A Projection-based Laplace Approximation for Spatial Latent Variable Models

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ABSTRACT

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Laplace method is a practical tool for obtaining maximum likelihood estimators for a broad class of latent variable models. The main idea is to approximate the integrand using a Gaussian distribution. However, with increasing observations, the Laplace approximation becomes infeasible because the dimension of the correlated latent variables grows, which results in the high-dimensional optimization problem. One important example is spatial latent variable models, which are widely used in many fields, such as ecology, epidemiology, and sociology. Spatial latent variable models are useful for investigating the relationship between spatial covariates or predicting the unobserved area. Here, we propose a fast Laplace approximation based on the dimension reduction of the latent variables. Our methods are faster and have fewer components to be tuned than simulation-based methods such as Markov chain Monte Carlo maximum likelihood and Monte Carlo expectation-maximization. Our approach can be applied to the large non-Gaussian spatial data sets, commonly used in modern environmental sciences. Especially, we show how we may understand spatial patterns of non-Gaussian responses for two case studies: confirmed COVID-19 cases in the United States and thickness of the Antarctic ice sheet. Through simulation studies under different scenarios, we investigate that our method can provide accurate maximum likelihood

estimations and predictions quickly. Our study can be broadly applicable for practical maximum likelihood inference for high-dimensional random effect models.

Keywords : Laplace method; numerical optimization; dimension reduction; spatial interpolation; spatial generalized linear mixed models

Chapter 1

Introduction

Latent variable models are useful when the underlying structures of interest are unobservable. Laplace methods (Tierney and Kadane, 1986) are practical tools for maximum likelihood estimation for such a class of models, such as longitudinal models (cf. Molenberghs and Verbeke, 2005) and generalized linear latent variable models (cf. Bianconcini and Cagnone, 2012). The likelihood evaluations for such models require integration with respect to latent variables. Laplace methods approximate the integrals through the Gaussian distribution by finding the optimized values of the latent variables for the given model parameters. However, when the dimension of the latent variables grows, they may be computationally infeasible. One such case is spatial latent variable models (or spatial generalized linear mixed models, SGLMMs), which are widely used to study observed data that have associated spatial locations (cf. Banerjee et al., 2014, Lawson et al., 2016). The maximum likelihood estimation of such models is challenging because the evaluation of the likelihood function requires high-dimensional integration as well as spatially correlated latent variables. These facts result in a high-dimensional optimization problem for the Laplace approximation, which is computationally infeasible. Here, we develop a practical Laplace approximation for high-dimensional spatial latent variable models. We replace high-dimensional integration with a reduced-dimensional representation based on the projection and provide a nested optimization method to find the maximum likelihood estimators (MLEs). We show that our approach is efficient at producing accurate estimations and predictions. We apply our method to two important environmental science problems and draw meaningful conclusions based on inference results.

The Bayesian framework is a popular approach for spatial latent variable models and a large

literature addresses the computational challenges in the Bayesian context. For instance, the predictive process approach (Banerjee et al., 2008) projects the original high-dimensional process onto a low-dimensional subspace at a specified set of locations. Nearest-neighbor Gaussian process approaches (Datta et al., 2016, Finley et al., 2019) can acheive scalability with sparse representation of precision matrices. (see Zhang et al. (2021) for multivariate extensions). To improve the mixing of Markov chain Monte Carlo (MCMC), several reparameterizations (cf. Rue and Held, 2005, Christensen et al., 2006) have been suggested. Combining such reparameterizations with an efficient subsampling strategy, Entezari et al. (2020) improve predictions of SGLMMs. Rue et al. (2009) develops the integrated nested laplace approximation (INLA), which allows practical Bayesian inference for non-Gaussian spatial data using a stochastic partial differential equation approximation to the latent Gaussian model. INLA has been widely used in many spatial and spatio-temporal applications with large number of observations (cf. Clifford et al., 2019, Forlani et al., 2020). Hughes and Haran (2013), Guan and Haran (2018) propose efficient projection-based approaches to address computational and inferential challenges under the Bayesian framework.

