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Design of on-farm precision experiments to estimate site-specific crop responses

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Abstract

Site-specific prescriptions require estimating response functions to controllable inputs across the field. The methodology of applying geographically weighted regression to on-farm precision experimentation studies opens new opportunities to study site-specific responses to inputs in farmers' fields by locally estimating the regression coefficients. However, the effect of the experiment's spatial layout, such as plot dimensions and randomization, and spatial structure of the yield response on the experiment performance are yet to be studied. Detailed information about these effects is needed to improve trial design to detect site-specific responses. A simulation study was conducted using 14,400 fields of 37 ha and 9-m resolution. Coefficients from a spatial variable response function were drawn from five random fields generated by unconditional Gaussian geostatistical simulations. Four levels of nitrogen were assigned to plots using 18 systematic and randomized chessboard designs with different plot sizes. Simulated yield data was obtained by combining the coefficients, treatment, and random error. The effect of spatial structure and the designs was assessed with measures of agreement between the true and estimated maps of regression coefficients. The ability to capture or approximate the true spatial pattern of the response function increased as the underlying response function's spatial structure increases. Overall differences in performance between design were observed across the spatial structure tested, mostly related to randomization and plot dimensions. In general best results were achieved by systematic designs with small or intermediate plot sizes ($r = 0.54 \pm 0.05$, MAE $= 0.005 \pm 0.0005$, SDR $= 0.81 \pm 0.06$, and CP $= 0.50 \pm 0.04$). Our methodology provides a path for testing designs under different spatial variability scenarios.

1 | INTRODUCTION

The goal of agricultural experimentation is to increase the scientific knowledge on the response of agricultural systems to manageable inputs such as seeds, fertilizers, pesticides, and ultimately to help farmers achieving higher yields and

Abbreviations: CP, coverage probability; DIFM, data-intensive farm management; GWR, geographically weighted regression; MAE, mean absolute error; MZ, management zone; OFPE, on-farm precision experimentation; PCA, principal component analysis; *r*, correlation coefficient; SDR, standard deviation ratio; SS, sum of squares; VRT, variable rate technology.

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sustainable systems by making better decisions under variable soil and weather conditions (Maat, 2011). Traditionally, these experiments are carried out at research centers using randomized and replicated small-plots designs with different levels of control of experimental conditions (Piepho et al., 2011). Although the precision and power achieved in these experiments could be high, the resulting recommendations are derived from inference extrapolations, which in many cases, result in uncertainty related to the variability of soil, weather, farming systems, and farmer skills (Marchant et al., 2019). In contrast, on-farm experiments, which are characterized by larger experimental units and simpler designs, are claimed to be more representative of real conditions but typically less precise and less powerful (Piepho et al., 2011). During the last decade, precision agriculture technologies (e.g., geopositioning systems, yield monitors, variable rate technology, etc.) have helped farmers and crop advisors to run farm-scale experiments almost effortlessly on their farms to compare different agronomic practices or to validate recommendations from research centers (Panten et al., 2010). At the same time, the structure of the data collected by machinery with this technology has challenged the classical statistical methods for small-plot agronomic experiments requiring new approaches (Hicks et al., 1997; Plant, 2007). For instance, in a recent simulation study, Alesso et al. (2019) showed that spatial autocorrelation, if not modeled, could reduce the efficiency of treatment effect estimators and increases the Type I error. Among the designs tested, those with smaller experimental units, and a larger number of replications, performed better.

As the spatial resolution at which inputs can be controlled within fields increases, farmers and agronomists are more interested in knowing about the responsiveness of each part of their fields instead of regional recommendations (Bullock & Bullock, 2000; Piepho et al., 2011; Pringle et al., 2004a) . Since the introduction of the precision agriculture concept, the management zone (MZ) approach has been widely applied as an interim approach between uniform and site-specific management (Whelan & Taylor, 2013). In this approach, within-field variability is clustered into zones with similar characteristics, which are assumed to also share the same response to inputs, and thus the same management requirements. If combined with on-farm experiments, this MZs may help to understand the responses at the subfield scale, and if treatments × zones interaction exist, there would be room for developing crop response functions for each zone (Bishop & Lark, 2006; Piepho et al., 2011). Although the MZ approach is intuitive and straightforward, the primary assumption behind it, that is, homogeneity of responses within MZ and heterogeneity between MZ, is not always met or verified. In addition, to increase the spatial resolution at which a crop can be managed, information about how crop yield responds to varying treatments and how those responses vary over space is required (Bullock & Bullock, 1994).

Core Ideas

- Application of geographically weighted regression estimate site-specific responses.
- On-farm Precision Experiment designs can be compared with simulation studies.
- Systematic treatment assignments are more favorable than random treatment assignment.
- Medium to smaller plots size increase trial performance compared with large plot size.
- Prior knowledge of spatial structure improves the performance of the experimental design.

Alternative on-farm experimental designs and analytical methods aimed to quantify the spatial variability of treatment effects or to estimate site-specific response functions have been proposed in the literature. These approaches were generally based on randomized or systematic experimental designs such as strip-plots (Kyveryga et al., 2009; Scharf et al., 2005), chessboard (Kindred et al., 2015), or whole-block (Panten & Bramley, 2012) designs carried out at field scale. Continuous variability of the field is broken down into smaller units or polygons matching the spatial resolution at which management is to be applied, and the response for each unit is estimated. As only the response to one treatment level can be measured at the same time for each unit, the treatment effects at untested locations have to be estimated. Some methods based on geostatistical interpolations were proposed to estimate responses at untested locations and fitted response functions using the actual response and those interpolated (Bishop & Lark, 2006; Panten et al., 2010; Pringle et al., 2004b). To avoid interpolations, Scharf et al. (2005) randomly assigned treatments to field length strip plots and then divided these strips into blocks for estimating the response function using the information of blocks of data within the strips. In a similar fashion, Kyveryga et al. (2009) proposed a method to assess the spatial distribution of the effects within the field using a paired comparison between systematically assigned plots. Compared to the MZ method, these approaches have increased the spatial resolution of the information gained from on-farm experiments. However, they involve several steps and assumptions, including interpolation procedures and estimation based on a few nearby observations. Recently, Trevisan et al. (2020) have introduced the application of geographically weighted regression (GWR) to on-farm precision experiment data collected from the Data-Intensive Management Project (DIFM) (Bullock et al., 2019). The authors showed the potential of GWR for developing prescription maps based on site-specific information rather than on subfield areas.

