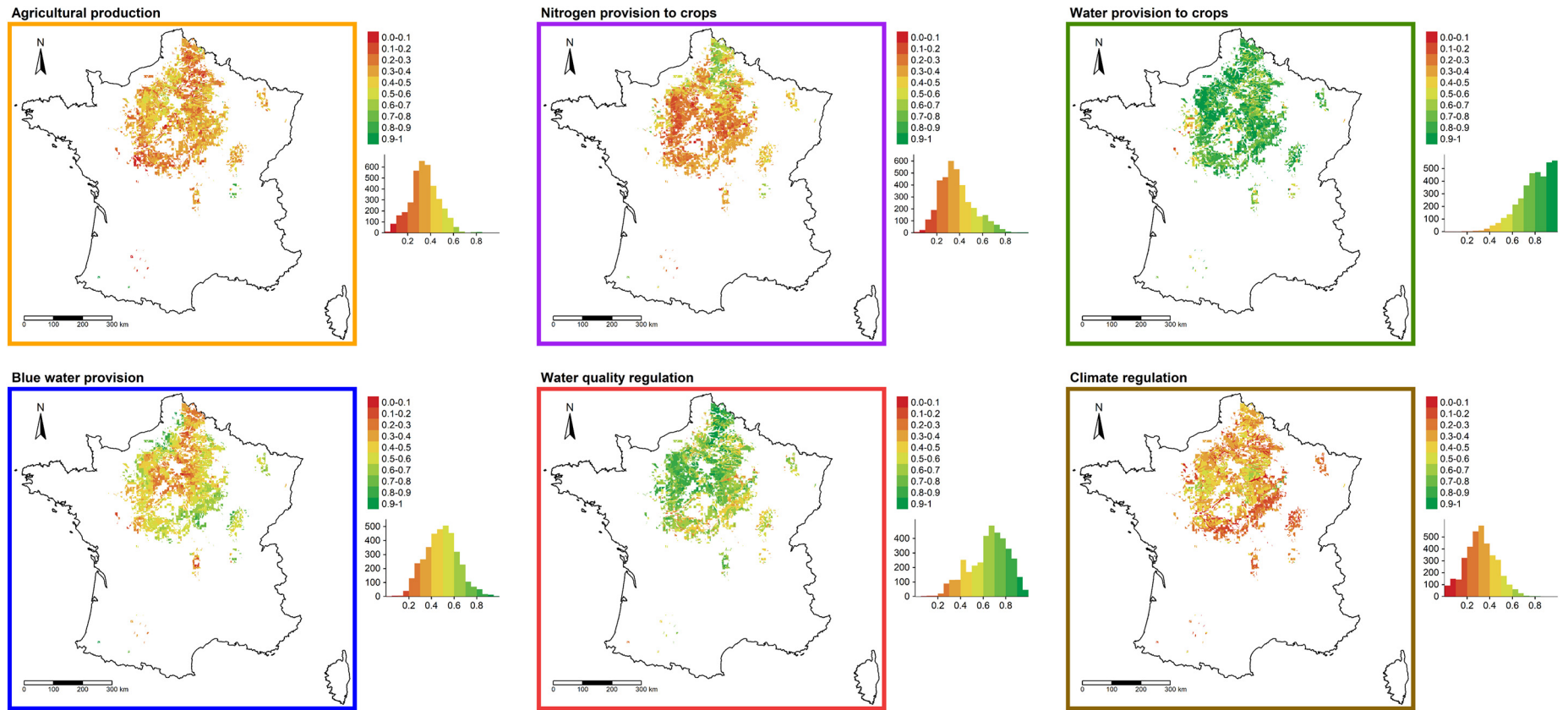


Fig. 1. Spatial distribution of levels of agricultural production and the five investigated ecosystem services (ES) in the arable area of the "modified oceanic climate of the central and northern plains", at the resolution of pedoclimatic units ($n = 3748$). Levels are normalized from 0 (red) to 1 (green). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

