Kathmandu University Journal of Science, Engineering and Technology, Vol. 20, No. 2, June 2026

Kathmandu University
Journal of Science, Engineering and Technology

Weighted D-optimal design for spatial regression model in the presence of heteroscedasticity

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Abstract

In experimental designs, classical D-optimal design methods rely on homoscedastic and independent error assumptions. In this study, a spatial regression model with heteroscedastic errors was considered and proposed using weighted D-optimal designs as a result. The study proposed a weighted D-optimal design framework that explicitly incorporates spatial epistemic uncertainty derived from an Integrated Nested Laplace Approximation – Stochastic Partial Differential Equation (INLA–SPDE) model. Spatial dependence through a latent Gaussian field represented by the SPDE approach. Epistemic uncertainty is measured using the posterior variance of the spatial field and is integrated into the D-optimality criterion through location-specific weights. This weighting scheme prioritizes candidate locations with higher predictive uncertainty, thereby targeting regions where additional observations are expected to yield the greatest information gain. The proposed method is applied to spatial data on malaria prevalence among children under 5 years in Nigeria. Results showed substantial spatial heterogeneity in predictive variance, with higher uncertainty concentrated in regions with sparse observations. The weighted D-optimal design allocates sampling points preferentially to these high-uncertainty areas, in contrast to classical D-optimal designs that tend to favour well-sampled regions. Ranking and priority analyses further confirm the internal consistency and transparency of the proposed approach. Overall, the study demonstrates that incorporating spatial epistemic uncertainty into D-optimal design leads to more informative and efficient sampling strategies for spatial regression models under heteroscedasticity and non-normal errors.

Keywords: Weighted D-optimal design; Heteroscedastic regression; Spatial design; Epistemic uncertainty.

1. Introduction

In statistical modelling, optimal experimental design plays a vital role in selecting sampling locations that maximizes the information content of data collected under limited resources [1, 2]. Among the widely used criteria, D-optimal design focuses on maximizing the determinant of the Fisher information matrix, thereby minimizing the generalized variance of parameter estimates [3]. The assumptions of classical optimal design theory originated from the work of Kiefer and Fedorov were built on independence, homoscedastic and normally distributed error. However, in many real-world applications, these assumptions are violated. Classical D-optimality has been successfully applied in regression settings under assumptions mentioned above; homoscedastic errors, independent observations, and well-specified linear predictors. However, many real-world applications—particularly in environmental, demographic, and spatial studies—violate these assumptions [4, 5]. The presence of heteroscedasticity, where the variance of the error term varies with location or covariate level and non-normal error distribution such as heavy-tailed or skewed residuals, challenges the efficiency and robustness of the traditional D-optimal designs [6, 7, 8]. Spatial data often exhibit heteroscedasticity, where error variance varies across locations, as well as nonnormally distributed errors arising from measurement error, aggregation effects, or latent processes. In addition, spatial dependence introduces structured uncertainty that is not adequately captured by classical design frameworks. [9] developed D-optimal design in linear model with different heteroscedasticity structures; three correction methods were adopted from weighted least square method for heteroscedasticity problem, and it was found that the correction method tagged HCW1 performed better. The weighted D-optimal design was introduced in which appropriate weights are incorporated into the information matrix to reflect the varying precision of observations. The method of weighted least squares is commonly used to deal with heterogenous residual variances [10]. [11] applied weighted D-optimal design to 2 and 3 variables with 2, 3 and 4 blocks and they compared the results with corresponding standard D-optimal designs in terms of the DN-efficiencies. Weighted designs provide improved parameter estimation efficiency under heteroscedastic conditions by emphasizing regions of higher information content [12]. Nevertheless, most existing weighted D-optimal designs still rely on the assumption of independent observations and therefore do not capture the additional layer of complexity introduced by spatial dependence among errors.

To address these limitations, recent advances in spatial statistics have emphasized the role of stochastic modelling frameworks such as Gaussian random fields and the Stochastic Partial Differential Equation (SPDE) approach, implemented via Integrated Nested Laplace Approximation (INLA). These methods provide a computationally efficient way to obtain posterior distributions of spatial processes and their associated uncertainties. In particular, they enable the decomposition of predictive uncertainty into components attributable to inherent variability and model uncertainty. Despite these developments, limited attention has been given to integrating uncertainty decomposition into optimal design criteria, especially in the presence of heteroscedastic and non-normally distributed errors. Most existing approaches either ignore spatially varying uncertainty or treat it in an ad hoc manner, potentially leading to suboptimal allocation of sampling effort.

