Flexible Basis Representations for Modeling High-Dimensional Hierarchical Spatial Data

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Abstract

Nonstationary and non-Gaussian spatial data are prevalent across many fields (e.g., counts of animal species, disease incidences in susceptible regions, and remotely-sensed satellite imagery). Due to modern data collection methods, the size of these datasets have grown considerably. Spatial generalized linear mixed models (SGLMMs) are a flexible class of models used to model nonstationary and non-Gaussian datasets. Despite their utility, SGLMMs can be computationally prohibitive for even moderately large datasets. To circumvent this issue, past studies have embedded nested radial basis functions into the SGLMM. However, two crucial specifications (knot placement and bandwidth parameters), which directly affect model performance, are typically fixed prior to model-fitting. We propose a novel approach to model large nonstationary and non-Gaussian spatial datasets using adaptive radial basis functions. Our approach: (1) partitions the spatial domain into subregions; (2) employs reversible-jump Markov chain Monte Carlo (RJMCMC) to infer the number and location of the knots within each partition; and (3) models the latent spatial surface using partition-varying and adaptive basis functions. Through an extensive simulation study, we show that our approach provides more accurate predictions than competing methods while preserving computational efficiency. We demonstrate our approach on two environmental datasets - incidences of plant species and counts of bird species in the United States.

Keywords: Bayesian Hierarchical Spatial Models; Non-Gaussian Spatial Models; Nonstationary Spatial Processes; Reversible-Jump MCMC; Spatial Basis Functions; Spatial Partitioning; Spatial Statistics.
1 Introduction

Discrete non-Gaussian spatial datasets (counts, binary responses, extreme values) are prevalent across a number of disciplines, such as ecology (Guan and Haran, 2018), public health (Ejigu et al., 2020), and atmospheric sciences (Sengupta et al., 2016; Heaton, Christensen and Terres, 2017). Modeling such datasets can be important for scientific applications, particularly in making predictions at unobserved locations and assessing prediction uncertainty. However, traditional regression models, which assume independent and identically distributed errors, may be inappropriate for these data (Schabenberger and Gotway, 2005; Banerjee, Carlin and Gelfand, 2003; Cressie, 1993) as they neglect spatial autocorrelation.

Spatial generalized linear mixed models (SGLMMs) (Diggle, Tawn and Moyeed, 1998; Haran, 2011) are a flexible class of spatial models that extend to non-Gaussian observations. Within SGLMMs, the spatial dependence is captured via location-specific random effects that are modeled as a latent Gaussian process (GP). Despite their flexibility, standard implementation of SGLMMs incurs a computational cost that is cubic in the data size, which can be computationally prohibitive for modeling modern spatial datasets. Additionally, the high-dimensional spatial random effects are typically highly correlated; thereby resulting in slow mixing Markov chain Monte Carlo (MCMC) algorithms (Haran, Hodges and Carlin, 2003).

Computationally-efficient approaches have been developed to reduce the dimensionality of the spatial random effects, speed up large matrix operations, or both. These include low-
rank approximations and basis representations (Cressie and Johannesson, 2006; Banerjee et al., 2008; Finley et al., 2009), sparse covariance and precision matrices (Furrer, Genton and Nychka, 2006; Datta et al., 2016; Vecchia, 1988; Zilber and Katzfuss, 2021), spatial partial differential equations (Lindgren, Rue and Lindström, 2011), spatial partitioning (Lee and Park, 2023; Heaton, Christensen and Terres, 2017), and more. Two prominent examples include nearest-neighbor Gaussian processes (NNGP) (Datta et al., 2016) and Integrated nested Laplace approximations (INLA) (Lindgren and Rue, 2015). NNGP approximates the GP using a sparse Cholesky factorization of the true precision matrix. Sparsity is induced by directed acyclical graphs that connect neighboring locations. While NNGP preserves the flexibility and interpretability of GP models, the SGLMM framework requires the inference of all $N$ spatial random effects. This can be prohibitive for large discrete non-Gaussian spatial datasets. Moreover, the spNNGP (Finley et al., 2009) package currently accommodates binary and Gaussian spatial data only; hence, it cannot directly model count observations (Dovers et al., 2023). INLA employs stochastic partial differential equations to provide fast and accurate numerical approximations of posterior distributions. INLA provides approximations of the marginal posterior distribution, rather than the joint distribution; hence, it may potentially underestimate the uncertainty in estimation and predictions (Ferkingstad and Rue, 2015).

In this manuscript, we focus on basis representation approaches which approximate the latent spatial process using a linear combination of spatial radial basis functions (e.g., bisquare, Wendland basis, and thin-plate-splines) (Sengupta and Cressie, 2013; Katzfuss, 2017; Cressie and Johannesson, 2008; Lee and Park, 2023). Two key components of radial
basis functions are the knots (centers of the basis functions) and the associated bandwidth (or smoothing) parameters. The bandwidth defines the “spread” of the radial basis function and also tunes the tradeoff between the goodness-of-fit and the roughness of the resulting basis approximation (Kato and Shiohama, 2009). Poorly specified knots and bandwidths can result in inaccurate representations of the latent spatial surface (Sheather and Jones, 1991). Since specifying these parameters can be challenging, past studies (Cressie and Johannesson, 2008; Katzfuss and Cressie, 2011, 2012) have typically fixed them prior to model fitting. As a result, the spatial basis functions are constructed without any feedback or influence from the observed data.

To address these challenges, we propose a computationally efficient, yet flexible approach for modeling nonstationary non-Gaussian spatial data. Our method addresses the two limitations (knot placement and bandwidth specification) by allowing the spatial radial basis functions to adapt to the observations. Our method partitions the spatial domain into disjoint subregions and allows the bandwidths to vary across each subregion. For each partition, we employ a reversible jump Markov chain Monte Carlo (RJMCMC) algorithm (Green, 1995) to infer the number and placement of knots. The proposed approach allows for more flexibility than using fixed basis functions and scales well to large datasets.

The outline of the remainder of the paper is as follows. In Section 2, we introduce SGLMMs and basis-expansion SGLMMs and discuss important modeling and computational challenges. In Section 3, we propose our approach (Adapt-BaSeS) and provide implementation details. We demonstrate our approach via a simulation study in Section 4 and real-world applications in Section 5. Concluding remarks and directions for future
2 Spatial Generalized Linear Mixed Models

SGLMMs (Diggle, Tawn and Moyeed, 1998) are a class of flexible models for modeling spatially-dependent non-Gaussian data. These models are a special case of generalized linear mixed models, where the random effects exhibit spatial correlation. Conditioned on the random effects, the observations are assumed to be independent and follow a location-specific probability distribution. SGLMMs have been used extensively in the literature to model non-Gaussian spatially-correlated data (Hughes and Haran, 2013; Zilber and Katzfuss, 2021; Zhang, 2002).

Let \( \{ Z(s) : s \in D \} \) denote the non-Gaussian observations on the spatial domain \( D \subset \mathbb{R}^d, d \in \mathbb{N} \). At \( N \) locations, we have observations \( Z = (Z(s_1), \ldots, Z(s_N))^\top \), where \( Z(\cdot) \sim F(\cdot) \) for some distribution \( F \). The conditional mean is modeled as \( g(\mathbb{E}[Z(s_i)]) := \eta(s_i) \) for \( i = 1, \ldots, N \), where \( g(\cdot) \) is a link function and \( \eta(\cdot) \) is the linear predictor. For location \( s_i \), the linear predictor is defined as

\[
\eta(s_i) := X(s_i)^\top \beta + W(s_i),
\]

where \( X(s_i) \) is a vector of covariates with regression coefficients \( \beta \), and \( W(s_i) \) represents the spatially-correlated random effect, often modeled as a zero-mean GP \( W(\cdot) \sim \mathcal{GP}(0, K) \), where \( K \) is a covariance function with marginal variance \( \sigma^2 \) and a correlation function \( C \), i.e., \( K(s_1, s_2) = \sigma^2 C(s_1, s_2), s_1, s_2 \in D \). The correlation function \( C : (D \times D) \to [-1, 1] \) is assumed to be known up to some parameters \( \theta \). A commonly used class of covariance
functions, which assumes stationarity and isotropy, is the Matérn class (Williams and Rasmussen, 2006), defined as,

$$\mathcal{M}_\nu(h) = \frac{2^{1-\nu}}{\Gamma(\nu)} \left( \frac{\sqrt{2\nu d}}{\rho} \right)^\nu K_\nu \left( \frac{\sqrt{2\nu d}}{\rho} \right), \quad \nu, \rho > 0,$$

where $d = ||s_i - s_j||$ denotes the Euclidean distance between pairs of locations, $\rho$ is the spatial range parameter, $\nu$ is the smoothness parameter, $\Gamma(\cdot)$ is the gamma function, and $K_\nu(\cdot)$ is the modified Bessel function of the second kind of order $\nu > 0$.