In this manuscript, we focus on developing a practical maximum likelihood approach for high-dimensional spatial latent variable models based on the Laplace method. Bayes approaches are convenient for constructing hierarchical spatial models. For instance, we can consider flexible link functions (Li et al., 2019) or incorporate spatially varying coefficient (Berrett et al., 2020) for spatial latent variable models. On the contrary, frequentist methods may provide faster alternatives and can be convenient by avoiding the need to tune MCMC algorithms. Several maximum likelihood approaches have been developed for spatial latent variable models. Zhang (2002) developed Monte Carlo expectation maximization (MCEM), which uses Monte the Carlo version of the conditional expectation in the E-step. Recently, Tadayon and Torabi (2019) propose MCEM for non-Gaussian spatial data with covariatemeasurement error. Christensen (2004) proposed Markov chain Monte Carlo maximum likelihood (MCML), which maximizes the Monte Carlo approximated log-likelihood function. However, these approaches are computationally infeasible for large data sets because Monte Carlo approximations require simulating high-dimensional latent variables. Instead of simulation-based methods, Evangelou et al. (2011), Bonat and Ribeiro (2016) provide the Laplace approximation for the conditional distribution of the latent variables. These

approaches approximate the integration in the likelihood function through a Gaussian distribution, which require optimized values of the latent variables. For large data sets, such optimization becomes computationally demanding or even unstable. Recently, to address such challenges, Guan and Haran (2019), Park and Haran (2020) develop the projection-based MCEM and MCML, respectively. Although their approaches are computationally feasible for large non-Gaussian spatial data sets, both require several components to be tuned. For instance, users need to decide the number of Monte Carlo samples as well as to check the convergence of their iterative approaches manually. Furthermore, obtaining accurate standard errors is challenging in practice.

The main contribution of this manuscript is to develop a projection-based Laplace method that is computationally efficient as well as easy to implement for practitioners. Our algorithms can be applied to both continuous and lattice spatial domains. Especially, we focus on analyzing two scientific data sets: (1) *US COVID-19 data* contain a number of confirmed cases from US counties. Analyzing the spatial patterns of confirmed cases is important for detecting disease hotspots, which is useful for issuing public health advisories. (2) *Antarctic ice sheet data* represent binary ice thickness (ice-no ice) patterns. Understanding ice thickness distribution is crucial for informative projections of global sea-level rise. For both data sets, we have thousands of non-Gaussian spatial observations; inference for such data sets is computationally challenging. The proposed method allows us to carry out accurate maximum likelihood inference quickly. The outline of the rest of the manuscript is as follows. In Chapter 2, we introduce the Laplace approximations for spatial latent variable models and discuss their computational challenges. In Chapter 3, we propose the projection-based Laplace approximation to maximum likelihood inference and describe the implementation details. In Chapter 4, we present the estimation and prediction performance for our method using simulation studies. In Chapter 5, we show the application of our methods to real data sets with large observations. We conclude with a discussion and summary in Chapter 6.

The work of this manuscript including the contents, figures, and tables has already been submitted to *Environmetrics*.