Recent advances in spatial statistics emphasize the importance of distinguishing between aleatoric uncertainty [13], which re-

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flects inherent random variability in the data-generating process, and epistemic uncertainty, which arises from limited knowledge about the underlying spatial process. While aleatoric uncertainty is irreducible, epistemic uncertainty can be reduced through improved sampling strategies. Despite its relevance, epistemic uncertainty is rarely incorporated explicitly into optimal design criteria for spatial regression models.

In many scientific and environmental investigations, data are collected over spatially distributed regions where observations at nearby locations tend to be more similar than those far apart. Such spatial dependence arises naturally in fields such as soil science, agriculture, hydrology, epidemiology, and environmental monitoring. Ignoring this spatial structure may lead to inefficient parameter estimates, misleading inferences, and suboptimal experimental designs. Consequently, there has been increasing interest in developing optimal design strategies that explicitly account for spatial correlation in the modelling process [14, 15]. Spatial regression models provide a natural extension of classical linear models by incorporating a spatial covariance structure into the error term. In such models, the covariance between observations depends on their spatial separation, often described by a parametric variogram or correlation function (e.g., exponential, Gaussian, or Matérn). The inclusion of this spatial dependence modifies the Fisher information matrix and consequently alters the criterion for optimal design selection. A design that is optimal under independence may perform poorly when spatial correlation is present, underscoring the need for spatially informed design criteria.

Despite significant progress in both spatial statistics and optimal design theory, limited attention has been given to the integration of weighted D-optimal design with spatial regression models, especially under heteroscedastic and non-normal error structures. This gap is particularly relevant in environmental and agricultural research, where measurement variability and spatial correlation coexist. There is therefore a strong motivation to extend weighted D-optimal design methodologies to explicitly accommodate spatial dependence and deviations from normality.

The present study develops a Weighted D-Optimal Design framework for Spatial Regression Models with Heteroscedastic errors. The proposed approach generalizes the conventional D-optimal criterion by incorporating a spatial covariance matrix and a variance-dependent weighting scheme, allowing for efficient parameter estimation under complex error structures. The performance of the proposed design is evaluated and compared with conventional D-optimal and spatially naive designs using real spatial data. The weights are constructed from spatial epistemic uncertainty. Using the Integrated Nested Laplace Approximation (INLA) framework coupled with the Stochastic Partial Differential Equation (SPDE) approach, we obtain spatially resolved posterior variances that quantify epistemic uncertainty across the study region [16, 17, 18]. These posterior variances are then incorporated into the D-optimality criterion to guide the selection of informative sampling locations.

The main contributions of this work are threefold. First, we develop a unified framework that integrates heteroscedastic spatial regression and optimal design. Second, we demonstrate how INLA–SPDE posterior variance can be operationalized as epistemic weights in a weighted D-optimal design. Third, we apply the proposed methodology to spatial data from Nigeria, illustrating how uncertainty-aware design leads to more efficient and informative spatial sampling strategies compared with classical D-optimal designs.

2. Material and method

2.1. Spatial regression Model with heteroscedastic rrrors

Let y_{s_i} denote the response observed at spatial location s_i for $i = 1, 2, \cdots, n$. The spatial regression model is specified as

$$y_{s_i} = x_{s_i}^T \beta + u_{s_i} + \varepsilon_{s_i}, \tag{1}$$

where $x(s_i)$ is a vector of observed covariates, β is the corresponding vector of fixed-effect coefficients, and $u(s_i)$ denotes a latent spatial effect capturing structured spatial dependence. The error term $\varepsilon(s_i)$ is assumed to satisfy

$$\varepsilon(s_i) \sim N\big(0,\, \sigma_{s_i}^2\big)\,, \tag{2}$$

allowing the error variance to vary across space. This formulation explicitly accommodates heteroscedasticity, relaxing the constant-variance assumption underlying classical regression and optimal design methods [3]. s is the spatial location; the covariance of the errors is not $\sigma^2 I$ but a spatial covariance:

$$\mathrm{Cov}\,(\varepsilon) = \mathcal{C}(s_i, s_j), \tag{3}$$

and the heteroscedastic variance is $\mathrm{Var}(\varepsilon_{s_i}) = \sigma_{s_i}^2$.