For a finite vector of locations $\mathcal{S} = (s_1, \ldots, s_N)$, the spatial random effects $W = (W(s_1), \ldots, W(s_N))^\top$ follows a multivariate normal distribution $W \mid \sigma^2, \theta \sim \mathcal{N}(0, K)$, where $K$ is an $N \times N$ covariance matrix whose entries are $K(s_i, s_j)$. Let $\eta := (\eta(s_1), \ldots, \eta(s_N))^\top$ denote the vector of transformed site-specific conditional means, such that each observation $Z(s_i)$ is conditionally independent given $\eta(s_i)$. Let $X$ be the covariate matrix of stacked $X(s_i)$ vectors. Then under the Bayesian hierarchical framework, SGLMMs are structured as follows:

**Data Model:**

$$Z(s_i) \mid \eta(s_i) \sim F(\eta(s_i))$$

$$g(\mathbb{E}[Z \mid \beta, W]) := \eta = X\beta + W$$

(1)

**Process Model:**

$$W \mid \sigma^2, \theta \sim \mathcal{N}(0, K)$$

**Parameter Model:**

$$\sigma^2 \sim p(\sigma^2), \theta \sim p(\theta),$$

with prior distributions $p(\sigma^2)$ and $p(\theta)$ specified by the practitioner.

Despite their flexibility, SGLMMs are subject to a myriad of limitations. In many cases, SGLMMs assume a second-order stationary and isotropic GP for the spatial random effects $W$, where the covariance function depends solely on pairwise Euclidean distances. This assumption can be overly restrictive or unrealistic (Risser, 2016), especially for large
and heterogeneous spatial domains (Katzfuss, 2013). Furthermore, evaluating the density $W \sim N(0, K)$ in SGLMMs requires $O\left(\frac{1}{3}N^3\right)$ operations and $O(N^2)$ memory, which can be computationally prohibitive for large datasets. SGLMMs are often overparameterized, since all $N$ highly-correlated random effects must be inferred. This can result in slow-mixing Markov chains in the MCMC algorithm (Haran, 2011).

### 2.1 Basis Function Representations

Basis representation approaches have been widely used for modeling complex spatial processes due to their flexibility and computational efficiency (Cressie and Wikle, 2011; Cressie, Sainsbury-Dale and Zammit-Mangion, 2022; Bradley, Cressie and Shi, 2011). These approaches represent the spatial process $W(\cdot)$ as a linear combination of $M$ basis functions $\Phi(s) = (\Phi_1(s), \ldots, \Phi_M(s))^\top$ with corresponding basis coefficients $\delta = (\delta_1, \ldots, \delta_M)^\top$ such that,

$$W(s) \approx \sum_{m=1}^{M} \Phi_m(s)\delta_m = \Phi(s)^\top\delta, \quad s \in D,$$

where $\delta \mid \Sigma_\delta \sim \mathcal{N}_M(0, \Sigma_\delta)$. Through dimension-reduction, we set $M \ll N$ to reduce the associated computational costs. Let $\Phi$ be an $N \times M$ matrix with columns indicating the basis functions and rows indicating the locations. Then by construction of (2), the approximated covariance matrix of $W$ is $\Phi\Sigma_\delta\Phi^\top$. This does not solely depend on the distance between locations and is hence nonstationary. Furthermore, evaluating the density $\delta \mid \Sigma_\delta \sim \mathcal{N}_M(0, \Sigma_\delta)$ only involves matrix operations on matrices of size $M \times M$, which requires $O\left(\frac{1}{3}M^3\right)$ operations and $O(M^2)$ storage.

Different types of basis functions have been used, including radial basis functions, such
as multi-resolution basis functions (Sengupta et al., 2016; Cressie and Johannesson, 2008; Katzfuss and Cressie, 2011, 2012), Fourier basis functions (Xu, Wikle and Fox, 2005), eigenfunctions (Holland et al., 1999), and the predictive-process approach (Banerjee et al., 2008). Multi-resolution basis function approaches employ multiple layers of nested basis functions with varying resolutions to capture spatial structures from very fine to very large scale. For example, Sengupta et al. (2016) utilize a “quad-tree” structure comprised of low- and high-resolution bisquare basis functions. Fourier basis functions are comprised of sine and cosine curves to represent the spatial variability (Royle and Wikle, 2005) and are particularly useful when dealing with periodic or cyclical spatial patterns. The eigenfunction approach employs eigenvectors of the empirical covariance matrix as basis functions to capture the major modes of spatial variation present in the data. The predictive-process approach considers both $\delta$ and $W$ to be parameterized according to a “parent process,” for which a parametric covariance model is chosen. Given the so-called “parent process” $W(\cdot)$, the predictive process is defined as, $W^*(\cdot) = \mathbb{E}(W(\cdot) \mid W(u_1), \ldots, W(u_M))$, where $\mathcal{K} = \{u_1, \ldots, u_M\}$ is a set of knots. Conditional on $\sigma^2$, $\theta$, and $\mathcal{K}$, the covariance function $K(s_1, s_2)$ can then be approximated by $\Phi(s_1)^\top \Sigma^{-1} \Phi(s_2)$, where $\Phi(s) = (K(s, u_1), \ldots, K(s, u_M))^\top$ for $s \in \mathcal{D}$ and $\Sigma = (K(u_i, u_j))_{i,j=1,\ldots,M}$.

In this manuscript, we focus on radial basis functions (e.g. Gaussian, bisquare, thin-plate-splines), which are usually parameterized by knots and bandwidth parameters. Despite their flexibility and low costs, radial basis functions require the user to pre-specify the: (1) number of knots; (2) knot locations; and (3) bandwidth parameters. For example, Sengupta et al. (2016) fix the bandwidths and knots associated with each resolution of
nested layers of bisquare basis functions. Similarly, Nychka et al. (2015) employ fixed compactly supported radial basis functions to capture multiple scales of spatial dependency. This pre-specification can potentially constrain the hierarchical spatial model to a fixed set of basis functions without any feedback or influence from the observed data. Given the challenge of appropriately specifying the number and placement of knots in spatial data, it is crucial to employ adaptive methods for knot selection.

3 Adapt-BaSeS: Adaptive Basis Selection and Specification

Our proposed method, Adaptive Basis Selection and Specification (Adapt-BaSeS), is a flexible yet computationally efficient method for modeling nonstationary and non-Gaussian spatial data. The utility of Adapt-BaSeS comes from the adaptive tuning of radial basis functions, specifically the number and placement of knots as well as the bandwidths. Let $\mathcal{K} = (\mathbf{u}_1, \ldots, \mathbf{u}_M)$ be a vector of $M$ knots over the spatial domain $\mathcal{D}$ and let $\epsilon > 0$ be the bandwidth parameter. Then the Gaussian radial basis function corresponding to knot $\mathbf{u}_m$ is defined as:

$$\Phi_m(s) = \exp(-\epsilon ||s - \mathbf{u}_m||^2)).$$ (3)

The choice of $\epsilon$ is crucial, as large values can lead to overfitting (Chaudhuri et al., 2017) and sharp localized peaks, while small values can oversmooth the latent spatial surface. Improper specification of the bandwidth parameters can lead to inaccurate predictions and improper approximations of the latent spatial surfaces (Sheather and Jones, 1991;
Adapt-BaSeS addresses these challenges by embedding an adaptive basis selection and specification mechanism within the SGLMM framework. First, we partition the spatial domain into disjoint subregions using an agglomerative clustering algorithm (Heaton, Christensen and Terres, 2017). Next, we fit a hierarchical spatial model with partition-specific and adaptive radial basis functions to model the observed data. Our algorithmic approach employs a RJMCMC algorithm (Green, 1995) to select key features of the radial basis functions (e.g., knot locations, total number of bases, and bandwidths) with clear feedback from the data. To the best of our knowledge, this study is the first to allow for both adaptive bandwidths and knots for basis-representation SGLMMs.