In a nutshell, GWR is one of the spatially varying coefficient models proposed for the direct estimation of these site-specific functions. Unlike other methods that involve several steps and assumptions, the GWR allows estimating functions where the parameters of the models vary in space, and they can be mapped and interpreted as a spatial variable (Fotheringham et al., 2002). This method applies a weighted least squares estimation to neighboring subsamples where weights are estimated via a distance-decay kernel within a bandwidth. Although initially designed to deal with the lack of stationarity issues, this method has been applied for making spatial inferences in several fields beyond geography (Wheeler & Calder, 2007). As reported by several authors, the inference about local coefficients is sensitive to the bandwidth selection and kernel functions which may result in the detection of misleading relationships (Bivand et al., 2013; Páez et al., 2011) and several methods to calibrate these aspects were reported (Farber & Páez, 2007).

Despite the potential of GWR for developing site-specific prescription maps (Rakshit et al., 2020; Trevisan et al., 2020), the effect of the experimental designs and the underlying spatial structure on the ability of this model to approximate the true spatial pattern of crop responses is yet to be explored. As the true underlying spatial structure of the crop response function is always unknown, we propose an in silico study to assess the effect of combinations of plot sizes and randomization on the GWR results assuming several spatial structure scenarios for those function coefficients. The main goal of this study is to assess the impact of experimental designs and the underlying spatial structure on the ability of GWR models to estimate the spatially variable response functions. Results from this exercise would help the optimization of OFPE methods for supporting site-specific decisions and build confidence in the methods applied for their analysis.

2 | MATERIALS AND METHODS

2.1 | Hypothetical experimental conditions

A simulation study was conducted to evaluate the effect of experimental designs on the ability of on-farm precision experiments to capture the spatial variability of crop response functions under different spatial variability scenarios. Hypothetical experiments aimed to estimate the yield response of corn (*Zea mays* L.) to nitrogen applications on a 432 m width by 864 m long experimental field (37 ha) were simulated. The following machinery configurations were assumed to be available for running the experiment and collecting the data: (a) a tractor powered with automatic guidance; (b) a 12-row 76 cm spacing applicator with variable rate technology (VRT); (c) and a combine harvester equipped with a 12-row header, yield monitor system, and automatic guidance. Based on combine specifications, the minimum width of the experimental units was the combined cut swath, which is equal to 9 m. The dimension of the field was approximately equivalent to 48 and 96 times the header width, respectively. A total of 4,608 data points were simulated for each combination of spatial scenario and experimental design described in the following section. The extent of the experimental field is comparable with fields from the DIFM project (Bullock et al., 2019) and provided the minimum size of the field for a realistic representation of different spatial patterns and allocation of experimental unit sizes while keeping the number of data points and computational time low. In real scenarios, coarser resolutions could be expected due to wider machinery footprints (header or planter widths) and the smoothing process along with harvest direction (Lark et al., 1997; Marchant et al., 2019).

2.2 | Experimental designs

The simulated treatments consisted of four nitrogen rates (0, 50, 100, and 150 kg N ha^{-1}) applied during the planting operation. These treatments were applied at a minimum spatial resolution of 9 m perpendicular to planting direction due to the dimensions of the header, which matches the applicator. The minimum resolution along planting direction was 36 m for allowing enough time (about 18 s) for the actuators for changing the rate on-the-go and the delays for the grain threshing and yield monitor system. As a result, the smallest and largest experimental unit sizes were about 324 to 1,296 m^2. Six spatial layouts (L1–L6) with a different number and size of experimental units were applied in a systematic (R0), partially (R1), and completely random (R2) fashion. Designs with restricted randomization (R1) were obtained by dividing the field in three zones and randomizing treatments within each zone independently. The combination of plot sizes and randomization resulted in 18 designs, which are summarized in Table 1 and displayed in Figure 1b.

In non-spatial experiments, some sort of blocking is desirable for controlling nuisance factor that can alter treatment responses (Piepho et al., 2011). In spatial experiments like those simulated in this study, the rationale behind the use of blocks or zones for restricting the randomization, even though the underlying trend is not evident or unknown, is related to the need of avoiding spatial clustering of treatment levels and thus getting a more spatially balanced distribution of treatments.

2.3 | Yield data simulation procedure and model assumptions

Corn yield response to nitrogen rates was simulated assuming a linear model with spatially variable coefficients within the

TABLE 1 Summary of the characteristics of the experimental designs evaluated

Code[a]	Layout	Randomization	Replications	Plot width	Plot length	Plot aspect ratio	EU area[b]
				m			m^2
L1R0	1	no	288	9	36	4	324
L2R0	2	no	144	9	72	8	648
L3R0	3	no	144	18	36	2	648
L4R0	4	no	72	18	72	4	1,296
L5R0	5	no	96	27	36	1.3	972
L6R0	6	no	48	27	72	2.6	1,944
L1R1	1	partial	288	9	36	4	324
L2R1	2	partial	144	9	72	8	648
L3R1	3	partial	144	18	36	2	648
L4R1	4	partial	72	18	72	4	1,296
L5R1	5	partial	96	27	36	1.3	972
L6R1	6	partial	48	27	72	2.6	1,944
L1R1	1	complete	288	9	36	4	324
L2R1	2	complete	144	9	72	8	648
L3R1	3	complete	144	18	36	2	648
L4R1	4	complete	72	18	72	4	1,296
L5R1	5	complete	96	27	36	1.3	972
L6R1	6	complete	48	27	72	2.6	1,944

[a] Code = identification code of the experimental design.
[b] EU area = area in m^2 of each experimental unit.

field:

$$y_i(s_i) = \beta_0(s_i) + \beta_1(s_i)\, x_i + \varepsilon_i \quad (1)$$

where $y_i(s_i)$ is the yield response at the site $s_i = (u_i, v_i)$ defined by u_i and v_i spatial coordinates; $\beta_0(s_i)$ and $\beta_1(s_i)$ are the regression coefficients for site s_i; x_i is the nitrogen rate; and the error term which is assumed to be independent and normally distributed with mean 0 and constant variance. Most of the corn yield response functions to nitrogen applications reported in bibliography involve some linear and quadratic or plateau feature. However, the importance of these terms depends on the range of the rates explored and the variability of soil and weather conditions. In this study, a linear function was assumed in order to simplify the yield simulation process as implemented by Evans et al. (2020) and Trevisan et al. (2020).