The latent spatial effect $u(s_i)$ is modelled as a Gaussian random field with Matérn covariance structure. Following [16], the Gaussian field is represented as the solution to a stochastic partial differential equation (SPDE), yielding a computationally efficient Gaussian Markov random field approximation defined on a triangulated mesh over the study region.

Bayesian inference for the latent field, fixed effects, and hyperparameters is carried out using the R package with Integrated Nested Laplace Approximation (INLA) framework [18]. INLA provides accurate posterior marginal approximations without reliance on Markov chain Monte Carlo methods, making it well suited for large-scale spatial applications.

2.2. Predictive variance decomposition and weight construction

In spatial regression models, uncertainty in prediction arises from two main sources: aleatoric and epistemic uncertainty. Distinguishing between these components is essential for constructing weights in the proposed weighted D-optimal design.

Let Y_s denote the response at spatial location $s \in \mathcal{D}$. Under the spatial model,

$$Y_s = X_s^T \beta + \omega_s + \varepsilon_s, \tag{4}$$

where $X_s^T \beta$ is the fixed effect component, ω_s is the spatial random field, and $\varepsilon_s \sim N(0, \sigma_\varepsilon^2)$ is the measurement error.

The posterior predictive variance at location s, obtained via INLA-SPDE, can be expressed as

$$\mathrm{Var}(Y_s \mid \mathcal{D}) = E\big[\sigma_\varepsilon^2 \mid \mathcal{D}\big] + \mathrm{Var}\Big(X_s^T \beta + \omega_s \mid \mathcal{D}\Big)\,. \tag{5}$$

Thus, we define the aleatoric variance as

$$V_a^s = E\big[\sigma_\varepsilon^2 \mid \mathcal{D}\big]\,, \tag{6}$$

and epistemic variance as

$$V_e^s = \mathrm{Var}\Big(X_s^T \beta + \omega_s \mid \mathcal{D}\Big)\,. \tag{7}$$

The epistemic component captures uncertainty due to limited data and spatial prediction, while the aleatoric component reflects irreducible noise.

For each candidate design point s_i, we compute

$$V_e^{s_i} = \mathrm{Var}(Y_{s_i}) - E\left[\sigma_\varepsilon^2 \mid \mathcal{D}\right], \tag{8}$$

where $\mathrm{Var}(Y_{s_i})$ is the posterior predictive variance reported by INLA. To incorporate uncertainty, a combined weighting scheme is used in the design criterion:

$$\omega_i = \frac{V_e^{s_i}}{V_a^{s_i} + V_e^{s_i}}. \tag{9}$$

This formulation ensures that locations with high epistemic uncertainty receive larger weights and regions with predominantly aleatoric noise are down-weighted.

Classical D-optimal design seeks to maximize the determinant of the Fisher information matrix,

$$\Phi_D = \det\left(X^T X\right), \tag{10}$$

implicitly assuming homoscedastic and independent errors. To account for spatially varying uncertainty, a diagonal weighting matrix is introduced, with elements derived from normalized posterior variances of the latent spatial field.

The weighted D-optimality criterion is defined as

$$\Phi_{D_w} = \det\left(X^T W X\right), \tag{11}$$

where $W = \mathrm{diag}(\omega_1, \omega_2, \cdots, \omega_n)$ and ω_i are derived from the variance decomposition. This modification prioritizes design points with higher epistemic uncertainty, leading to improved learning of the spatial process. Locations with higher epistemic uncertainty receive greater weight. This criterion prioritizes candidate sampling locations that are expected to yield the greatest reduction in spatial uncertainty.

The generalized Fisher Information Matrix is

$$M(\xi) = X^T \mathcal{C}^{-1} X, \tag{12}$$

which is exactly what a weighted D-optimal design maximizes.

3. Results and discussion

3.1. Fixed Effects Estimates

Table 1: Results of fixed effects for the spatial model.