3.1 Spatial Partitioning

Let \( Z = (Z(s_1), \ldots, Z(s_N))^\top \) denote observations at locations \( s_i \in \mathcal{D} \). We use an agglomerative clustering approach (Heaton, Christensen and Terres, 2017) to partition the spatial locations into \( K \) disjoint subregions \( \{\mathcal{D}_k\}_{k=1}^K \) such that \( \bigcup_{k=1}^K \mathcal{D}_k = \mathcal{D} \) and \( \mathcal{D}_{k_i} \cap \mathcal{D}_{k_j} = \emptyset \) for all \( k_i \neq k_j \). To accomplish this, the dissimilarity between \( Z(s_i) \) and \( Z(s_j) \) is:

\[
d_{ij} = \min_{\mathcal{D}_k} \{d(Z(s_i), Z(s_j)) \mid s_i, s_j \in \mathcal{D}_k \} = \frac{|Z(s_i) - Z(s_j)|}{||s_i - s_j||},
\]

where \( ||s_i - s_j|| \) is the Euclidean distance between the points \( s_i \) and \( s_j \). An agglomerative clustering approach is then used, where \( K = N \) clusters are initialized such that each observation starts as its own cluster. Clusters are then linked together based on the smallest dissimilarity and spatial contiguity is enforced by only clustering Voronoi neighbors. This process is then repeated until the desired \( K \) partitions is reached. We then let \( Z_k = \)
\{Z(s_i) : s_i \in D_k \subset D\} for i = 1, \ldots, N_k denote the N_k observations belonging to the k-th partition, such that N = \sum_{k=1}^{K} N_k. Alternatively, dissimilarity can be defined using the residuals from a regression with non-spatial errors (Heaton, Christensen and Terres, 2017). For non-Gaussian data, we find that this alternative approach outperforms clustering based on the observations themselves.

Figure 1: Illustration of spatial partitioning. (a) Spatial observations. (b) Observations partitioned into 4 subregions; different colors indicate disjoint partitions. (c) Case for 8 partitions. (d) Case for 16 partitions.

### 3.2 Bayesian Hierarchical Model

For partition k = 1, \ldots, K, the conditional mean \( \mathbb{E}[Z_k | \beta_k, \delta_k, \epsilon_k, K_k, \gamma] \) is modeled as,

\[
g(\mathbb{E}[Z_k | \beta_k, \delta_k, \epsilon_k, K_k, \gamma]) := \eta_k = X_k \beta_k + \Phi_k(\epsilon_k, K_k) \delta_k + H_k \gamma, \tag{4} \]

where
where $X_k$ is an $N_k \times P$ covariate matrix with corresponding regression coefficients $eta_k = (\beta_{k1}, \ldots, \beta_{kP})^\top$, $K_k = (u_{k,1}, \ldots, u_{k,r_k})$ is a vector of partition-specific knots, $\epsilon_k$ is a partition-specific bandwidth parameter, $\Phi_k(\epsilon_k, K_k)$ is an $N_k \times r_k$ adaptive radial basis function matrix with basis coefficients $\delta_k = (\delta_{k1}, \ldots, \delta_{kr_k})^\top$, and $H_k$ is a basis function matrix with global coefficients $\gamma = (\gamma_1, \ldots, \gamma_G)^\top$.

For the combined vector of observations $Z = (Z_1^\top, \ldots, Z_K^\top)^\top$, (4) implies that,

$$g(\mathbb{E}[Z \mid \beta, \delta, \epsilon, K, \gamma]) := \eta = X\beta + \Phi(\epsilon, K)\delta + H\gamma,$$

where $X$ is a block-diagonal matrix with matrices $X_k$ on the main diagonal, $\beta = (\beta_1^\top, \ldots, \beta_K^\top)^\top$, $\epsilon = (\epsilon_1, \ldots, \epsilon_K)$, $\Phi(\epsilon, K)$ is a block-diagonal matrix with matrices $\Phi_k(\epsilon_k, K_k)$ on the main diagonal, $\delta = (\delta_1^\top, \ldots, \delta_K^\top)^\top$, and $H$ is an $N \times G$ matrix stacking the individual $H_k$ matrices. The parameter $\epsilon_k$ determines the smoothness of the basis functions associated with the $k$-th partition. By allowing $\epsilon_k$ to vary across partitions, our approach can capture the smooth and rough surfaces of the heterogeneous spatial domain.

Since the basis functions (3) are infinitely differentiable, it is possible that the surfaces resulting from the basis expansions will be infinitely smooth. However, we find that letting $\epsilon_k$ be sufficiently large obviates this challenge in practical applications. In many applications, it may be desirable to have global regression coefficients such that $\beta = \beta_1 = \cdots = \beta_K$. In that setting, $X$ would be an $N \times P$ matrix stacking the $X_k$
matrices. Using Adapt-BaSeS, the hierarchical spatial model is:

**Data Model:**
\[ Z(s_i) \mid \eta(s_i) \sim F(\eta(s_i)) \]
\[ g(\mathbb{E}[Z \mid \beta, \delta, \epsilon, K, \gamma]) := \eta = X\beta + \Phi(\epsilon, K)\delta + H\gamma \]

**Process Model:**
\[ \delta_k \mid \tau_k^2 \sim N(0, \tau_k^2 I) \]
\[ \gamma \mid \rho^2 \sim N(0, \rho^2 I) \]

**Parameter Model:**
\[ \beta_k \sim p(\beta_k), \epsilon_k \sim p(\epsilon_k), \tau_k^2 \sim p(\tau_k^2), \]
\[ K_k \sim p(K_k), \rho^2 \sim p(\rho^2), \]

where \( I \) denotes the identity matrix. We complete the hierarchical spatial model by specifying the prior distributions for the model parameters \( \beta_k, \epsilon_k, \tau_k^2, \rho^2 \), and \( K_k \). We can reduce computational costs by limiting the number of basis functions \( r_k \) within each partition to be small and by specifying the covariance matrices \( \Sigma_{\delta_k} \) and \( \Sigma_{\gamma} \) to be diagonal (Lee and Park, 2023; Higdon, 1998; Lindgren, Rue and Lindström, 2011; Nychka et al., 2015). It can also be possible to introduce a covariance structure for the basis coefficients, such as an exponential covariance function (Heaton et al., 2019). However, this would result in additional computational overhead. Conditional on \( \gamma \), the parameters \( \beta_k, K_k, \delta_k, \epsilon_k, \) and \( \tau_k^2 \) can be estimated independently for each partition. Hence, the MCMC updates of these parameters can be done in parallel to facilitate computational efficiency.

### 3.3 The Reversible-Jump MCMC Algorithm

We propose a RJMCMC algorithm (Algorithm 1) to select the number and placement of knots within each partition. For a given partition \( k \), we take the number of knots \( r_k \) to be random, from some countable set \( S_k = \{0, \ldots, R_k\} \), where \( R_k \) is the number of
candidate knots in partition $k$. Let $M_{r_k}$ denote the model with exactly $r_k$ knots and let $K_k(r_k) = \{u_{k,1}, \ldots, u_{k,r_k}\}$ denote the knots. We generate samples from the joint posterior of $(r_k, K_k(r_k))$. To account for the varying dimensionality, we must develop appropriate reversible jump moves. For this problem, possible transitions are: (1) add a knot (birth step), (2) delete a knot (death step), and (3) move a knot. These independent move types are randomly chosen with probability $b_{r_k}$ for the move $r_k$ to $r_k + 1$ (birth step), $d_{r_k}$ for the move $r_k$ to $r_k - 1$ (death step), and $\eta_{r_k}$ for the move step. These probabilities must satisfy $b_{r_k} + d_{r_k} + \eta_{r_k} = 1$. For this choice, we define $b_0 = d_{R_k} = 1$ and $b_{r_k} = d_{r_k} = \eta_{r_k} = 1/3$ otherwise.

### 3.3.1 Prior Specifications

We specify a truncated Poisson prior distribution for $r_k$, such that

$$p(r_k) \propto \lambda^{r_k} \exp(-\lambda) \frac{r_k!}{r_k!} 1_{\{0, \ldots, R_k\}}(r_k).$$

The choice of $\lambda$ is a compromise between model flexibility and model parsimony. A small value of $\lambda$ reflects a strong incidence of smoothness whereas a large value may cause the model to fit the data too closely. The choice of $\lambda$ will be discussed later.

For a given $r_k$, the knots are taken to be randomly uniformly selected with state space the candidate knots $R_k = \{u_{k,1}, \ldots, u_{k,R_k}\}$, where $u_{k,1}, \ldots, u_{k,R_k}$ are distributed equidistantly over subregion $D_k$. Given $r_k$, the prior distribution for $K_k(r_k) = \{u_{k,1}, \ldots, u_{k,r_k}\}$ is then given by

$$p(K_k(r_k) \mid r_k) = \left(\frac{R_k}{r_k}\right)^{-1} r_k!(R_k - r_k)! \frac{1}{R_k!}. $$

A commonly used prior for regression coefficients of a generalized linear model is the
multivariate normal distribution \( \delta_k \mid r_k \sim \mathcal{N}(0, \Sigma_{\delta_k}) \) (Gamerman, 1997). Following Biller (2000), we assume the basis coefficients \( \delta_k \) are uncorrelated, i.e., \( \Sigma_{\delta_k} = \tau_k^2 I \).