First, the spatial distribution of each regression coefficients of Equation 1 was simulated independently by an unconditional Gaussian geostatistical simulation procedure (Webster & Oliver, 2007). Five spatial variability scenarios, that is, random fields, for each regression coefficient, were created assuming they are a realization of a first-order stationary random process with the following general linear model:

$$\beta_j(s_i) = \mu_j + \varepsilon(s_i)$$

where $\beta_j(s_i)$ is the true value of the j regression coefficient at location $s_i = (u_i, v_i)$; μ_j is the overall mean value of the j regression coefficient over the experimental field, and $\varepsilon(s_i)$ the random term having a Normal distribution with expectation equal to 0 and a spatial variance–covariance matrix as a function of distances. Note that for scenarios with range = 0 (no spatial autocorrelation) the variance–covariance matrix is not spatial and $\varepsilon_i(s_i)$ simplifies to ε_i. The spatial autocorrelation was assumed to be isotropic and depicted by a spherical covariance model without nugget effect and ranges of 0, 50, 100, 200, and 400 m (Equation 2). Along with the exponential model, the spherical is one of the models used in literature to represent both soil and yield properties (Richter et al., 2015; Thöle et al., 2013; Webster & Oliver, 2007).

$$C(h) = \begin{cases} \sigma^2_{sill}\left(\frac{3h}{2a} + \frac{1h^3}{2a^3}\right) & 0 \le h \le a \\ 0 & h > a \end{cases} \quad (2)$$

where C(h) is the spatial covariance function between pairs distanced by h units; a is the range of spatial dependence, σ^2_{sill} is the total variance of the process, assumed to be 30% around the mean, 5 Mg ha^{-1} and 0.03Mg kg N^{-1} for $\beta_0(s_i)$ and $\beta_1(s_i)$, respectively.

For each scenario, a single realization of $\beta_0(s_i)$ and $\beta_1(s_i)$ were independently drawn, and they were assumed to be

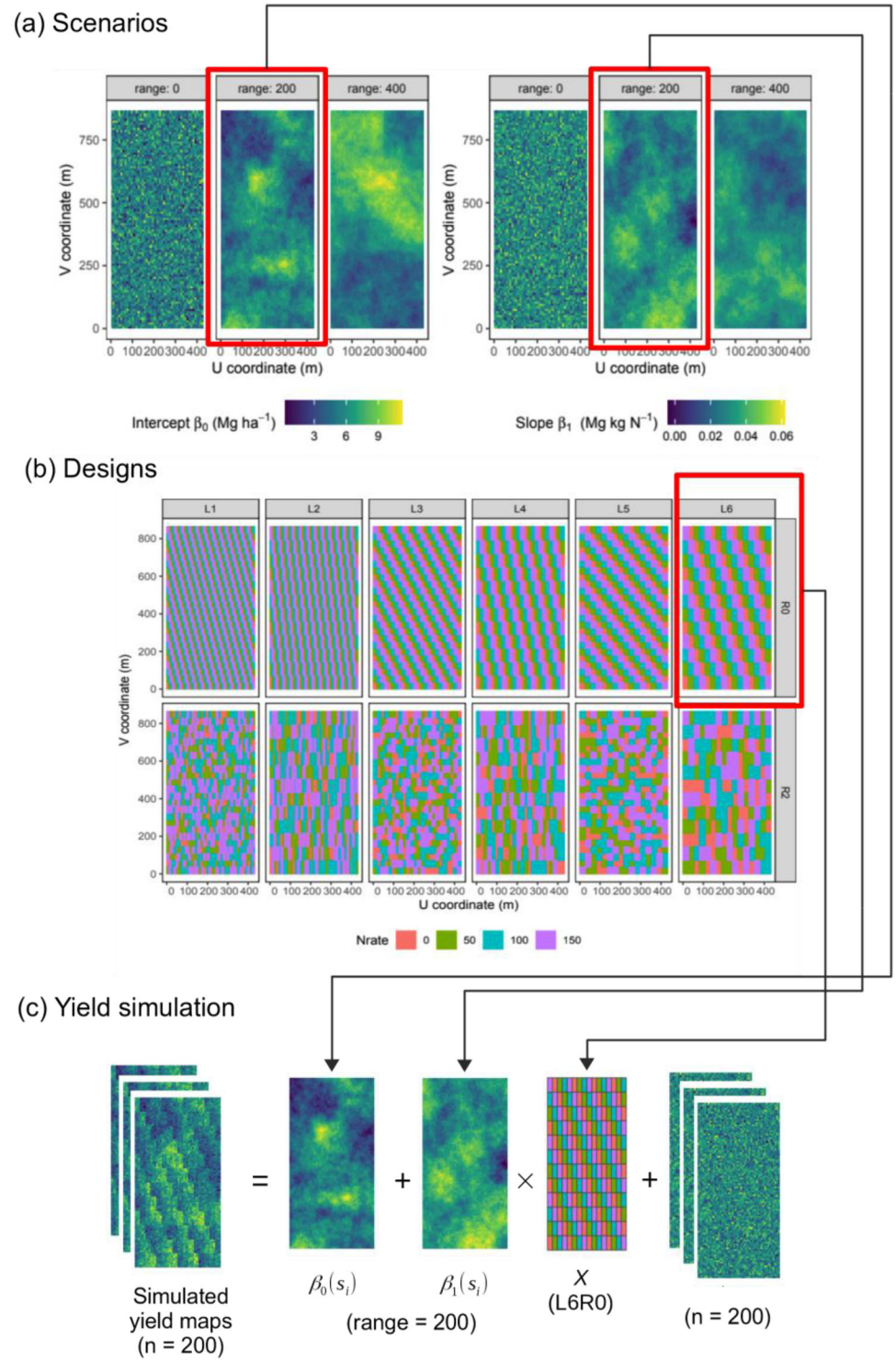

FIGURE 1 Description of (a) the spatial variability scenarios (ranges 50 and 100 were omitted due to space restrictions), (b) experimental design (blocked design R1 was omitted due to space restrictions), and (c) the yield simulation process. The example illustrates the simulation of yields for the design L6R0 applied to scenario 6 (range 200)

the true regression coefficient map of the spatially variable function (Figure 1a). Correlations between these maps for scenarios with no trend were negligible (Pearson's correlation coefficients between −0.16 and 0.07). By combining the information from these maps, simulations allowed to represent a wide range of patterns in the linear response. For example, locations with low intercepts and slopes could represent situations where another limiting factor is governing the yield response, and the application of inputs will not produce an increase in the yields. In locations where these limiting factors