Chapter 2

Model Specification

2.1 Spatial Latent Variable Models

The Spatial generalized linear mixed models (SGLMMs) consist of the fixed effect for explaining the mean trend and random effect for capturing the spatial correlation. SGLMMs have been developed both for point-referenced data in a continuous domain (Diggle et al., 1998) and for areal data in a lattice domain (Besag, 1974). Let $\mathbf{Z}$ be the n-dimensional observations at locations $\mathbf{s} \in R^{n\times 2}$. $\mathbf{X} \in R^{n\times p}$ is the matrix of spatial covariates depending on the locations. At each coordinate we can consider spatially correlated random effects $\mathbf{W} \in R^n$. Depending on the spatial domain of interest, random effects are modeled differently. For a continuous domain, $\mathbf{W}$ is often modeled as a second-order stationary Gaussian process with mean zero and covariance kernel $\mathbf{K}_{\boldsymbol{\theta}}(\mathbf{h}) = \mathbf{K}_{\boldsymbol{\theta}}(W(\mathbf{s}+\mathbf{h}), W(\mathbf{s}))$. For instance, with the parameter $\boldsymbol{\theta} = (\sigma^2, \phi)$, the Matérn class (Stein, 2012) covariance kernel is widely used, where σ^2 controls the overall variance of the process, and ϕ determines the range of spatial correlation. Let $\mathbf{C}_{\boldsymbol{\theta}} = \sigma^2\mathbf{R}_\phi$ be the $n \times n$ covariance matrix obtained from the kernel $\mathbf{K}_{\boldsymbol{\theta}}(\mathbf{h})$ defined above. Here $\mathbf{R}_\phi$ is a positive definite correlation matrix. Then the distribution of $\mathbf{W}$ is $f_W(\mathbf{W}|\boldsymbol{\theta}) \propto |\mathbf{C}_{\boldsymbol{\theta}}|^{-1/2} \exp(-\frac{1}{2}\mathbf{W}^\top\mathbf{C}_{\boldsymbol{\theta}}^{-1}\mathbf{W})$. To account for measurement errors, the independent nugget effect can be added into this model. For a lattice domain, $\mathbf{W}$ follows a Gaussian Markov random field (GMRF) (Besag, 1974) with mean zero. GMRF is defined by its neighbor structure using the $n \times n$ adjacency matrix $\mathbf{A}$: $A_{i,j} = 1$ if the ith location and jth location are neighbors, and 0 otherwise. Then, $f_W(\mathbf{W}|\boldsymbol{\theta}) \propto \boldsymbol{\theta}^{\text{rank}(\mathbf{Q})/2} \exp(-\frac{\theta}{2}\mathbf{W}^\top\mathbf{Q}\mathbf{W})$, where $\mathbf{Q}$ =diag$(\mathbf{A}\mathbf{1}) - \mathbf{A}$ and $\boldsymbol{\theta}$ determines the smoothness of the process.

With the spatial random effects defined above, we can write a link function as

$$g\{E[\mathbf{Z}|\mathbf{W},\boldsymbol{\beta}]\} = \mathbf{X}\boldsymbol{\beta} + \mathbf{W}. \tag{2.1}$$

Here, the observed response $\mathbf{Z}$ is conditionally independent for the given $\mathbf{W}$ and $\boldsymbol{\beta}$. We assume that the conditional distribution of $\mathbf{Z}$ is from the exponential family as

$$f_{\mathbf{Z}|\mathbf{W}}(\mathbf{Z}|\mathbf{W},\boldsymbol{\beta}) = \exp(\mathbf{Z}^\top(\mathbf{X}\boldsymbol{\beta} + \mathbf{W}) - \mathbf{1}^\top b(\mathbf{X}\boldsymbol{\beta} + \mathbf{W}) + \mathbf{1}^\top c(\mathbf{Z})), \tag{2.2}$$

where $b(\cdot), c(\cdot)$ are known. With the model parameters $\boldsymbol{\psi} = (\boldsymbol{\beta}, \boldsymbol{\theta})$, the likelihood function can be written as

$$L(\boldsymbol{\psi}|\mathbf{Z}) = \int_{R^n} f_{\mathbf{Z}|\mathbf{W}}(\mathbf{Z}|\mathbf{W},\boldsymbol{\beta}) f_{\mathbf{W}}(\mathbf{W}|\boldsymbol{\theta}) d\mathbf{W}. \tag{2.3}$$

The number of random effects grows with the size of the data, which makes evaluating the likelihood function difficult. Therefore, the direct maximization of (2.3) is infeasible.