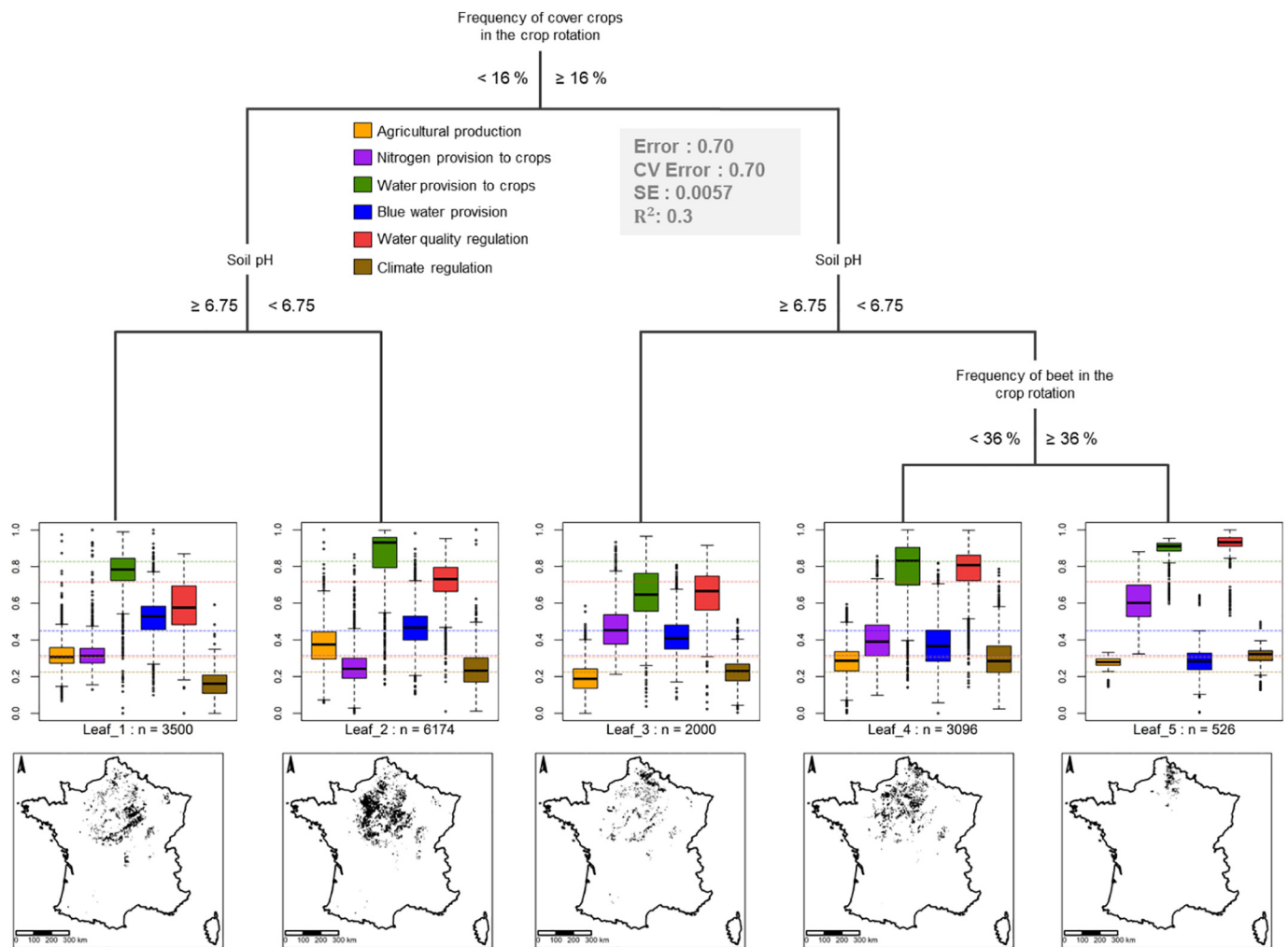


Fig. 2. Multivariate regression tree (MRT) results and mapping of production situations. The regression tree must be read from the top (root) to the bottom (leaf). It shows drivers of ecosystem services (ES) bundles, the bundles, and their associated maps. Each leaf in the tree (i.e. ES bundles) shows the number of associated production situations (n). Drivers of ES bundles and associated thresholds are specified along the branches of the tree. Statistical indices are shown in the gray box. Error = residual error (calculated with the same data used to fit the model), CV Error = mean residual error calculated following a 10-fold cross validation procedure to avoid overfitting, SE = standard error of the 10 CV errors. Cross-validated $R^2 = 1 - \text{CV Error}$ = percentage of variance explained by the tree, which ranged from 0 (poor set of predictors) to 1 (perfect set of predictors). For each leaf (ES bundles), the boxplots compare agricultural production and ES levels for normalized values ranging from 0 to 1. The central solid line in each box is the median of ES values of production situations in each leaf, and dots represent outliers (values outside the whisker range). The edges of each box are 25th and 75th percentiles. Boxplot whiskers are maximum and minimum values. Dashed horizontal lines behind boxplots represent the median agricultural production and ES values of all production situations investigated. This median value was used as a reference to compare ES levels among the leaves. The spatial distribution of each terminal group characteristic is shown in the maps.