### 3.3.2 Algorithm

At each step of the RJMCMC algorithm, we propose one of three modifications to the current set of \( r_k \) knots for each partition \( k \):

1. **Add a knot (birth step):** Draw a new knot \( u_{k,r_k+1} \) uniformly with probability \( 1/(R_k - r_k) \) from the set of the \( R_k - r_k \) vacant knots. Let \( K^*_k = K_k \cup \{u_{k,r_k+1}\} \) be the proposed set of knots, which now has size \( r^*_k = r_k + 1 \).

2. **Delete a knot (death step):** Select a knot \( u_{k,J} \) uniformly at random from one of the \( r_k \) current knots, so it is drawn with probability \( 1/r_k \). Then set \( K^*_k = K_k \setminus \{u_{k,J}\} \) and \( r^*_k = r_k - 1 \).

3. **Move a knot (move step):** Select a knot \( u_{k,J} \) uniformly at random to be deleted, and then select a new location \( u_{k,r_k+1} \) from the vacant knots (i.e., where to move the old knot). This results in \( K^*_k = \{u_{k,r_k+1}\} \cup K_k \setminus \{u_{k,J}\} \) and \( r^*_k = r_k \).

Note that when we propose to add a knot \( u_{k,r_k+1} \), a corresponding basis coefficient \( \delta^*_{k,r_k+1} \) will also need to be proposed. Similarly, if we propose to delete a knot \( u_{k,J} \), the current basis coefficient \( \delta_{k,J} \) will be set to 0. If we propose to move a knot, we will propose changing the current basis coefficient from \( \delta_{k,J} \) to \( \delta^*_{k,r_k+1} \). Complete details of the RJMCMC algorithm can be seen in Algorithm 1. Proposition 1 asserts that a sufficient choice for the acceptance probability is given by (6); hence fulfilling the detailed balance condition.
Proposition 1. The detailed balance condition is satisfied by setting the acceptance probability to be \( \min\{1, \alpha\} \), where

\[
\alpha = \frac{L(Z_k \mid \mathcal{K}^*_k, \delta^*_k) \pi(\mathcal{K}^*_k, \delta^*_k) Q(\mathcal{K}^*_k, \mathcal{K}_k)}{L(Z_k \mid \mathcal{K}_k, \delta^*_k) \pi(\mathcal{K}_k, \delta^*_k) Q(\mathcal{K}_k, \mathcal{K}^*_k)},
\]

and the proposal ratio is given by,

\[
Q(\mathcal{K}^*_k, \mathcal{K}_k) \quad Q(\mathcal{K}_k, \mathcal{K}^*_k) = \begin{cases} 
\frac{R_k - r_k}{r_k + 1} \times \mathcal{N}(\delta^*_{r_k, r_k + 1}; 0, \sigma^2), & r_k^* = r_k + 1 \\
\frac{r_k}{R_k - r_k + 1} \times \mathcal{N}(\delta^*_k, J; 0, \sigma^2), & r_k^* = r_k - 1 \\
\frac{\mathcal{N}(\delta^*_k, J; 0, \sigma^2)}{\mathcal{N}(\delta^*_{r_k, r_k + 1}; 0, \sigma^2)}; & r_k^* = r_k,
\end{cases}
\]

and the prior ratio is given by,

\[
\pi(\mathcal{K}^*_k, \delta^*_k) \quad \pi(\mathcal{K}_k, \delta^*_k) = \begin{cases} 
p\left(\frac{r_k + 1}{r_k - r_k + 1}\right) \times \mathcal{N}(\delta^*_{r_k, r_k + 1}; 0, \tau^2_k), & r_k^* = r_k + 1 \\
p\left(\frac{r_k - 1}{r_k}\right) \times \mathcal{N}(\delta^*_{r_k, r_k + 1}; 0, \tau^2_k), & r_k^* = r_k - 1 \\
\frac{\mathcal{N}(\delta^*_k, J; 0, \tau^2_k)}{\mathcal{N}(\delta^*_{r_k, r_k + 1}; 0, \sigma^2)}; & r_k^* = r_k,
\end{cases}
\]

where \( \sigma^2 \) is the proposal variance for the basis coefficients. For the special cases where \( r_k = 0 \) or \( r_k = R_k \), the respective proposal ratios can be shown to be \( R_k/\left(3 \mathcal{N}(\delta^*_{r_k, r_k + 1}; 0, \sigma^2)\right) \) and \((R_k \mathcal{N}(\delta^*_k, J; 0, \sigma^2))/3\).

Proof: See Supplement S5.

3.4 Prediction

Let \( N_O \) denote the number of observations used for model-fitting and let \( N_P \) denote the number of observations used for validation. Upon fitting the hierarchical spatial model on the vector of observed locations \( S_O = (s_1, \ldots, s_{N_O}) \), a natural extension is to infer the linear predictor \( \eta(\cdot) \) at a vector of prediction locations \( S_P = (s_1, \ldots, s_{N_P}) \). Letting \( s^* \in S_P \),
Algorithm 1 RJMCMC Algorithm

1: for $i \leftarrow 1$ to $B$ do
2: Metropolis-Hastings updates for $\beta_k$, $\epsilon_k$, and $\gamma$
3: Gibbs updates for $\tau^2_k$ and $\rho^2$
4: for Partition $k \leftarrow 1$ to $K$ do
5: Propose to: (1) add; (2) remove; or (3) move a knot with equal probability $p$
6: Denote proposed vector of knots and coefficients as $K^*_k$ and $\delta^*_k$, respectively
7: Generate $U \sim \text{Unif}(0, 1)$
8: Accept $K^*_k$ and $\delta^*_k$ if $U < \min\{1, \alpha\}$ where $\alpha$ is defined in (6).
9: end for
10: end for

be an arbitrary unobserved location residing in partition $k$, we write:

$$
\eta(s^*) = X_k(s^*)^\top \beta_k + \Phi_k(s^*; \epsilon_k, K^*_k)^\top \delta_k + H_k(s^*)^\top \gamma,
$$

where $X_k(s^*)$ is the covariate vector evaluated at location $s^*$, $\Phi_k(s^*; \epsilon_k, K^*_k)$ is the adaptive basis function vector with corresponding basis coefficients $\delta_k$, and $H_k(s^*)$ is the global basis function vector with corresponding global basis coefficients $\gamma$. We approximate the posterior predictive distribution for $\eta(s^*)$ using posterior samples \{\(\beta_k, \epsilon_k, \delta_k, K_k, \gamma\}\}. As with the parameter estimation, we note that the predictions are made within each cluster and hence can be done in parallel to promote computational efficiency. Furthermore, the posterior distribution allows for uncertainty quantification by evaluating the variance of the posterior samples.

### 3.5 Implementation Details

Our method requires tuning three parameters: (1) the number of partitions $K$; (2) the prior rate parameter $\lambda$ for the number of basis functions to be used within each partition; and (3) the prior distribution for the partition-specific bandwidths $\epsilon = \{\epsilon_k\}^K_{k=1}$. Selecting
a small value of $K$ may not be adequate for approximating nonstationary spatial processes because there may be several heterogeneous subregions within the spatial domain. On the other hand, selecting a large value of $K$ may result in many partitions with a small number of observations $N_k$. In our simulation study, we compare the performance of our method with various choices of $K$. For the partition-specific bandwidths, we specify a uniform prior $\epsilon_k \sim \text{Unif}(\alpha, \beta)$ to allow for control over the range of possible values $\epsilon_k$ can take on. For $\mathcal{D} = [0, 5]^2$, a sensitivity analysis suggests that $\alpha = 0.01$ and $\beta = 3$ provides a suitable range of values for $\epsilon_k$ to accommodate both smooth and rough partitions. A truncated Poisson distribution with prior rate parameter $\lambda$ is used for the number of basis functions for each partition. A sensitivity analysis suggests that results are relatively insensitive to choices of $\lambda$ in the range 5-20 so we choose $\lambda = 5$ to promote parsimony and computational efficiency. We set the priors for $\beta$ and $\tau^2_k$ following (Hughes and Haran, 2013): $\beta \sim \mathcal{N}(0, 100\mathcal{I})$ and $\tau^2_k \sim \text{IG}(0.5, 2000)$. The latter prior is desirable because it corresponds to the prior belief that the fixed effects are sufficient for explaining the data. For the global basis function matrix $H$, we use three layers of nested bisquare basis functions (Sengupta et al., 2016).