Variables	Mean	SD	95% Credible Interval
Intercept	-2.9183	18.2592	$(-38.7227,\ 32.8861)$
Age	0.0319	0.0043	$(0.0234,\ 0.0404)$
Sex1	-1.4918	18.2580	$(-37.2940,\ 34.3100)$
Sex2	-1.4264	18.2580	$(-37.2280,\ 34.3750)$
Medu	-0.3096	0.0847	$(-0.4755,\ -0.1432)$
Wealth	-0.2509	0.0697	$(-0.3871,\ -0.1135)$
Hhsize	-0.0783	0.0179	$(-0.1134,\ -0.0430)$
Net	0.0272	0.0624	$(-0.0950,\ 0.1490)$
Residence	0.6370	0.2040	$(0.2359,\ 1.0390)$

Table 1 presents the posterior summaries of the fixed effects obtained from the spatial regression model with heteroscedastic and nonnormally distributed errors. The results show that age has a positive and statistically significant effect on the response variable, with a posterior mean of 0.032 and a 95% credible interval that excludes zero (0.023, 0.040). This indicates a robust increasing relationship between age and the outcome after accounting for spatial dependence and heteroscedasticity. In addition, residence type (residence2) shows a positive and statistically significant effect, implying systematic differences between residential categories even after adjusting for spatial effects.

Several socioeconomic variables exhibit negative associations. Maternal education (medu) shows a negative and significant effect (posterior mean $= -0.310$; 95% credible interval: -0.476 to -0.143), suggesting that higher levels of maternal education are associated with lower values of the response variable. Similarly, household wealth and household size both have negative and statistically meaningful effects, with their respective credible intervals lying entirely below zero, indicating consistent protective or reducing influences.

The effects of sex categories (sex1 and sex2) are characterized by large posterior standard deviations and wide credible intervals spanning zero, suggesting substantial uncertainty in their estimated effects. This variability may be attributable to heteroscedastic noise, limited information in certain subgroups, or spatial confounding. Likewise, the effect of net is not statistically significant, as its credible interval includes zero.

Overall, the fixed effects results demonstrate that the proposed spatial regression framework is capable of identifying meaningful covariate effects under heteroscedasticity and non-normal errors, while appropriately quantifying uncertainty through posterior credible intervals. These estimates form the basis for the subsequent construction of the weighted D-optimal design.

3.2. Spatial Prediction and Uncertainty Maps

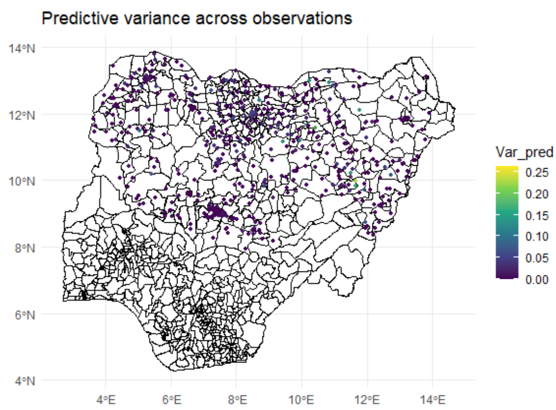

Figure 1: Spatial prediction and uncertainty maps.

Figure 1 displays the spatial distribution of the predictive variance across observation locations. The map reveals clear spatial heterogeneity in uncertainty, reflecting the combined effects of heteroscedastic measurement noise and spatial dependence captured through the SPDE model. Regions with relatively high predictive variance (shown in lighter colors) are predominantly concentrated in parts of the northern and north-eastern areas of the study region, whereas lower variance values are observed in the southern zones where observations are denser.

The spatial pattern indicates that predictive uncertainty is not uniformly distributed, but instead varies systematically with location. Areas exhibiting higher predictive variance are likely associated with sparser sampling coverage and increased variability in the underlying process, while areas with lower variance benefit from greater information content and stronger local support from nearby observations. This behaviour is consistent with expectations under heteroscedastic spatial regression models.

Importantly, the predictive variance surface provides critical guidance for optimal sampling design. Locations characterized by elevated variance represent regions where additional observations are most informative for reducing uncertainty. Consequently, this spatial variance map forms the basis for constructing the weighting scheme used in the weighted D-optimal design, ensuring that sampling effort is preferentially allocated to areas with greater uncertainty rather than uniformly across space.

3.3. Weighted D-optimal design points

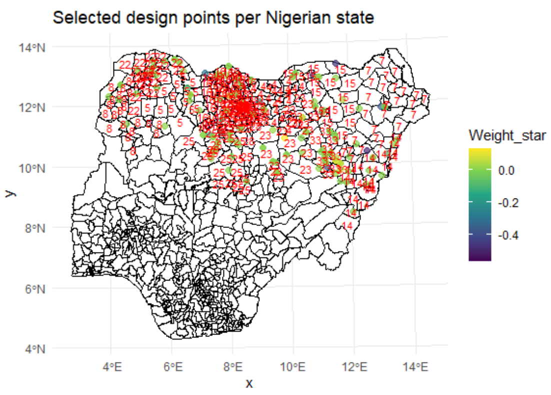

Figure 2: Some selected weighted D-optimal design points.