(<160 kg/ha) (Fig. S1). Like for leaf 1, the soil was slightly alkaline ($\text{pH} > 7$), but particularly calcareous (CaCO_3 content of about 15%), and had a lower clay content (<15%) than the other leaves. The available water capacity was also low (<100 mm), as for leaf 1.

- Leaf 4: medium frequency of cover crops in the center of the study area

In leaf 4 production situations ($n = 3096$), water quality regulation, N provision to crops, and climate regulation levels were moderately high. Agricultural production and blue water provision were moderately low, with a median level of water provision to crops. Thus, production situations in this leaf had a synergistic relationship between water quality regulation, N provision to crops, and climate regulation. However, these three ES had a trade-off relationship with agricultural production and blue water provision. Like for leaf 3, production situations in this leaf were characterized mainly by a long crop rotation associated with a medium frequency of cover crops and a medium mean mineral/organic fertilization (<160 kg/ha). The only difference with the rotations in leaf 3 was the presence of spring pea instead of sunflower.

The soil was slightly acidic ($\text{pH} < 6.75$) without CaCO_3 , like for leaf 2, but the available water capacity was moderately high (about 170 mm).

- Leaf 5: high frequency of cover crops in the northeastern region of the study area

In leaf 5 production situations ($n = 526$), water quality regulation, N provision to crops, climate regulation, and water provision to crops were particularly high. Agricultural production and blue water provision were low. Thus, there was a strong synergistic relationship among all regulating ES, except blue water provision. However, these four ES had a trade-off relationship with agricultural production and blue water provision. Production situations were characterized mainly by a short crop rotation, such as wheat-beet, and associated with a high frequency of cover crops and a medium mean mineral/organic fertilization (<160 kg/ha), like for leaves 3 and 4. SOC inputs to the soil profile (about 4 t ha^{-1}) and available water capacity (>200 mm) were higher than those in the other leaves. The soil was slightly acidic ($\text{pH} < 6.75$) without CaCO_3 , like for leaves 2 and 4.

Table 3

Qualitative interpretation of results of the multivariate regression tree. Green “++” and “+” symbols correspond to higher and moderately higher, respectively, agricultural production and ecosystem services in the leaf than in the other leaves. The “=” symbol indicates a median supply, while the red “--” and “-” symbols correspond to a lower and moderately lower supply, respectively.

	Leaf 1	Leaf 2	Leaf 3	Leaf 4	Leaf 5
	Frequency of cover crops in the crop rotation (< 16%)		Frequency of cover crops in the crop rotation (≥ 16%)		
Tree characteristics	Soil pH (≥ 6.75)	Soil pH (< 6.75)	Soil pH (≥ 6.75)	Soil pH (< 6.75)	
				Frequency of beet in the crop rotation (< 36%)	Frequency of beet in the crop rotation (≥ 36%)
Ecosystem service					
Agricultural production	=	+	--	-	-
Nitrogen provision to crops	=	-	++	+	++
Water provision to crops	-	++	--	=	++
Blue water provision	+	=	-	-	--
Water quality regulation	--	=	-	+	++
Climate regulation	-	=	=	+	++

4. Discussion

4.1. Drivers of relationships between ecosystem services

Our results suggest that in non-irrigated temperate cropping systems, crop rotation, cover crop frequency, N fertilization practices, and certain key soil properties or components (e.g. pH, CaCO₃ content, available water capacity) are major drivers of multiple ES. Except for available water capacity, these relevant drivers are manageable and thus can be modified via adapted management strategies (Dominati et al., 2010; Robinson et al., 2013). However, altering drivers such as pH and CaCO₃ content significantly often requires large amounts of inputs and/or time, which can involve prohibitive costs in the long term. Moreover, these two drivers may serve as proxies for other fertility-related soil properties that can co-vary with them, such as cation exchange capacity or soil texture, which are much more difficult (if not impossible) to alter. Our results provide practical information for landscape management and spatial planning. They can help landscape managers and stakeholders identify which ES bundles can be developed more than others for a given study area, although it is rarely as simple to achieve.