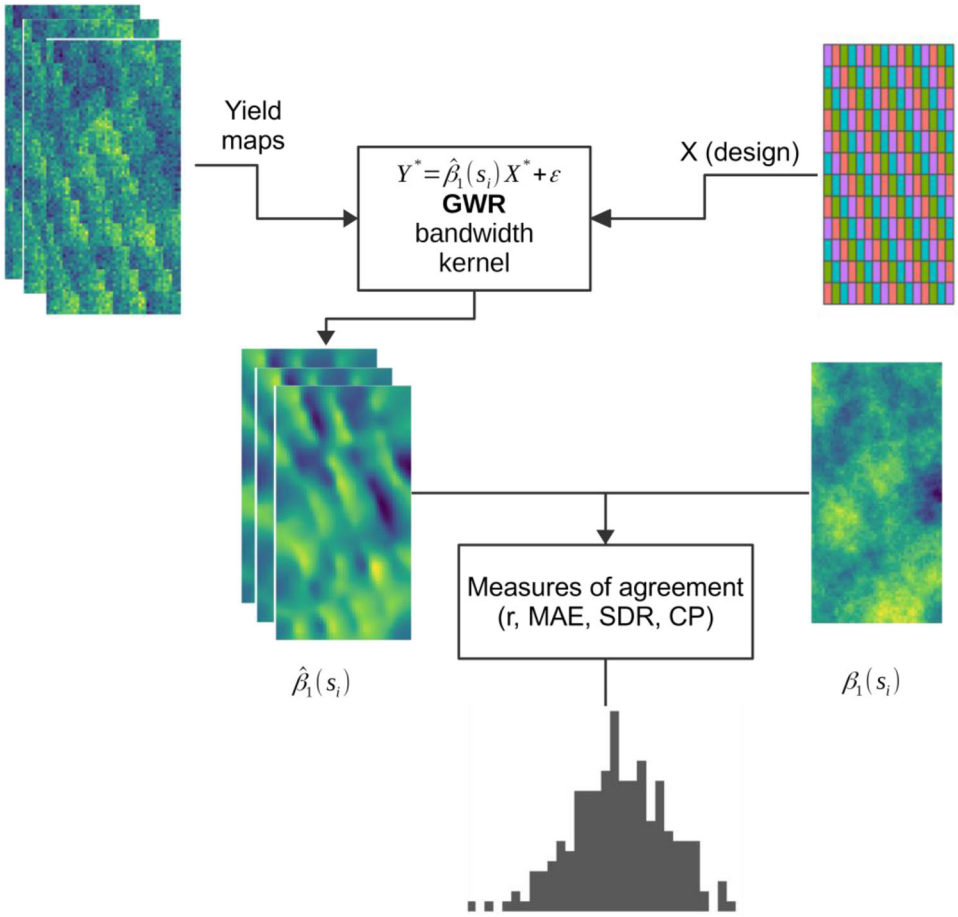

FIGURE 2 Description of the process for the simulation of geographically weighted regression (GWR) coefficient distributions from simulated yield maps and designs. The example continues the case for design L6R0 applied on scenario 6 (range 200)

are not present, the same initial yield but with higher response rate could be observed, which is the expected response for the input application to be warranted. Finally, a high intercept and low slope could represent situations where the soil provides enough nutrients to achieve a high base yield without input addition and the addition of input does not result in an increased yield.

The random fields used here for geostatistical simulation aimed to cover a wide range of spatial variability scenarios observed in the fields, ranging from purely random to well-structured variation with large-scale patterns. The pure nugget effect scenario (range = 0 m) represents the situation where crop response to nitrogen varies within the field in a way that is not spatially structured so that there is no need for local coefficients for the regression model. In contrast, in the fifth scenario (range = 400 m) the variation of the yield response is assumed to be spatially structured and local coefficients for the regression model would be warranted. In both cases, regression coefficients vary around the overall mean value.

Finally, for each scenario, corn yield data were simulated 200 times over the 4,608 grid points by plugging the information of the spatial variability of regression coefficients, the nitrogen rates from the experimental designs and a random error with mean 0 and variance assumed to be $(1.5\ \text{Mg ha}^{-1})^2$ into the model from Equation 1 (Figure 1c). In total, 18,000 yield data set were simulated.

2.4 | Data analysis

Each simulated yield data set containing 4,608 data points (each pixel is 81 m^2) was analyzed by fitting the geographically weighted regression (GWR) (Fotheringham et al., 2002) model from Equation 1 (Figure 2) but using centered data (treatments and yield) and omitting the intercept term. Regression coefficients at each location were estimated using a weighted least squares estimator based on the information of the nearby locations:

$$\hat{\beta}(s_i) = \left(\mathbf{X}^T \mathbf{W}(s_i) \mathbf{X}\right)^{-1} \mathbf{W}(s_i) \mathbf{y} \quad (3)$$

where **y** represents the vector of yield response, **X** a matrix of predictors, in this case, the treatments levels, $\hat{\beta}(s_i)$ represents the vector of estimates of $\hat{\beta}_1$ at location si, and $\mathbf{W}(s_i)$, is an **n** by

n matrix whose off-diagonal elements are zero, and diagonal elements denote the geographical weighting of each of the n observed data for point s_i. Three kernel density functions with adaptive bandwidth were tested:

$$\text{exponential kernel } w\left(s_i, s_j\right) = \exp\left(\frac{-d\left(s_i, s_j\right)}{b\left(s_i\right)^{ad}}\right) \quad (4)$$

$$\text{gaussian kernel } w\left(s_i, s_j\right) = \exp\left[\frac{-1}{2}\left(\frac{d\left(s_i, s_j\right)}{b\left(s_i\right)^{ad}}\right)^2\right] \quad (5)$$

$$\text{bisquare kernel } w\left(s_i, s_j\right) = \left[1 - \left(\frac{d\left(s_i, s_j\right)}{b\left(s_i\right)^{ad}}\right)^2\right] \text{ if } d\left(s_i, s_j\right) < b \text{ and 0 otherwise} \quad (6)$$

where the $w(s_i, s_j)$ is the weight of the data from location s_i in relation to s_j, $d(s_i, s_j)$ is the Euclidean distance between a location s_i and s_j; and $b(s_i)^{\text{ad}}$ is the adaptive bandwidth parameter for site s_i. Due to the impact of the number of neighbors on the estimation bias and variance of the estimators, the number of neighbors was selected by the adaptive algorithm to be about 3% of total observations, that is, 138 neighbors. Based on plot dimensions and the grid spatial resolution, this amount of neighbors allowed each treatment to be represented within the search radius from the target point. As a result, 54,000 GWR models were estimated, and the estimated regression coefficients and the local coefficient of determination (R^2) were retained for further analysis.

When applied to data with predictors far enough from 0, the GWR, as any linear regression procedure, is known to produce some degree of correlation between coefficient estimates, that is, intercept and slopes. As the true coefficient maps used for simulation yield datasets were assumed to be uncorrelated, fitting the GWR model to the non-centered data would result in forcing the algorithm to balance error between these two estimates, resulting in underestimation of the agreement between model estimates and true coefficients.