Figure 2 illustrates the spatial distribution of the selected design points obtained from the weighted D-optimal design across Nigerian states. The selected locations are not uniformly distributed over space; instead, they exhibit clear clustering in regions identified as having higher predictive variance and greater uncertainty in the spatial regression model. The map displays candidate and selected sampling locations overlaid on administrative boundaries of Nigeria. Red points indicate the chosen design locations under the weighted D-optimal criterion. The color scale represents the normalized weights (weight_star) derived from epistemic uncertainty, where lighter color indicates higher weights (greater model uncertainty) and darker color indicates lower weights. Regions with higher weights are prioritized in the sampling design due to increased epistemic uncertainty. A substantial concentration of design points is observed in the northern and central parts of the country, particularly in areas that correspond to elevated predictive variance in Figure 1. This indicates that the weighted D-optimal criterion effectively prioritizes regions where additional sampling is expected to yield the greatest information gain. In contrast, fewer design points are allocated to the southern regions, where predictive variance is relatively low and the existing observations provide stronger local support.

The spatial allocation of design points demonstrates the advantage of incorporating weights derived from heteroscedastic and spatial uncertainty into the D-optimality criterion. By emphasizing locations with larger variance, the proposed approach departs from classical unweighted D-optimal designs that tend to favour regions with dense existing data. Instead, the weighted design promotes a more informative and efficient sampling strategy that directly targets uncertainty reduction in spatial prediction. Notably, higher-weight regions are concentrated in northern areas, reflecting greater predictive uncertainty and motivating denser sampling in these locations.

Overall, the selected design points reflect a principled balance between spatial coverage and information efficiency, reinforcing the suitability of weighted D-optimal design for spatial regression models operating under heteroscedasticity and nonnormally distributed errors.

Table 2 presents the ranking and priority scores of candidate design locations derived from the weighted D-optimal design procedure. The ranking is based on a composite weighting scheme that integrates information from the predictive variance, Fisher information contribution, and uncertainty-based weights. Locations with lower rank values (e.g., Rank 1–10) represent the highest-priority sampling points under the proposed design framework.

The top-ranked locations are characterized by relatively high predictive variance and correspondingly large uncertainty weights (Weight-Uncertainty), indicating areas where additional observations are expected to provide substantial gains in information. For instance, the highest-ranked location (Rank 1) exhibits the largest priority score and a comparatively high predictive variance, confirming its importance for reducing spatial uncertainty. Similar patterns are observed across the top-ranked locations, where elevated values of predicted variance and priority consistently align.

The weighting components reveal that both the Fisher-based weight (weight_fisher) and the uncertainty-based weight contribute meaningfully to the final composite weight. While weight_fisher reflects the contribution of each location to parameter estimation efficiency, weight_uncertainty emphasizes regions with higher predictive uncertainty arising from heteroscedasticity and spatial variability. The resulting standardized weights (weight_standard) ensure comparability across locations and form the basis for the final ranking.

Overall, the rank and priority table provide a transparent and quantitative mechanism for identifying optimal sampling locations. The strong agreement between high-ranking locations, elevated predictive variance, and the spatial clustering of selected design points demonstrates the internal consistency of the proposed weighted D-optimal design approach. These results further support the effectiveness of incorporating heteroscedastic and spatial uncertainty into optimal design construction for spatial regression models with nonnormally distributed errors.

This study develops and applies a weighted D-optimal design framework for spatial regression models in the presence of heteroscedasticity and nonnormally distributed errors. By integrating spatial modelling via the INLA–SPDE approach with a variance-informed weighting scheme, the proposed method addresses key limitations of classical optimal design techniques when applied to realistic spatial data.

A central finding of this work is that accounting for heteroscedasticity and spatially varying uncertainty substantially alters the allocation of optimal design points. Unlike unweighted D-optimal designs, which tend to favour regions with dense observations and lower variability, the weighted approach reallocates sampling effort toward locations exhibiting higher predictive variance. This ensures that additional data collection is targeted at regions where uncertainty is greatest and where the potential information gain is highest.

The results further demonstrate that nonnormally distributed errors can be accommodated within the spatial regression framework without compromising interpretability or design efficiency. The posterior summaries of the fixed effects show that meaningful covariate relationships can still be identified, while the predictive variance surface captures both measurement-level heteroscedasticity and uncertainty arising from spatial dependence. This dual consideration is particularly important in applied settings, where assumptions of constant variance and normality are often violated.