The crop rotation is a strong driver of ES since it determines water, N, and C cycles over cropping seasons and years (Lin, 2011; Kremen and Miles, 2012; Duru et al., 2015). The effects of pH, followed by CaCO₃ content (a surrogate in our analysis, Fig. S3 in Supplementary material), are recognized as key drivers of soil organic matter mineralization (Clivot et al., 2017) and thus of ES related to N and C cycles (here, N provision to crops, water quality regulation, and climate regulation). Available water capacity influences water flows in the soil (i.e. the higher the available water capacity, the lower the percolation) and, as expected, blue water provision and water quality regulation (O'Geen et al., 2010).

4.2. Relationships between agricultural production and regulating services

From analyzing the MRT, we identified trade-offs and synergies between agricultural production and ES and their spatial distribution over the study area. Although directly comparing our results to the many bundles identified in the literature is difficult due to the diversity of landscapes studied, statistical methods used, and the ES considered (Saidi and Spray, 2018), many of our results are consistent with those of other studies. In their reviews, Lee and Lautenbach (2016) and Saidi and Spray (2018) indicated that most case studies show a synergistic relationship between several regulating ES and a trade-off between regulating and provisioning ES. Demestihis et al. (2017) demonstrated that agricultural production and regulating ES could conflict in agroecosystems. In our study, this synergy between regulating ES and the trade-off with agricultural production varied greatly among the leaves. In leaves 4 and 5, as shown in the general review of Abdalla et al. (2019), cover crops simultaneously increase N provision to crops (green manure effect), water regulation (decrease N leaching), and climate regulation (SOC sequestration) but this effect was not observed in leaf 3. In the three leaves with a high frequency of cover crops (3, 4 and 5), we observed a lower mean level of agricultural production, which could be due to a negative effect of cover crops, as observed by Abdalla et al. (2019).

Our results also identified a major trade-off between agricultural production and the N provision to crops for all leaves in nearly all areas of the study, except leaf 1. In leaves 3, 4, and 5, the N provision to crops was higher than the median, while agricultural production was lower. This result may be explained by combined effects of i) a higher yield of wheat and sugar beet (leaves 4 and 5), ii) the presence of crops with low energy production – due either to low yield (sunflower) or low energy content (sugar beet and winter wheat) – in the

crop rotation, iii) the presence of peas in the rotation (low yield and low energy content) (leaf 4), and iv) the fact that cover crops support SOC storage (Jarecki and Lal, 2003; Lee et al., 2019) and then function as “green manure” (Jarecki and Lal, 2003). In leaf 2, the trade-off is the opposite of those in leaves 3, 4, and 5: a high level of agricultural production and a low level of N provision to crops. This trade-off may exist because farmers compensate for lower N fertility of the soil applying more N fertilizer, as indicated by the high mean mineral/organic fertilization ($> 175 \text{ kg/ha}$) in these production situations.

4.3. Trade-offs between regulating services

In ES bundles of leaves 1 and 5, a trade-off appeared between water provision to crops and blue water provision. For leaf 5, as shown in the meta-analysis of Meyer et al. (2018) for temperate climates, the high frequency of cover crops reduced water drainage and thus the blue water provision. For leaf 1, the low available water capacity ($< 100 \text{ mm}$) contributed to the low water retention in the soil, thus promoting water drainage into deeper layers. The moderate magnitude of this drainage, and thus blue water provision, can be explained by the climate of these production situations in the study area which is one of the driest areas in France, annual rainfall of less than 700 mm (Joly et al., 2010). This low rainfall associated with low available water capacity could also explain the moderately low level of water provision to crops.