4 Simulation Study

In this section, we demonstrate the Adapt-BaSeS approach through an extensive simulation study featuring multiple spatial data classes and dependence structures. To benchmark performance, we compare our approach with two competing methods.
4.1 Simulation Study Design

Let \( s_i \in D = [0, 5]^2 \subset \mathbb{R}^2 \) for \( i = 1, \ldots, N \) denote the spatial locations and let \( S = (s_1, \ldots, s_N) \). On these locations, let \( Z = (Z(s_1), \ldots, Z(s_N))^\top \) denote the vector of response variables (i.e., the data). For model fitting, we use \( N_O = 5,000 \) observations and reserve \( N_P = 1,000 \) observations for validation. We consider both binary and count data, with the associated spatial random effects generated from both nonstationary and stationary spatial processes. Observations are generated using the SGLMM framework described in (1) with \( X_1, X_2 \sim \text{Unif}(-0.5, 0.5) \) and \( \beta = (1, 1) \). We study our method for \( K = \{9, 16, 25, 36, 49\} \) partitions. All together, we study a total of \( 5 \times 2 \times 2 = 20 \) implementations.

The nonstationary spatial random effects \( W = \{W(s_i) : s_i \in D\} \) are generated by smoothing several locally stationary processes (Fuentes, 2001). Further details are provided in the supplementary material. The stationary spatial random effects are generated using an exponential covariance function with scaling parameter \( \phi = 1 \) and partial sill parameter \( \sigma^2 = 1 \). The binary datasets use a Bernoulli data model and a logit link function and the count datasets are generated using a Poisson data model and a log link function. For each data generation mechanism (4 total), we generate 100 replicate data sets.

We fit the model using the hierarchical framework outlined in (5). We generate 100,000 samples from the posterior distribution \( \pi(\beta, \epsilon_k, K_k, \delta_k, \tau_k^2, \rho^2) \) for \( k = 1, \ldots, K \) using the RJMCMC algorithm described in Algorithm 1. To evaluate predictive performance, we compute the average root cross-validated mean squared prediction error (rCVMSPE), defined as \( \text{rCVMSPE} = \left( \frac{1}{N_P} \sum_{i=1}^{N_P} \left( Z_i - \hat{Z}_i \right)^2 \right)^{1/2} \), the area under the receiver operating curve (AUC) for the binary case, and the walltime (computation time) required to run...
100,000 iterations of the RJMCMC algorithm.

Fitting a “gold standard” SGLMM (1) is prohibitive due to the overparameterized model and large matrix operations. Hence, we compare our approach with two competing methods: the NNGP approach and a fixed bisquare basis function approach. The computation times are based on a single 2.4 GHz Intel Xeon Gold 6240R processor provided by GMU’s HOPPER high-performance computing infrastructure.

4.2 Simulation Study Results

Table 1 and Table 2, respectively, present the rCVMSPE and AUC for Adapt-BaSeS and the competing approaches. The results indicate that our method yields more accurate predictions than the competing methods across different values of $K$, data classes, and covariance structures. Paired $t$-tests were performed to compare the sets of rCVMSPE’s between our approach and the competing methods. The corresponding $p$-values were found to be statistically significant, with $p < 0.001$ for each pairwise comparison. Predictive performance generally improves as we increase the number of partitions $K$. However, the predictive standard deviations generally increase with larger $K$. For one simulated nonstationary dataset, we present the posterior predictive log intensity surface (Figure 2) and the posterior predictive probability surface (Figure 3) obtained from the implementation yielding the lowest rCVMSPE ($K = 49$). Based on a visual inspection, our method successfully captures the nonstationary behavior of the true latent spatial process in both cases. Plots illustrating the prediction standard deviations can be found in the supplementary material.

The model-fitting walltimes are reported in the supplementary material. The proposed
approach exhibits higher computational costs than the fixed basis function approach. However, our method is more computationally efficient than the NNGP approach. The shorter walltimes for the fixed basis function approach are expected since the spatial basis functions are fixed prior to model-fitting. In contrast, our proposed method modifies the spatial basis functions at each iteration of the RJMCMC algorithm, leading to increased computational costs. Despite the longer walltimes, our approach offers additional flexibility in modeling the latent spatial process and yields more accurate predictions. Importantly, both approaches provide substantial improvements in computational efficiency over the “gold standard” SGLMM (1), which would be computationally infeasible for a dataset with $N_O = 5,000$ observations.

| Method  | Nonstationary | Stationary |
|---------|---------------|------------|
|         | Poisson       | Binary     | Poisson     | Binary |
| Bisquare| 1.817 (0.140) | 0.478 (0.045) | 1.754 (0.143) | 0.460 (0.044) |
| NNGP    | 0.474 (0.131) | 0.474 (0.131) | 0.458 (0.123) | 0.458 (0.123) |
| $K = 9$ | 1.719 (0.156) | 0.470 (0.042) | 1.709 (0.128) | 0.453 (0.043) |
| $K = 16$| 1.700 (0.174) | 0.468 (0.043) | 1.650 (0.180) | 0.451 (0.042) |
| $K = 25$| 1.688 (0.192) | 0.466 (0.045) | 1.648 (0.195) | 0.450 (0.044) |
| $K = 36$| 1.682 (0.206) | 0.465 (0.048) | 1.639 (0.213) | 0.449 (0.047) |
| $K = 49$| 1.680 (0.224) | 0.464 (0.052) | 1.633 (0.232) | 0.448 (0.051) |

Table 1: Average rCVMSPRE for the simulation study. Columns correspond to the data class and spatial dependence structure. Results are presented for various choices of $K$. Top rows correspond the fixed basis functions approach and NNGP. Average standard deviation of the predictions are provided in parentheses.
Table 2: Out-of-sample area under the receiver operating curve (AUC)

| Method   | Nonstationary | Stationary |
|----------|---------------|------------|
| Bisquare | 0.663         | 0.711      |
| NNGP     | 0.679         | 0.716      |
| $K = 9$  | 0.693         | 0.731      |
| $K = 16$ | 0.700         | 0.736      |
| $K = 25$ | 0.706         | 0.740      |
| $K = 36$ | 0.709         | 0.742      |
| $K = 49$ | 0.711         | 0.743      |

5 Applications

In this section, we apply the Adapt-BaSeS to two real-world spatial datasets: binary incidence of dwarf mistletoe in Minnesota (Hanks, Hooten and Baker, 2011) and counts from the North American Breeding Bird Survey (BBS) (Ziolkowski et al., 2022).
5.1 Binary Data: Parasitic Infestation of Dwarf Mistletoe

The dwarf mistletoe is a parasitic species that extracts key resources from its host, such as the black spruce species (Geils and Hawksworth, 2002). This infestation poses economic challenges, because black spruce is a valuable resource for producing high-quality paper. We apply our method to analyze dwarf mistletoe incidence data in Minnesota, obtained from the Minnesota Department of Natural Resources operational inventory (Hanks, Hooten and Baker, 2011). The dataset contains binary incidence of dwarf mistletoe at $N = 25,431$ locations, with dwarf mistletoe being present at 2,872 of these locations. We fit the model on $N_O = 12,931$ observations and set aside $N_P = 12,500$ observations for validation. We consider several covariates as inputs to our model, including: (1) the average age of trees in years; (2) basal area per acre of trees in the stand; (3) average canopy height; and (4) volume of the stand measured in cords. We study the performance of our method for $K \in \{9, 16, 25, 36\}$.
For each implementation, we compute the rCVMSPE and the AUC for the binary classification (Table 3). We observe that increasing the number of partitions improves the predictive performance of our proposed approach. Specifically, using $K = 36$ partitions yields the highest AUC value and the lowest rCVMSPE. In contrast, the fixed basis function approach provides less accurate predictions compared to our proposed method, across all four partition levels. Figure 4 displays the predictive probability surface and the true binary observations for the validation sample, for the case of $K = 36$.

| Method  | rCVMSPE   | AUC  |
|---------|-----------|------|
| Bisquare | 0.308 (0.015) | 0.734 |
| $K = 9$ | 0.300 (0.017) | 0.764 |
| $K = 16$ | 0.296 (0.022) | 0.785 |
| $K = 25$ | 0.295 (0.023) | 0.790 |
| $K = 36$ | 0.294 (0.024) | 0.793 |

Table 3: rCVMSPE and AUC for the dwarf mistletoe dataset. Results are presented for varying number of partitions $K$. The top row corresponds to the fixed basis function approach. The average standard deviation of the predictions are provided in parentheses.