The ranking and priority analysis highlight the practical value

Table 2: Ranking and Priority Analysis.

S/N	Rank	Pred. Variance	Wt-Uncertainty	Wt-Fisher	Weight	Wt-Standard	Priority
1	0.127659	0.137699	0.244536	0.827309	0.018961	0.154306	6352
2	0.121770	0.148397	0.235325	0.811781	0.022022	0.150003	6284
3	0.116001	0.100914	0.232470	0.808058	0.010184	0.143555	6126
4	0.116001	0.100914	0.232470	0.808058	0.010184	0.143555	6132
5	0.116001	0.100914	0.232470	0.808058	0.010184	0.143555	6146
6	0.112923	0.121150	0.225466	0.800019	0.014677	0.141151	6096
7	0.111193	0.119973	0.222841	0.797302	0.014393	0.139462	6100
8	0.109696	0.118768	0.220555	0.795039	0.014106	0.137975	6098
9	0.108018	0.127087	0.216711	0.791418	0.016151	0.136487	7457
10	0.107658	0.135673	0.214914	0.789795	0.018407	0.136311	6280

of the proposed design strategy. By combining Fisher information–based measures with uncertainty-driven weights, the resulting priority scores provide a transparent and quantitative basis for selecting sampling locations. The strong alignment between high-ranked locations, elevated predictive variance, and the spatial clustering of selected design points confirms the internal coherence of the method and its suitability for guiding data collection decisions.

From an applied perspective, the proposed weighted D-optimal design offers a flexible and robust tool for spatial sampling in complex environments, such as large and heterogeneous regions. By explicitly incorporating heteroscedasticity, spatial dependence, and non-normal error structures, the method better reflects the realities of environmental, demographic, and socio-economic data. This makes it particularly useful for large-scale surveys and monitoring studies where efficient allocation of limited sampling resources is critical.

Despite its advantages, this study has some limitations. The weighting scheme relies on model-based estimates of predictive variance, which may be sensitive to prior specification and model assumptions. In addition, the analysis focuses on a single spatial scale, and extensions to multiscale or spatio-temporal designs warrant further investigation. Future research could also explore alternative optimality criteria, such as A- or I-optimality, and assess their performance under similar heteroscedastic and non-normal settings. Overall, this work contributes to the growing literature on optimal experimental design for spatial models by demonstrating that weighted D-optimal design provides a principled and effective approach when classical assumptions are violated. The proposed framework bridges spatial statistics and optimal design theory and offers a practical pathway for improving sampling efficiency in complex spatial regression problems.

4. Conclusion

This study proposed and implemented a weighted D-optimal design framework for spatial regression models operating under heteroscedasticity and nonnormally distributed errors. By integrating spatial modelling through the INLA–SPDE approach with a variance-informed weighting scheme, the methodology extends classical optimal design theory to settings where key modelling assumptions—such as constant variance—are violated. The results demonstrate that incorporating spatially varying predictive variance into the D-optimality criterion leads to a fundamentally different and more informative allocation of design points. Rather than concentrating sampling effort in regions with dense observations and low uncertainty, the weighted design prioritizes locations characterized by elevated predictive variance, thereby targeting areas where additional data collection is expected to yield the greatest reduction in uncertainty. This behaviour was consistently reflected in the predictive variance maps, the spatial distribution of selected design points, and the ranking and priority analysis. The proposed framework also showed that meaningful fixed-effect relationships can be reliably estimated even in the presence of heteroscedastic errors, while spatial dependence is appropriately accounted for through the latent Gaussian field. The decomposition of uncertainty into aleatoric and epistemic components provides a clear conceptual basis for design weighting and reinforces the importance of focusing sampling resources on reducible, model-based uncertainty. Overall, this work contributes to the literature on spatial optimal experimental design by offering a principled and flexible approach that bridges spatial Bayesian modelling and weighted D-optimal design. The methodology is particularly relevant for large-scale spatial studies where resources are limited and uncertainty is unevenly distributed across space. Future research may extend this framework to spatio-temporal settings, alternative optimality criteria, or adaptive design strategies that update weights sequentially as new data become available. Survey designers are encouraged to consider weighted designs in settings where spatial heterogeneity in uncertainty is expected.

Acknowledgement

There is no support from any individual or organization.

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