2.5 | Design comparisons

The agreement between the estimated regression coefficients obtained by GWR model for each realization and true coefficient used in the simulation procedure was assessed by computing the correlation coefficient (r), the mean absolute error (MAE), coverage probability (CP) and standard deviation ratio (SDR):

$$r = \frac{\sigma_{\hat{\beta}_1(s_i)\beta_1(s_i)}}{\sigma_{\hat{\beta}_1(s_i)}\sigma_{\beta_1(s_i)}} \quad (7)$$

$$\text{MAE} = \frac{1}{N}\sum\left|\hat{\beta}_1\left(s_i\right) - \beta_1\left(s_i\right)\right| \quad (8)$$

$$\text{CP}(d) = P\left[\left|\hat{\beta}_1\left(s_i\right) - \beta_1\left(s_i\right)\right| \le d\right] \quad (9)$$

$$\text{SDR} = \frac{\sigma^2_{\hat{\beta}_1(s_i)}}{\sigma^2_{\beta_1(s_i)}} \quad (10)$$

The r indicates the degree of linear association exists between the GWR estimated and true coefficients. Absolute values near the unity indicate that there exists a perfect linear relationship between them but not necessarily implies that these estimates are accurate. The MAE represents the average absolute distance between the GWR estimated coefficients and the true value over the entire field for each realization. Ideally, this measure should be near 0, but the smaller the value, the smaller is the bias, and higher is, on average, the agreement between estimated and true regression coefficients. Besides, for each realization, CP was estimated by computing the proportion of sites where the estimates of the regression coefficients were equal or less than ±15% of the true value. In other words, this measure represents the proportion of the field where the differences between model estimates, and true values are lesser than a predefined error margin. Finally, the SDR was computed to assess if the variability of the GWR estimates under- or over-estimate of the spatial variability of the true coefficients.

As a result, for each combination of spatial structure (ranges) and design distribution of 200 values of each measure was computed (Figure 2). The distribution of each measure was summarized by descriptive statistics and correlation. The effects of experimental designs and the underlying spatial variability scenarios on the ability of the model to capture the spatial variability of the true response were assessed by fitting a linear model using the measure as a response variable. The importance of factors on these measures was assessed by computing main and total sensitivity indices from ANOVA Sum of Squares (SS) of a 5 (range) x 18 (design) full factorial model (Wallach et al., 2006). For a given factor, the main sensitivity index relates to the SS associated with its main effect on the total SS.

In contrast, the total sensitivity index of a given factor accounts for the SS associated with the main effect of that factor and also any interaction involving it. Thus the higher the main or total sensitivity index, the higher the direct or direct and indirect importance of the factor on the results. The SS associated with design factors were further partitioned into specific contrast for assessing the effect of the randomization and plot dimensions.

The comparisons between designs at each spatial structure scenario were summarized through principal component analysis (PCA). The distribution of measures for each combination of designs and spatial structure scenarios was aggregated by their means, and principal components were extracted from the correlation matrix. Finally, the scores for designs with different plot width and length were related to the size of the underlying spatial structure.

2.6 | Software

Data manipulation, visualization, and modeling were performed using the statistical language R (R Core Team, 2020) and functions from packages gstat (Pebesma, 2004), dplyr (Wickham et al., 2017), ggplot2 (Wickham, 2009), and GWmodel (Gollini et al., 2015; Lu et al., 2014).

3 | RESULTS AND DISCUSSION

The average local coefficients of determination (R^2) ranged from .27 to .49. Regardless the kernel chosen or the design simulated, the moderate to a low amount of variance explained by these models is related to the amount of variation left on the residuals. In this case, the simulations assumed an error (residual) variability about 1.5 Mg ha^{-1}, which represents 30% of the mean yield without N addition, that is, the intercept. Simulations using a lower amount of residual variability could result in higher R^2 values. However, this assumption was meant for testing the designs under high variability scenarios, which could cover real on-farm experiments. As the regression coefficients estimated by GWR depend on the weighting kernel function (Fotheringham et al., 2002; Páez et al., 2011), the analysis was performed on the GWR models with bisquare kernel provided they maximized the local R^2 with values between .31 to .49 among designs and spatial structure scenarios.

The overall distributions of the measures of the agreement are summarized in Table 2. The correlation coefficients between GWR estimates and true values differed from the rest of the measures. The lowest values for CP, *r*, and SDR were associated with scenarios with no spatial structure, no matter the design. In contrast, the highest values for CP and *r* were obtained mostly under combinations of highly structured spatial variability scenarios and systematic designs with small plots sizes. The SDR rates larger than 1 were mostly found in designs with large plots. Finally, the MAE showed a similar pattern of CP but the opposite.

TABLE 2 Summary statistics of the measures of agreement computed between the true and GWR estimates of the slope of the response function from Equation 1]

Measure of agreement	Min.	Mean	Median	Max.	CV (%)
r	0	0.42	0.44	0.88	60
MAE	0.0028	0.0079	0.0081	0.0129	25
SDR	0.434	1.13	1.13	2.51	38
CP	0.23	0.39	0.35	0.78	0.27

Note. Min. = minimum; Max. = maximum; CV = coefficient of variation; *r* = coefficient of correlation; MAE = mean absolute error; SDR = standard deviation ratio; CP = coverage probability;

TABLE 3 Correlation matrix between measures of agreement computed between the true and GWR estimates of the slope of the response function

	r	MAE	SDR
MAE	−0.58		
SDR	0.39	0.43	
CP	0.71	0.94	0.21

Note. *r* = coefficient of correlation; MAE = mean absolute error; SDR = standard deviation ratio; CP = coverage probability.

The overall ability of the GWR model to capture the underlying spatial pattern of the response function is strongly correlated to the distance between the estimated coefficients and the true ones, accounted by MAE and CP (Table 3). Thus, as the correlation between the true and estimated coefficients increases, and the average error decreases, the proportion of the experimental area with estimates within 15% about the true values increases. In contrast, the SDR showed a low correlation with the rest of the measures indicating that it carries additional information.

3.1 | Impact of spatial structure and design on results

Sensitivity analysis from SS provided information about the relative importance of the design and spatial structure on GWR results. The importance of these factors varied regarding the measure considered, although some similarities were found (Figure 3). In all cases, the small difference between the main and total sensitivity index reflects the amount of SS accounted for by the interaction.

The effect of the spatial structure of the true parameter accounted for 76% of the variability of the correlation (*r*)