In ES bundles of leaves 1, 4 and 5, major trade-off appeared between water quality regulation and blue water provision. Certain soil properties (e.g. available water capacity) and agricultural practices (e.g. frequency of cover crops, N mineral fertilization) were major drivers of this trade-off (Fig. S1 in the Supplementary materials). In leaf 1, the high blue water provision and low water quality regulation were associated with low available water capacity ($< 100 \text{ mm}$) and high N fertilization ($> 170 \text{ kg N ha}^{-1}$), while the lack of cover crops resulted in high N leaching. Conversely, in leaf 4 and 5, the low water provision and high water quality regulation corresponded to cropping systems with moderate fertilization ($< 160 \text{ kg N ha}^{-1}$), cover crops, and grown on soils with high available water capacity ($> 150 \text{ mm}$).

4.4. Methodological advantages of multivariate regression trees

In this study, we present an innovative use of MRT to identify key ES bundles and their drivers. One main advantage of the MRT method is its ability to identify relations, non-linear effects, and threshold effects when analyzing trade-offs/synergies. For example, the MRT distinguished effects of pH over a threshold of 6.75. From a management perspective, this threshold is relevant because it can be considered the level required to promote expression of a certain ES bundle. Finally, the MRT method does not require or assume any specific distributions within the data (Smith et al., 2019), is simple to apply to datasets and is available in free software, such as R.

4.5. Limitations and uncertainties of the MRT-based approach

The low R^2 (0.30) value in our study reflects the low explanatory power of the tree. This low R^2 is related in part to the number of leaves set in the final tree. To assess the influence of this choice, we explored the optimal tree size that avoided overfitting (i.e. the “1se” criterion (Breiman et al., 1984)) using an internal cross-validation procedure. The resulting deeper tree contained 13 leaves and had an R^2 of 0.40 (results not shown). Even with this optimal tree, most of the variability remained unexplained, which justified our choice of a five-leaf tree that balanced descriptive power and interpretability of the results. This unexplained variability may be related to the specific characteristics of each production situation, since ES in agricultural systems depend greatly on adapting agricultural practices to site-specific characteristics (Duru et al., 2015). To overcome this limitation, our

large-scale approach could be combined with more focused and detailed analysis of particular situations. The former would be helpful for designing regional policies or landscape management strategies, while the latter would be more useful for designing management strategies of specific situations.

The classic interpretation of trade-offs or synergies in each leaf of the tree is usually based on visually interpreting the relative sizes of bars plotted by the MRT method (Fig. S4 in the Supplementary material). This interpretation could be more subjective than interpretations based on more quantitative methods, such as pairwise correlation of ES. One issue is how to define the boundary between a high vs. low level of ES objectively. To address this issue, we replaced the usual bar plots with boxplots and thus used the median of each ES value from the entire sample as a reference. By comparing the median of each ES per leaf with the median of the same ES for all leaves, we objectively determined the relative level of each ES (Table 3) within leaves. However, as a boundary, it assumes that all production situations within the PCUs can produce the same level of each ES, while according to our results, some production situations (e.g. within leaf 3) have limited ability to provide certain ES.

Despite these limits, this study was the first to analyze and quantify relationships between agricultural production and some regulating ES in a variety of production situations in France. Our results provide farmers and agricultural policy makers with basic information about manageable drivers and associated target levels (thresholds) that can be used to design ecosystem management strategies that promote a balanced bundle of ES.

4.6. Relative influence of manageable and non-manageable drivers in MRT

To assess the extent to which adding non-manageable drivers to the final tree might decrease the unexplained variance, in addition to the final tree (Fig. 2), we generated a new five-leaf tree that also considered drivers related to the climate (precipitation, average temperature, and precipitation minus evapotranspiration) and additional non-manageable soil properties (clay content and available water capacity). In this new tree (Fig. S5 in the Supplementary material), clay content and available water capacity appeared as key variables, but the tree's explanatory power (41%) increased by only 11 percentage points. The climate variables tested may have added little explanatory power because we investigated production situations in the same climate type (i.e. little climate variability). Interestingly, comparison of the two trees developed shows that manageable drivers (e.g. cover crop frequency) influence ES relationships greatly and that farmers have opportunities to manage them.

This new tree confirmed our hypothesis about the source of unexplained variance, which was related more to the high diversity of the production situations investigated than to the potential exclusion of key drivers in the tree. Thus, one way to decrease the unexplained variance would be to focus analysis on a lower diversity of production situations.