5.2 Count Data: North American Breeding Bird Survey 2018

The Bird Breeding Survey (BBS) (Ziolkowski et al., 2022) is an annual roadside survey that involves trained observers monitoring the abundance of bird populations in North America. The sum of counts serves as an index of species abundance along the route for that specific year. The particular BBS dataset includes Blue Jay (Cyanocitta cristata) bird counts at a total of $N = 1,593$ locations, covering eastern and central regions of the United States. We use $N_O = 1,000$ observations to fit the model and reserve $N_P = 593$ for validation. We fit the model with only the spatial random effects (i.e., the conditional mean is modeled as
Figure 4: Illustration of the dwarf mistletoe occurrence dataset for $K = 36$. True observations (left) and posterior predictive probability surface (right) for the validation sample.

$g(\mathbb{E}[Z(s_i)]) = W(\cdot)$ and does not include spatial covariates).

Table 4 displays the rCVMSPE for each implementation. We find that our method consistently outperforms the fixed basis function approach. For the case of $K = 9$ partitions, Figure 5 displays the true count observations and the predictive intensity surface, obtained from $k$-fold cross-validation. The predictive intensity map reveals that Blue Jays are most abundant in the southeastern and northeastern regions of the United States.

| Method  | rCVMSPE    |
|---------|------------|
| Bisquare| 8.735 (0.706) |
| $K = 5$ | 8.599 (0.735)  |
| $K = 6$ | 8.583 (0.857)  |
| $K = 7$ | 8.537 (0.892)  |
| $K = 8$ | 8.515 (1.013)  |
| $K = 9$ | 8.572 (0.904)  |

Table 4: rCVMSPE for the Blue Jay spatial count dataset. Results are presented for varying $K$. Results from fixed basis functions are in the top row. Average standard deviation of predictions are in parentheses.
6 Discussion

We propose a data-informed, flexible, and computationally efficient method to model high-dimensional non-Gaussian spatial observations with nonstationary spatial dependence structures. Past studies have used spatial radial basis functions; thereby accounting for nonstationarity and reducing computational costs. However, these studies generally fix crucial components of the basis functions, such as the number of basis functions, placement of basis knots, and bandwidth (smoothing) parameters, perhaps arbitrarily, before fitting the model.

Our fast yet flexible method partitions the spatial domain into disjoint subregions using an agglomerative spatial clustering algorithm (Heaton, Christensen and Terres, 2017). We then employ a RJMCMC algorithm to select critical features (knots and bandwidths) of
the basis functions within each partition. Results from both our simulation study and real-world applications demonstrate that our approach performs well in both inference and predictions over competing methods, while also preserving computational efficiency.

While our proposed adaptive framework primarily focuses on Gaussian radial basis functions, it can be extended to accommodate a wider range of radial basis functions. This includes thin-plate-spline basis functions, multiquadric radial basis functions, and bisquare basis functions, among others. Though our approach offers a significant speedup compared to the “gold standard” SGLMM (1), the computational speedup can be further enhanced by embedding sparse basis functions such as the Wendland basis functions (Nychka et al., 2015) or multi-resolution approximation (M-RA) basis functions (Katzfuss, 2017), which can drastically reduce the number of floating point operations. In a similar strain, the embarrassingly parallel matrix operations can be distributed across available processors (Guan and Haran, 2018) in high-performance computing systems.

**Supplementary Material**

The supplementary material includes: (1) details on the construction of the bisquare basis functions as well as a visualization of the multi-resolution “quad-tree” structure; (2) details on the clustering algorithm (Heaton, Christensen and Terres, 2017); (3) model-fitting walltimes for the simulation study; (4) a proof of the detailed balance proposition; and (5) visualizations of the prediction standard deviation surfaces.
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Supplementary Material for Flexible Basis Representations for Modeling High-Dimensional Hierarchical Spatial Data

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1 Reversible Jump MCMC

Given the challenge of visually determining the appropriate number and placement of knots in spatial data, it is crucial to employ adaptive methods for knot selection. One such method is the reversible jump Markov chain Monte Carlo (RJMCMC) sampler (Green, 1995), which provides a flexible framework for Markov chain Monte Carlo simulation by allowing the dimension of the parameter space to vary at each iteration.

The RJMCMC sampler is particularly useful for model selection tasks, as it enables the Markov chain to explore parameter subspaces of different dimensions. This capability has led to successful application in various domains, including change-point analysis (Fan and Brooks, 2000), finite mixture models (Richardson and Green, 1997), time series models with an unknown number of components (Brooks, Giudici and Roberts, 2003), variable selection in regression models (Nott and Leonte, 2004), and knot selection in curve fitting (Denison, Mallick and Smith, 1998).

Let $y$ be a vector of observations, and let $\mathcal{M} = \{\mathcal{M}_1, \mathcal{M}_2, \ldots\}$ denote a countable collection of candidate models, indexed by a model indicator $k \in \mathcal{K}$, for some countable set $\mathcal{K}$. 

Let $y$ be a vector of observations, and let $\mathcal{M} = \{\mathcal{M}_1, \mathcal{M}_2, \ldots\}$ denote a countable collection of candidate models, indexed by a model indicator $k \in \mathcal{K}$, for some countable set $\mathcal{K}$.
Each model $M_k$ has an $n_k$-dimensional vector of unknown parameters, $\theta_k \in \Theta_k \subset \mathbb{R}^{n_k}$, where $n_k$ can vary with $k$. The joint distribution of $(k, \theta_k, y)$ is modeled as,

$$p(k, \theta_k, y) = p(k)p(\theta_k | k)p(y | k, \theta_k),$$

where $p(k)$ is the model probability, $p(\theta_k | k)$ is the parameter prior given the model, and $p(y | k, \theta_k)$ is the likelihood. Inference about $k$ and $\theta_k$ is based on the joint posterior $p(k, \theta_k | y) \propto p(k, \theta_k, y)$, which is known as the target distribution. For convenience, we abbreviate $(k, \theta_k)$ as $x$, and $p(k, \theta_k | y) = p(x | y)$ as $\pi(x)$. Given $k$, $x$ lies in $C_k = \{k\} \times \Theta_k$, while generally, $x \in \mathcal{C} = \bigcup_{k \in \mathcal{K}} C_k$.

In order to traverse freely across the combined parameter space $\mathcal{C}$, we need a method that moves between parameter subspaces $\mathcal{A}, \mathcal{B} \subset \mathcal{C}$ of possibly different dimension. To that end, we consider different move types $m$, and for each of these move types we construct a transition kernel $P_m$, which satisfies the detailed balance condition,

$$\int_{\mathcal{A}} \int_{\mathcal{B}} \pi(dx)P_m(x, dx') = \int_{\mathcal{B}} \int_{\mathcal{A}} \pi(dx')P_m(x', dx)$$

for all $\mathcal{A}, \mathcal{B} \subset \mathcal{C}$. This means that the equilibrium probability that the state of the chain is in a general set $\mathcal{A}$ and moves to a general set $\mathcal{B}$ is the same as with $\mathcal{A}$ and $\mathcal{B}$ reversed. To construct the MCMC sampler, consider $x = (k, \theta_k)$ to be the current state of the Markov chain. Following the Metropolis-Hastings algorithm, a move of type $m$ is proposed to a new state $x' = (k', \theta_{k'})$ according to the proposal density $q_m(x, dx')$. As usual with the Metropolis-Hastings algorithm, the detailed balance condition (1) is enforced through the acceptance probability, where the move to the candidate state $x'$ is accepted with probability

$$\alpha_m(x, x') = \min \left\{ 1, \frac{\pi(dx')q_m(x', dx)}{\pi(dx)q_m(x, dx')} \right\},$$

otherwise, remain at the current state $x$. At each step of the RJMCMC algorithm, Brooks et al. (2011) divide the types of moves $m$ into two major categories:
• **Within-model moves:** fix the model index $k$ and update the parameters $\theta_k$ following standard Gibbs or Metropolis-Hastings algorithms.

• **Between-model moves:** jointly update the state $x = (k, \theta_k)$ by proposing a new state $x' = (k', \theta_{k'}) \sim q_m(x, dx')$ and “matching dimensions” before accepting with probability $\alpha_m(x, x')$.

While the within-model moves are straightforward, the between-moves are more complicated as they involve a “dimension matching” component (Green, 1995). Suppose that the current state $x = (k, \theta_k)$ has dimension $n_k$ under the current model $M_k$, and the proposed state $x' = (k', \theta_{k'})$ under model $M_{k'}$ has dimension $n_{k'}$, where $n_k \neq n_{k'}$. In order to “match dimensions” between the two model states, introduce an auxiliary variable for the transition $m$ from model $M_k$ to model $M_{k'}$ denoted $u \sim g_m$ and of dimension $r_m$ where the density $g_m$ is known. The new state $\theta'_{k'}$ is constructed as $(\theta'_{k'}, u') = h_m(\theta_k, u)$ for some suitable deterministic function $h_m$. The reverse move from $x'$ to $x$ needs to be defined symmetrically by generating random numbers $u'$ of dimension $r'_m$ from the joint distribution $g'_m$ needed for the reverse move, to move from $\theta'_{k'}$ to $\theta_k$, using the inverse function $h'_m$ of $h_m$. In order for the transformation from $(\theta_k, u)$ to $(\theta'_{k'}, u')$ to be a diffeomorphism, meaning the transformation and its inverse are differentiable, it must be the case that $n_k + r_m = n_{k'} + r'_m$.