2.2 Laplace Approximation and Computational Challenges

Laplace approximations have been studied for maximum likelihood inference of SGLMMs. Evangelou et al. (2011), Bonat and Ribeiro (2016) use the Laplace method, which approximates the integrand using a Gaussian distribution. These works are closely related to the idea of INLA (Rue et al., 2009) in Bayes approaches. Let $Q(\mathbf{W})$ be the sum of the log-likelihood from exponential families and the multivariate normal log-likelihood for the latent variable $\mathbf{W}$. $Q(\mathbf{W})$ is a unimodal and bounded function of n-dimensional random effects $\mathbf{W}$. Then, using the Laplace method, the likelihood function in (2.3) can be approximated as

$$L(\boldsymbol{\psi}|\mathbf{Z}) = \int_{R^n} \exp\left(Q(\mathbf{W})\right) d\mathbf{W} \approx (2\pi)^{n/2} \left| -\frac{\partial^2 Q(\widehat{\mathbf{W}})}{\partial \mathbf{W} \partial \mathbf{W}^\top} \right|^{-1/2} \exp\left(Q(\widehat{\boldsymbol{W}})\right), \tag{2.4}$$

where $\widehat{\mathbf{W}}$ is the value that maximizes $Q(\mathbf{W})$. The Laplace approximation in (2.4) requires optimizing the integrand and calculating the second derivative of $Q(\mathbf{W})$ (Hessian matrix) for a fixed parameter value $\boldsymbol{\psi}$. However, since the dimension of the random effects grows with the number of observed locations, such optimizations do not generally work well for large data sets. To address these issues, we develop a projection-based Laplace method, as shown in the following section.

Chapter 3

Fast Laplace Approximation

3.1 Dimension Reduction through Projection

To address the computational and inferential challenges of such models, projection methods have been developed for both continuous (Guan and Haran, 2018) and lattice (Hughes and Haran, 2013) spatial domains. The main idea is to reduce the dimension of the latent variables from n to m based on $n \times m$ projection matrix $\mathbf{M}$. We note that m is much lower than n; for instance, in US COVID-19 data example (Section 5.1) we use $m = 207$ for $n = 3,108$.

In the continuous domain, the projection matrix is based on the covariance of the latent variable. For the zero-mean Gaussian process $\mathbf{W}$, the covariance matrix is $\mathbf{C}_{\boldsymbol{\theta}} = \sigma^2\mathbf{R}_\phi$, where σ^2 is the overall variance and ϕ is the range parameter. Taking the first m principal components of $\mathbf{R}_\phi$, the projection matrix $\mathbf{M} = \mathbf{U}_\phi\mathbf{D}_\phi^{1/2}$ is computed. Here, $\mathbf{U}_\phi$ is the $n \times m$ matrix of the first m eigenvectors of $\mathbf{R}_\phi$ and, $\mathbf{D}_\phi$ is the diagonal matrix with corresponding eigenvalues. Then the reduced-dimensional model is

$$\begin{aligned} g\{E[\mathbf{Z}|\boldsymbol{\beta}, \mathbf{M}, \boldsymbol{\delta}]\} &= \mathbf{X}\boldsymbol{\beta} + \mathbf{M}\boldsymbol{\delta} \\ \boldsymbol{\delta} &\sim N(0, \sigma^2\mathbf{I}). \end{aligned} \tag{3.1}$$

However, this requires the eigendecomposition of the $n \times n$ correlation matrix $\mathbf{R}_\phi$ for each ϕ update, which is computationally demanding for large spatial data. Therefore, Guan and Haran (2018) use a stochastic version of this for their implementation. We provide a summary of this in the supplementary material.