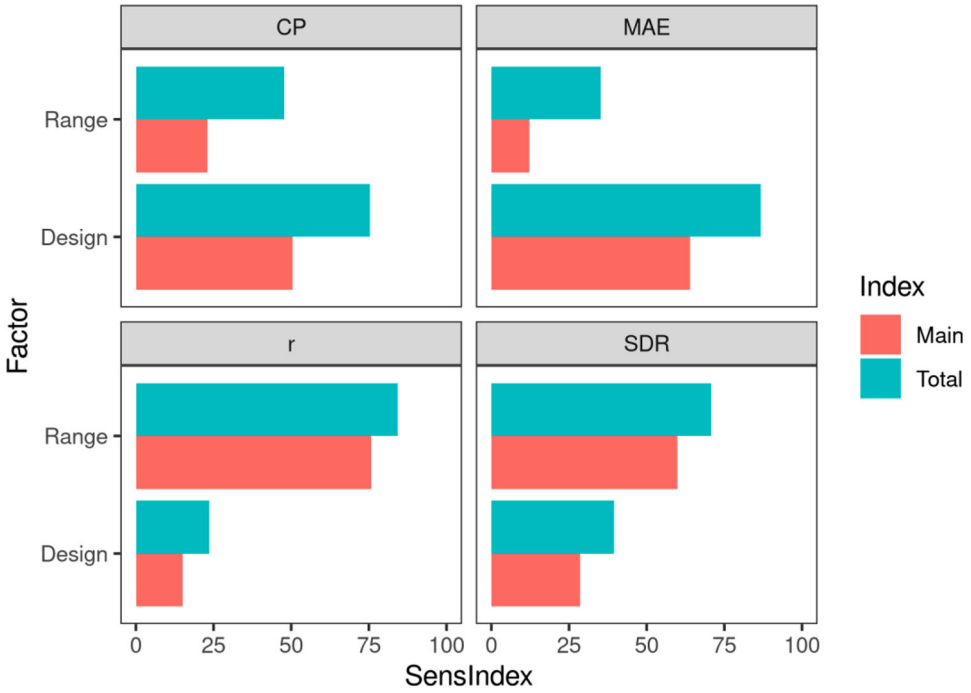

FIGURE 3 Effect of spatial structure (range) and experimental designs (design) on the amount of variability observed in the distribution of correlation coefficients (*r*), mean absolute error (MAE), standard deviation ratio (SDR), and coverage probability (CP)

between the estimates and the true values. Similarly, 60% of the variability of the ratios between the spatial variability of the true coefficients and the estimated by GWR was determined by the underlying spatial structure of the regression coefficient, but also 28% of such variation was accounted for by design. In contrast, the MAE and CP, which both measure the degree of bias of the estimates, were more related to the design. The main effect of the design represented 60 and 50% of the total variability, respectively. The partition of the SS associated with the design revealed that the plot width and randomization were the most critical factors impacting field design performance.

According to this analysis, the ability of the GWR model to capture the variability of the response function, that is, the amount and the spatial pattern, was mainly affected by the spatial structure of the underlying process. However, the overall accuracy of the coefficients estimated by the GWR model was affected mainly by the degree of bias introduced by design. Part of this behavior could be related to the fact that regression coefficients on Equation 1 are assumed to be deterministic functions of coordinates within the GWR estimation algorithm (Fotheringham et al., 2002). As the patterns of spatial variability increase in ranges, the lack of stationarity of the regression coefficients increases, and the GWR allowed capturing these smoother patterns. Conversely, the coefficients from Equation 1 are regarded as invariant within the neighborhood (Fotheringham et al., 2002); thus, the longer the range, the less spatial variability within the neighborhood, resulting in the estimated coefficients closer to the true ones. In a recent work, Rakshit et al. (2020) suggested that the upper bound for bandwidth selection for on-farm experiment designs should be based on maximum distances between all pairwise distances nearest treatments. Thus, the effect of the design through the randomization and plot width could be attributed to the distribution of the treatment plots within the search radius imposed by the bandwidth.

3.2 | Differences between designs by spatial structure scenarios

According to the PCA, 97% of the variability of the measures of agreement could be summarized into two principal components (Figure 4). The first PC accounted for 63% of the total variation and summarized the information related to the bias (MAE and CP), and the correlation between estimates and true values (Table 4). In contrast, the second PC represented mostly the variation on the SDR. According to the loading sign, positive scores on the PC1 are associated with correlation and bias higher and lower than the mean, respectively. In contrast, negative scores on the PC2 are related to the overestimation of the spatial variability of the regression coefficient.

The distribution of the observations within these two PC space showed some patterns related to the interaction between the designs (shape and colors), and the spatial structure (symbol size). As expected, under the no spatial structure scenario, the designs performed similarly with scores between −1.03

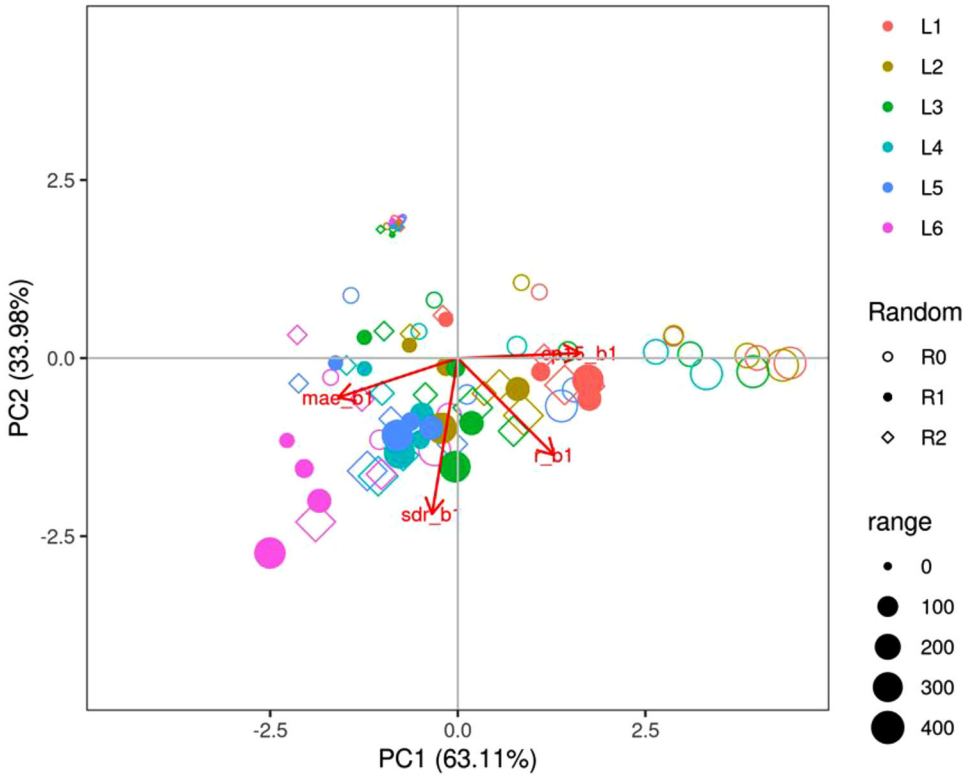

FIGURE 4 Effect of spatial structure and experimental designs on the correlation between estimated and true regression coefficients

TABLE 4 Loadings and correlation coefficients in parenthesis between measures of agreement and principal components (PC)

Measure of agreement	PC1	PC2
r	0.48 (0.77)	−0.52 (−0.60)
MAE	−0.60 (−0.96)	−0.21 (−0.24)
SDR	−0.13 (−0.21)	−0.83 (−0.97)
CP	0.62 (0.98)	0.03 (0.03)

Note. *r* = coefficient of correlation; MAE = mean absolute error; SDR = standard deviation ratio; CP = coverage probability.

and −0.73 on the PC1 and 1.73 to 1.97 on PC2, representing the lowest bound of the overall performance. As the spatial structure increases, systematic designs with small plots (L1, L2, L3, and L4) increased their scores on PC1, meaning higher values of correlation, CP, and lower MAE. However, at the same time, the small displacement along the direction associated with SDR means some improvement in the amount of variability captured by the GWR estimates. In contrast, all randomized designs, both fully and partially randomized, along with those systematic with large plot sizes tended to have low scores on PC1 and more considerable variation on PC2 as spatial structure increases. In terms of performance, although the spatial structure increases, these designs result in lower values of correlation, CP and higher MAE, and, more importantly, a higher degree of overestimation of the spatial variability of the regression coefficient.