When there are multiple possible moves $m$, we must generally also include the probability $j_m$ of choosing a specific move. The detailed balance requirement (1) can then be rewritten as

$$\int_A \int_B \pi(x) j_m(x) g_m(u) \alpha_m(x, x') dx du = \int_B \int_A \pi(x') j_m(x') g'_m(u') \alpha_m(x', x) dx' du'$$

for all $A, B \subseteq C$. Thus, a sufficient choice for the acceptance probability $\alpha_m$ corresponding to move type $m$ is given by

$$\alpha_m(x, x') = \min \left\{ 1, \frac{\pi(x') j_m(x') g'_m(u')}{\pi(x) j_m(x) g_m(u)} \left| \frac{\partial(\theta'_{k'}, u')}{\partial(\theta_k, u)} \right| \right\},$$

3
where the last factor corresponds to the Jacobian for the change of variable between $(\theta_k, u)$ and $(\theta'_k, u')$.

## 2 Bisquare Basis Functions

We employ the bisquare basis functions from (Sengupta and Cressie, 2013; Cressie and Johannesson, 2008) which take the form:

$$
\Phi_m(s) = \left\{ 1 - \left( \frac{||s - u_m||}{\gamma} \right)^2 \right\}^2 \mathbb{I}(||s - u_m|| < \gamma),
$$

where $u_m$ is the center of basis function $m$ and $\mathbb{I}(\cdot)$ is an indicator function. The knots associated with each basis function are constructed according to a multi-resolution “quad-tree” structure such that the knots associated with different resolutions do not overlap. In particular, we use three resolutions, where there are four knot locations $u_1, \ldots, u_4$ for the first resolution, 16 knots $u_5, \ldots, u_{20}$ for the second resolution, and 64 knots $u_{21}, \ldots, u_{84}$ for the third resolution. An illustration of the three resolutions of knot locations is provided in Figure 1. The bandwidth $\gamma$ for a specific resolution from Cressie and Johannesson (2008) is given by $\gamma = 1.5 \times$ minimum distance between knot locations.

We employ the multi-resolution bisquare basis functions into the Bayesian hierarchical framework for spatial generalized linear mixed models (SLGMMs) as follows:

**Data Model:**

$$Z(s_i) \mid \eta(s_i) \sim F(\eta(s_i))$$

$$g(\mathbb{E}[Z \mid \beta, \delta]) := \eta = X\beta + \Phi\delta$$

**Process Model:**

$$\delta \mid \tau^2 \sim \mathcal{N}(0, \tau^2 \mathcal{I})$$

**Parameter Model:**

$$\beta \sim p(\beta), \tau^2 \sim p(\tau^2),$$

where $\mathcal{I}$ denotes the identity matrix and $\Phi$ denotes the matrix of the multi-resolution bisquare basis functions. The hierarchical model is completed by assigning prior distributions for the model parameters $\beta$ and $\tau^2$. In the simulation study, we use the following
prior distributions for the model parameters: \( \beta \sim N(0, 100I) \) and \( \tau^2 \sim \text{IG}(0.5, 2000) \).

## 3 Spatial Clustering Algorithm

Here, we provide details on the clustering algorithm (Heaton, Christensen and Terres, 2017). We obtain residuals \( \epsilon \) from a nonspatial generalized linear model (GLM) fit with a response vector \( Z \in \mathbb{R}^N \) and a covariate matrix \( X \in \mathbb{R}^{N \times M} \). Let \( \epsilon_k \in \mathbb{R}^{N_k} \) denote the residuals belonging to the cluster (partition) \( S_k \). We can then define the dissimilarity between two clusters as

\[
d(S_{k_1}, S_{k_2}) = \left[ \frac{N_{k_1}N_{k_2}}{N_{k_1} + N_{k_2}} (\bar{\epsilon}_{k_1} - \bar{\epsilon}_{k_2})^2 \right] \frac{1}{\bar{E}},
\]

where \( \bar{\epsilon}_k \) is the average of the residuals in cluster \( k \) and \( \bar{E} \) is the average Euclidean distance between points in \( S_{k_1} \) and \( S_{k_2} \) amongst Voronoi neighbors. Heaton, Christensen and Terres (2017) define \( s_i \) and \( s_j \) to be Voronoi neighbors if they share a border in a Voronoi tessellation of the observation locations \( s_1, \ldots, s_N \). The spatial clustering algorithm is summarized in Algorithm 1.
Algorithm 1: Spatial clustering algorithm (Heaton, Christensen and Terres, 2017)

Initialize $S_k = s_k$ for $k = 1, \cdots, N$ such that each observation is its own cluster.

1. Find clusters $S_{k_1}, S_{k_2}$ having the minimum $d(S_{k_1}, S_{k_2})$ where $s_i \sim s_j$ (Voronoi neighbors) for $s_i \in S_{k_1}$ and $s_j \in S_{k_2}$

2. Combine two clusters

$$S_{\min\{k_1, k_2\}} = S_{k_1} \cup S_{k_2}$$

and set

$$S_{\max\{k_1, k_2\}} = \emptyset$$

Repeat 1-2 until we have $K$ clusters where $K < N$.

We note that Algorithm 1 becomes computationally expensive when the number of observations is large. Following suggestions in Heaton, Christensen and Terres (2017), we perform clustering after aggregating observations to a lattice $\{s^*_l\}_{L=1}^L$ ($L << N$). Here, $N_l = \{s_i : \|s_i - s^*_l\| < \|s_i - s^*_m\| \text{ for all } l \neq m\}$ is the subset of observations whose closest lattice point is $s^*_l$, and $\bar{\epsilon}(s^*_l) = |N_l|^{-1} \sum_{s_i \in N_l} \epsilon(s_i)$ is the average of the observed residuals in $N_l$. We then apply Algorithm 1 to $\{\bar{\epsilon}(s^*_l)\}_{l=1}^L$ rather than to $\{\epsilon(s_i)\}_{i=1}^N$. By specifying the number of lattice points $L$ to be much smaller than the number of observations $N$, the spatial clustering algorithm becomes computationally feasible. For example, in our simulation studies, we specify $L = 400$ for $N = 5,000$.

4 Computation: Model-Fitting Walltimes

In Table 1, we report the model-fitting walltimes (computation times). These include the time required for model initialization and running 100,000 iterations of the RJMCMC algorithm. The proposed approach exhibits higher computational costs compared to the fixed bisquare basis function approach. However, our method is more computationally efficient than the NNGP approach.
Table 1: Average walltime (seconds) for 100,000 iterations

| Method            | Nonstationary Poisson | Nonstationary Binary | Rough Stationary Poisson | Rough Stationary Binary |
|-------------------|------------------------|----------------------|--------------------------|-------------------------|
| Fixed (Bisquare)  | 192                    | 165                  | 184                      | 166                     |
| NNGP              | 2336                   | 2291                 | 2291                     | 2291                    |
| \(K = 9\)         | 754                    | 581                  | 726                      | 602                     |
| \(K = 16\)        | 739                    | 633                  | 748                      | 643                     |
| \(K = 25\)        | 775                    | 715                  | 791                      | 770                     |
| \(K = 36\)        | 833                    | 830                  | 860                      | 842                     |
| \(K = 49\)        | 931                    | 926                  | 958                      | 932                     |