4.7. Effectiveness of multivariate regression trees for evaluating ES trade-offs and synergies

According to Turkelboom et al. (2016), analysis of ES bundles should (i) predict where and when trade-offs might occur, (ii) identify how to reduce undesirable trade-offs and increase desirable synergies via management strategies, and (iii) promote transparent and honest dialogue between concerned stakeholder groups. Our MRT-based approach addresses these three topics:

- (i) It identifies production situations that provide different types of bundles. Since each situation is associated with a spatially explicit PCU, it was simple to map the spatial distribution of these bundles and the associated trade-offs and synergies. According

to Hauck et al. (2013), ES maps have an air of authority and are useful for governance and ecosystem management plans and their ES.

- (ii) The main strength of MRT, along with the use of boxplots to interpret the results, is its ability to identify and characterize the drivers of each ES bundle explicitly. For example, in leaf 5 we identified that high blue water provision and low water quality regulation were associated with patterns of the dominant crop rotation (e.g. sugar beet and cover crop frequency, short crop rotation such as wheat-beet) and associated management practices (e.g. N fertilization), which were related to certain soil properties (e.g. pH, available water capacity).
- (iii) As discussed in other studies (Hamann et al., 2010; Smith et al., 2019), the MRT approach is simple and intuitive to interpret, especially for non-scientists. The ease of interpretation is a major advantage that promotes dialogue between scientists and agricultural ecosystem managers (e.g. farmers and agricultural policy makers). Moreover, it facilitates discussion between stakeholders – such as ES beneficiaries – who can have contrasting interests in a region. For example, in our study, the ES bundles in leaf 2 could be interesting for farmers (due to an adequate supply of agricultural production) and agricultural landscape managers (due to a median supply of blue water associated with non-degradation of water quality).

Our results for ES relationships and their drivers are built upon a high diversity of non-irrigated cropping systems in the modified oceanic climate of France. However, their general representativeness of this type of agricultural system and of other systems (e.g. in a temperate climate) remains to be defined based on the results of future studies.

5. Conclusion

We developed an original MRT-based approach to identify trade-offs and synergies between ES. We demonstrated advantages of this approach for identifying relationships between agricultural production and five key soil ES provided by agricultural ecosystems in 15,296 production situations, distributed over the main arable area of France (mainly the Paris basin of production).

Our MRT-based approach identified the spatial distribution of ES bundles and their specific manageable drivers. For example, we demonstrated that synergies between water quality regulation, N provision to crops, and climate regulation were located mainly in the northeastern region of the study area and influenced mainly by agricultural practices such as the crop rotation (type of crop rotation and cover crop frequency) and soil properties (e.g. pH, available water capacity). We identified that cover crop frequency, while promoting the three ES, can drive the trade-off between water provision to crops and blue water provision (i.e. between an ES to farmers and one to society). Identifying the manageable drivers of ES bundles can help stakeholders define locally adapted management strategies (e.g. introducing cover crops) to reduce undesirable trade-offs between targeted ES and increase desirable synergies. Due to the mapping ability of the method, it can also promote dialogue between stakeholders, such as farmers and landscape managers, to identify priority regions for promoting bundles of ES.

Because the MRT-based approach considers non-linear relationships between ES and threshold effects of drivers, it can provide crucial information to decision-makers. However, its relatively low explanatory power highlighted the wide variety of ES relationships and their drivers among production situations. Increasing the explanatory power requires combining a large-scale approach to ES relationships with more focused and detailed analysis of particular situations. While the former would be helpful for designing regional policies or landscape management, the latter would provide useful local information to farmers and reflect their specific situations.

As our study was based on model output, an interesting next step would be to model effects of alternative cropping systems, such as including a large number of cover crops in the rotation, to evaluate their ability to modify the provision of certain ES. This approach could help stakeholders address current issues related to climate and/or land-use changes, such as identifying which cropping systems (crop rotation and management) can reduce trade-offs between ES, such as water provision to crops and blue water provision.

CRediT authorship contribution statement

Gregory Obiang Ndong: Conceptualization, Methodology, Investigation, Formal analysis, Software, Data curation, Visualization, Writing – original draft. **Jean Villerd:** Methodology, Formal analysis, Writing – review & editing. **Isabelle Cousin:** Conceptualization, Funding acquisition, Methodology, Project administration, Supervision, Validation, Visualization, Writing – review & editing. **Olivier Therond:** Conceptualization, Funding acquisition, Methodology, Project administration, Supervision, Validation, Visualization, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.scitotenv.2020.142815>.

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