3.3 | Relating experimental units dimensions and spatial structure

The effect of the experimental designs on the performance of GWR procedure to capture the underlying spatial pattern of the regression coefficient is shown in Figure 5. As the spatial structure increases from pure nugget to the maximum range simulated, the amount of variability captured by the model, and the overall accuracy of the estimates increases. For systematic designs with narrow plots, no matter the plot width, the scores on PC1 increase rapidly, turning into positive values for scenarios with spatial structure higher than 50 m. This gain on overall performance means that these designs can capture small-scale structures. A similar trend, although more smoothed, is observed for the PC2 with scores approaching to 1 beyond the range 100 m. Thus, when the spatial structure is higher than 100 m, the amount of spatial variability of the GWR estimates would be closer to the true spatial variability. In contrast, the impact of spatial structure on the performance of systematic designs with wider and longer plots is less evident. The measures of agreement related to PC1 increase beyond a spatial structure of 100 m but reach values lower than the mean (e.g., negative scores). The pattern observed on PC2 indicates that these designs consistently overestimate the true spatial variability of the regression coefficient as they resulted in negative scores on PC2. An interim situation is observed for wider but narrow plots.

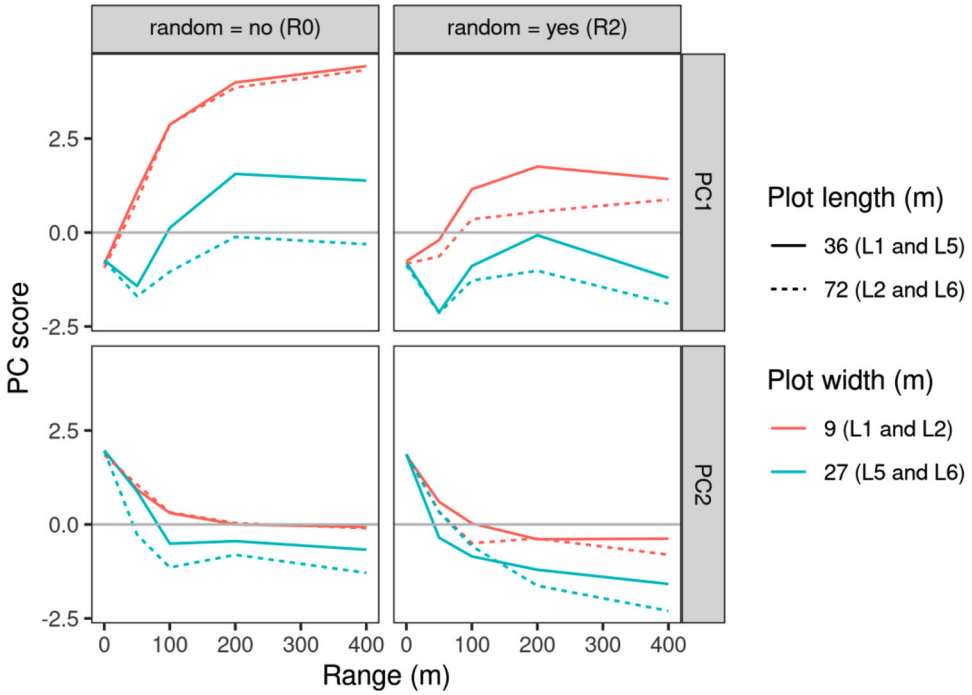

FIGURE 5 Effect of contrasting experimental designs on the performance of the geographically weighted regression (GWR) procedure to capture the underlying spatial pattern of the regression coefficient

When considering randomized designs, only the designs with narrow plots resulted in performance scores above the mean for *r*, MAE and CP, and slightly over unity for SDR. Even though, some improvement can be observed for shorter plots. In contrast, as the spatial structure increases, the amount of spatial variability observed in the GWR estimates increases up to a factor of 2 for designs with wider and longer plots.

As any simulation study, the assumptions made for the simulations, especially the hypothetical response and the amount of variability considered covered in the simulated scenarios, may condition or limit the generalization of their results. However, this novel approach combining statistical simulation and multivariate techniques provided useful insights for guiding the design of on-farm experiment. First, as showed in Figure 3, the underlying spatial structure plays a significant role in the ability of the GWR procedure to accurately estimate the spatial variability of the regression coefficients. In general, as the range of spatial structure increases, that is, more significant and smoother patterns, the agreement between GWR estimates tends to increase. Thus, confidence in the prescription maps based on these coefficients is conditioned by the degree on which the factors affecting crop response are spatially structured. Our results verified the rationale behind the opportunity index for site-specific management proposed by Pringle et al. (2003). Although this index is based on the amount and spatial structure of yield variability from uniform trials, our results suggest the need for a strong spatial structure for developing reliable prescriptions.

Second, the experimental design, through the plot dimensions and randomization, determines the spatial distribution of the treatment within the field, which affects the ability of the GWR procedure to accurately estimate the spatial variability of the regression coefficients. In this study we tested three types of randomizations: systematic, partially or blocked randomization, and full randomization. According to van Es, Gomes, Sellmann, and van Es (2007), experimental designs with some sort of blocking, that is, randomized complete block designs or Latin-square designs, are the most popular in field experiments. When applied properly, in non-spatial experiments these designs allow experimenters to control nuisance factors that can influence treatment responses but are not of interest (Piepho et al., 2011). In the context of spatial experiments, even though the underlying trend is not evident or unknown, some restrictions on the randomization are desirable in order to avoid spatial clustering of treatment levels and thus getting a more spatially balanced distribution of treatments (van Es et al., 2007). Our results showed that systematic designs provided better results for the estimation of the spatially variable regression coefficients. Among them, narrow plot designs produced better results in terms of correlation and MEA, although SDR < 1, resulting in some degree of underestimation. However, the results depend on the suitability of the designs to match the underlying spatial structure. Systematic