5 Proof of Proposition

In this section, we provide a proof establishing that the acceptance probability satisfies the detailed balance condition for the birth step. Given the \(r_k\) knots \(\mathcal{K}_k = (u_{k,1}, \ldots, u_{k,r_k})\), in the birth move we draw a new knot \(u^*\) uniformly with probability \(1/(R_k - r_k)\) from the set of the \(R_k - r_k\) vacant knot locations. Let \(\mathcal{K}^*_k = \mathcal{K}_k \cup \{u^*\}\) be the proposed set of knots, which now has size \(r_k^* = r_k + 1\). The resulting model is now defined by the new model indicator \(r_k + 1\), the new knots \(\mathcal{K}^*_k = (u^*_{k,1}, \ldots, u^*_{k,r_k+1})\) (with \(u^*_{k,i} = u_{k,i}\) for \(i \leq r_k\) and \(u^*_{k,r_k+1} = u^*\)), and the new basis coefficients \(\delta^*_k = (\delta^*_{k,1}, \ldots, \delta^*_{k,r_k+1})\), which must be adjusted appropriately. Formally, the birth move can be defined as a transition from state \(\theta = (r_k, \theta_{r_k})\) to state \(\theta^* = (r_k + 1, \theta^*_{r_k+1})\). With

\[
\theta_{r_k} = (\mathcal{K}_k, \delta_k, \beta_k, \gamma, \tau^2_k, \rho^2, \epsilon_k)
\]

and

\[
\theta^*_{r_k+1} = (\mathcal{K}^*_k, \delta^*_k, \beta_k, \gamma, \tau^2_k, \rho^2, \epsilon_k),
\]

there is a change in dimension from \(\dim(\theta_{r_k}) = 2r_k + P + G + 3\) to \(\dim(\theta^*_{r_k+1}) = 2r_k + P + G + 5\). For the birth move, we have to compute \(\theta^*_{r_k+1}\) as a function of \(\theta_{r_k}\) and two random
numbers $u^*$ and $u$, with $u_B = (u^*, u)$. The proposed knot $u^*$ is drawn uniformly with probability $p(u^*) = 1/(R_k - r_k)$ from the set of the $R_k - r_k$ vacant candidate knots. The new coefficient $\delta^*_{k,r_k+1}$ corresponding to the new knot $u^*_{k,r_k+1} = u^*$ is set equal to $u$ where $u \sim g(u)$, i.e., we simulate a value of $u$ from some proposal distribution $g$. We specify $u \sim \mathcal{N}(0, \sigma^2)$ where $\sigma^2$ can be tuned by the user to achieve a reasonable acceptance rate. Hence, we set

$$
\delta^*_{k,r_k+1} = u \\
\delta^*_k = \delta_{k,r_k} \\
\vdots \\
\delta^*_{k,1} = \delta_{k,1}
$$

This ensures that in the reverse death move, given the knot $u^*_{k,r_k+1}$ to be deleted, the computation of $\delta_k$ from $\delta^*_k$ is deterministic and the required dimension matching holds:

$$
u = \delta^*_{k,r_k+1} \\
\delta_{k,r_k} = \delta^*_{k,r_k} \\
\vdots \\
\delta_{k,1} = \delta^*_{k,1}
$$

The acceptance probability for the birth move can be expressed as

$$
\alpha(\theta_{r_k}, \theta^*_{r_k+1}) = \min\{1, \mathcal{L} \cdot \mathcal{A} \cdot \mathcal{P} \cdot \mathcal{J}\}.
$$
where \( \mathcal{L} \) is the likelihood ratio, \( \mathcal{A} \) is the prior ratio, \( \mathcal{P} \) is the proposal ratio, and \( \mathcal{J} \) is the Jacobian. The ratio of priors results in

\[
\mathcal{A} = \frac{\text{prior for } r_k + 1 \text{ knots}}{\text{prior for } r_k \text{ knots}} \times \frac{\text{prior for location of } r_k + 1 \text{ knots}}{\text{prior for location of } r_k \text{ knots}} \times \frac{\text{prior for proposed basis coefficient}}{\text{prior for current basis coefficient}} = \frac{p(r_k + 1)}{p(r_k)} \frac{r_k + 1}{R_k - r_k} \frac{\mathcal{N}(\delta^*_k, r_{k+1}; 0, \tau^2_k)}{\mathcal{N}(0; 0, \tau^2_k)},
\]

where the factor \( p(r_k+1)/p(r_k) \) depends on the alternative priors of \( r_k \): \( p(r_k) \propto \frac{\lambda^r}{r_k!} \mathbb{1}_{0,\ldots,R_k}(r_k) \) with prior rate parameter \( \lambda \). The corresponding proposal ratio \( \mathcal{P} \) is given by

\[
\mathcal{P} = \frac{d_{r_k+1}(1/(r_k + 1))}{b_{r_k}(1/(R_k - r_k))} \times \frac{1}{\mathcal{N}(\delta^*_{k, r_k+1}; 0, \sigma^2)} = \frac{d_{r_k+1}(R_k - r_k)}{b_{r_k}(r_k + 1)} \times \frac{1}{\mathcal{N}(\delta^*_{k, r_k+1}; 0, \sigma^2)}.
\]
Considering $\theta^*_{rk+1}$ as a function of $\theta_{rk}$ and $u_B$, the Jacobian is

$$J = \left| \frac{\partial \theta^*_{rk+1}}{\partial (\theta_{rk}, u_B)} \right|$$

$$= \left| \begin{array}{cccc}
\frac{\partial \delta^*_{k,1}}{\partial \delta_{k,1}} & \frac{\partial \delta^*_{k,2}}{\partial \delta_{k,1}} & \frac{\partial \delta^*_{k,3}}{\partial \delta_{k,1}} & \cdots & \frac{\partial \delta^*_{k,rk+1}}{\partial \delta_{k,1}} \\
\frac{\partial \delta^*_{k,1}}{\partial \delta_{k,2}} & \frac{\partial \delta^*_{k,2}}{\partial \delta_{k,2}} & \frac{\partial \delta^*_{k,3}}{\partial \delta_{k,2}} & \cdots & \frac{\partial \delta^*_{k,rk+1}}{\partial \delta_{k,2}} \\
\frac{\partial \delta^*_{k,1}}{\partial \delta_{k,3}} & \frac{\partial \delta^*_{k,2}}{\partial \delta_{k,3}} & \frac{\partial \delta^*_{k,3}}{\partial \delta_{k,3}} & \cdots & \frac{\partial \delta^*_{k,rk+1}}{\partial \delta_{k,3}} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{\partial \delta^*_{k,1}}{\partial u} & \frac{\partial \delta^*_{k,2}}{\partial u} & \frac{\partial \delta^*_{k,3}}{\partial u} & \cdots & \frac{\partial \delta^*_{k,rk+1}}{\partial u}
\end{array} \right|$$

$$= \left| \begin{array}{ccc}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{array} \right|$$

$$= 1.$$

The proof for both the move and death steps follows similarly.

6 Standard Deviation Surfaces

Figure 2 and Figure 3 illustrate example prediction standard deviation surfaces for the binary and count examples, respectively. It can be noted that regions with high predicted intensity exhibit correspondingly high standard deviations. Conversely, regions with both high and low predicted probabilities demonstrate lower standard deviations.

7 Generation of Nonstationary Spatial Random Effects

The nonstationary spatial random effects $W = \{W(s_i) : s_i \in D\}$ are generated by smoothing several locally stationary processes contained in disjoint subregions (Fuentes,
To do this, we partition the spatial domain $\mathcal{D}$ into four disjoint subregions $\mathcal{D}_1$, $\mathcal{D}_2$, $\mathcal{D}_3$, and $\mathcal{D}_4$, where $\mathcal{D}_1 = [0, 2.5]^2$, $\mathcal{D}_2 = [2.5, 5]^2$, $\mathcal{D}_3 = [0, 2.5] \times [2.5, 5]$, and $\mathcal{D}_4 = [2.5, 5] \times [0, 2.5]$. We then specify $C_1(\cdot)$, $C_2(\cdot)$, $C_3(\cdot)$, and $C_4(\cdot)$ to be stationary covariance functions associated with each of the four subregions. Each stationary covariance function comes from the Matérn class with smoothness $\nu = 0.5$, partial sill parameter $\sigma^2 = 1$, and respective range parameters $\phi_1 = 0.5$, $\phi_2 = 0.4$, $\phi_3 = 0.3$, and $\phi_4 = 0.2$. The nonstationary global covariance function is then constructed using the modeling framework of Nott and Dunsmuir (2002), where

$$C(s, t) = \sum_{i=1}^{4} \lambda_i(s) \lambda_i(t) C_i(s, t).$$

Here $\lambda_i(s)$ is a weight function based on the distance between location $s$ and the center of subregion $\mathcal{D}_i$ which we denote as $\mu_i$. The weight function is chosen such that $\lambda_i(s) \geq 0$, $\sum_{i=1}^{4} \lambda_i(s) = 1$, $\lambda_i(s)$ attains its maximum at $\mu_i$, and decays smoothly to zero as $||s - \mu_i|| \to \infty$. To ensure that $\lambda_i(s) \geq 0$, Nott and Dunsmuir (2002) employ the kernel function

$$\kappa_\eta(t) = \exp\left(-\frac{||t||^2}{\eta}\right),$$

Figure 2: Prediction standard deviation surface for the binary example.

2001).
where $\eta$ is a smoothing parameter (we specify $\eta = 6$), and then

$$
\lambda_i(s) = \frac{\kappa_\eta(s - \mu_i)}{\sum_{j=1}^4 \kappa_\eta(s - \mu_j)}.
$$

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