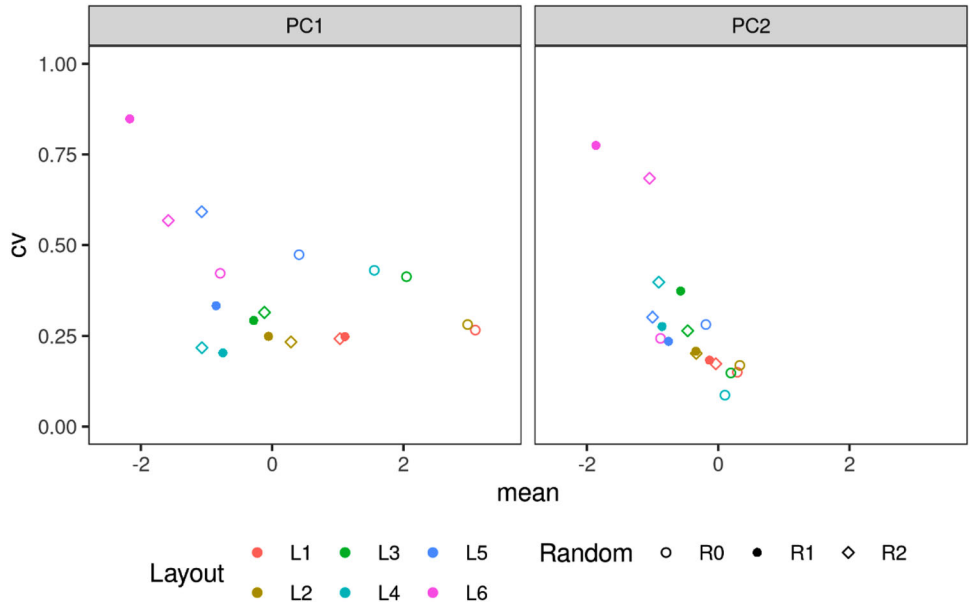

FIGURE 6 Mean and coefficient of variation of the principal component scores across the spatial structure simulated for each experimental design as a combination of spatial layouts and randomization

designs with large strip plots are popular in on-farm experiments (Griffin et al., 2004; Marchant et al., 2019; Whelan et al., 2012). These results confirm that systematic designs are more convenient for estimating local predictions of response curves, as suggested by other authors (Piepho et al., 2011; Pringle et al., 2004a).

Third, if we were able to have some idea of the spatial structure beforehand, the information about the interaction between designs and spatial structure showed in Figures 4 and 5 would be useful for designing the experiments. For example, results from DIFM (Trevisan et al., 2020) showed that the spatial structure for the optimal nitrogen rate would be around 200 m. In this case, using the results from PCA analysis, the best results in terms of measures of agreement here considered would be achieved using systematic designs L1R0 and L2R0. However, in a real setting, the scale of the underlying spatial structure is unknown. In such scenarios, the recommendation on the experimental design could be based on the results over a wide range of spatial structure scenarios. A summary of the PCA scores across the simulated spatial variability scenarios excluding the pure nugget is shown in (Figure 6). The latter scenario has been excluded as it would be an extreme case where GWR procedure does not make sense to be applied. The distribution of the points from Figure 6 shows that although systematic designs with narrow plots (L1R0, L2R0) produced the higher mean values and lower CV on PC1 scores, which is associated with high values of correlation and CP and low values of MAE, the estimated regression coefficients produced by these designs are on average less variable than those produced by designs with plots two times wider (L3R0 and L4R0) or randomized design with smallest plots (L1R1).

Four, our results suggested that the approximation of the spatial structure of a response before running the experiment in the whole field is a key aspect of on-farm experiments optimization. This information could be obtained either by using ancillary data correlated with these responses, for example, soil or landscape attributes strongly related to factors controlling crop response or using a two-stage approach. In the latter case, the first stage would consist of running a pilot trial using approaches similar to those proposed by Whelan et al. (2012) where treatments are assigned to a reduced number of plots arranged in blocks and distributed within the field. Then, fit the response function for each block (Kyveryga et al., 2009; Scharf et al., 2005) and analyze the spatial structure of these responses (Panten et al., 2010; Pringle et al., 2004b). Finally, the selection of the plot design could be based on the simulations performed for scenarios with similar spatial structures. Nevertheless, this approach would need to assume some specific form for the response function, that is, lineal, quadratic, etc., which must be regarded fixed in time. If the particular case of nitrogen fertilizer, most of the variation results from the interaction of site-specific conditions and weather. Thus, the underlying spatial pattern of the coefficients might not be the same across seasons. One way to address this issue would be to run the experiments over multiple years or instead regarding fixed this pattern incorporate this source of randomness into the yield data generation process by allowing the coefficients to vary not only spatially but also temporally.

Five, although the measures of agreement used in this work measure different aspects of the quality of GWR estimates, the PCA analysis showed a certain level of redundancy between them. The spatial structure and the experimental design affect mostly the amount of bias and the degree of correlation between estimates and true coefficients, but also the degree of under- or over-estimation of the spatial variability of the true coefficients. Prescription maps based on a biased crop response function could result in application rates that are below or above the optimal rate. In contrast, as the decision about the need for site-specific rates is based on the spatial variability of the estimated coefficients, departures from the true spatial variability of the coefficients may result in recommendations of uniform rates where variable rates are warranted. In that case, a low correlation between GWR estimates and true coefficients would result in the application of inputs based on misleading spatial patterns.

4 | CONCLUSION

On-farm experiments are valuable sources of information to help farmers in making data-driven decisions. The ability of the GWR model to capture the true spatial variability of the response function in the context of OFPE opens new opportunities to measure site-specific responses in farmer's fields and strengthen the knowledge on the impact of precision agriculture practices. In order to conduct more informative experiments, multiple field chessboard trial designs were compared in a wide range of spatial variability scenarios using a simulation approach based on principles of spatial field theory and assuming a simple response function.

Results indicated that the ability of GWR and OFPE trials of detecting linear site-specific responses is more related to the degree of spatial variability of those coefficients than the spatial arrangement of the treatments. However, experimental designs can have a significant impact on the quality of the results, and some differences related to the plot width were observed in favor of smaller plot sizes. Besides designs, systematic treatment assignment outperformed trial design by assigning treatments randomly. In a real farming scenario, the underlying response function and its true spatial pattern is often unknown ex-ante. However, by approximating the spatial structure of the response based on ancillary information or a two-stage approach, recommendations about designs could be developed.

Finally, our methodology provides a way for testing newer trial designs in new scenarios. Additional simulation studies should be conducted in order to assess the effect of other popular designs applied in on-farm experiments, for example, strip plots, or for experiments with simpler treatment structures, such as head-to-head comparisons. These results would help farmers and practitioners by giving insights about the impact of the trial designs they are employing to conduct their on-farm experiments.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

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