In the lattice domain, $\mathbf{M}$ is constructed based on the underlying graph structure as well as the covariates of interest. With the adjacency matrix $\mathbf{A}$, the Moran operator is $\mathbf{P}^{\perp}\mathbf{A}\mathbf{P}^{\perp}$, where $\mathbf{P} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ and $\mathbf{P}^{\perp} = \mathbf{I} - \mathbf{P}$. By taking the largest m principal components of $\mathbf{P}^{\perp}\mathbf{A}\mathbf{P}^{\perp}$, the projection matrix $\mathbf{M}$ can be constructed. Then the reduced-dimensional model in Hughes and Haran (2013) can be written as

$$\begin{aligned} g\{E[\mathbf{Z}|\boldsymbol{\beta}, \mathbf{M}, \boldsymbol{\delta}]\} &= \mathbf{X}\boldsymbol{\beta} + \mathbf{M}\boldsymbol{\delta} \\ f_{\boldsymbol{\delta}}(\boldsymbol{\delta}|\theta) &\propto \theta^{m/2} \exp(-\frac{\theta}{2}\boldsymbol{\delta}^{\top}\mathbf{M}^{\top}\mathbf{Q}\mathbf{M}\boldsymbol{\delta}). \end{aligned} \tag{3.2}$$

In what follows, we provide projection-based Laplace methods that can provide accurate estimation and prediction quickly. Compared with simulation-based methods such as MCEM (Guan and Haran, 2019) and MCML (Park and Haran, 2020), our methods can be an easier alternative in that users do not have to tune numerous components manually as in convergence analysis for Monte Carlo samples. Furthermore, our methods can provide accurate standard errors for covariance parameters.

3.2 Projection-based Laplace Method

Here, we describe a fast Laplace method for SGLMMs. We apply our method to both continuous and lattice domains. Based on the projection approaches described in the previous section, a reduced-dimensional representation of the likelihood function is

$$L(\boldsymbol{\psi}|\mathbf{Z}) = \int_{R^m} f_{\mathbf{Z}|\boldsymbol{\delta}}(\mathbf{Z}|\boldsymbol{\beta}, \mathbf{M}, \boldsymbol{\delta}) f_{\boldsymbol{\delta}}(\boldsymbol{\delta}|\boldsymbol{\theta}) d\boldsymbol{\delta} = \int_{R^m} \exp\left(Q(\boldsymbol{\delta})\right) d\boldsymbol{\delta}, \tag{3.3}$$

where

$$Q(\boldsymbol{\delta}) = \mathbf{Z}^{\top}(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\boldsymbol{\delta}) - \mathbf{1}^{\top}b(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\boldsymbol{\delta}) + \mathbf{1}^{\top}c(\mathbf{Z}) - \frac{m}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\boldsymbol{\delta}^{\top}\boldsymbol{\delta}. \tag{3.4}$$

$Q(\boldsymbol{\delta})$ is the sum of the log-likelihood from exponential families and the multivariate normal log-likelihood for the reduced dimensional random effects $\boldsymbol{\delta}$. For the Laplace approximation in (2.4), we need the optimized $\widehat{\boldsymbol{\delta}}$ from $Q(\boldsymbol{\delta})$ for the given model parameter $\boldsymbol{\psi}$. The projection-based Laplace method can dramatically reduce computational costs. This is because, compared with $Q(\mathbf{W})$ in

Bonat and Ribeiro (2016), solving $Q(\boldsymbol{\delta})$ is a much lower-dimensional ($m << n$) maximization problem. Even with long computing time, the estimates from the original method (Bonat and Ribeiro, 2016) are unstable for the problems considered in our manuscript ($n > 1,000$), because this requires high-dimensional optimization with each iteration. To obtain $\widehat{\boldsymbol{\delta}}$, we use the following iterative Newton-Raphson method as

$$\boldsymbol{\delta}^{+} = \boldsymbol{\delta} - \Big(\frac{\partial^2 Q(\boldsymbol{\delta})}{\partial\boldsymbol{\delta}\partial\boldsymbol{\delta}^{\top}}\Big)^{-1}\frac{\partial Q(\boldsymbol{\delta})}{\partial\boldsymbol{\delta}}, \tag{3.5}$$

where the first and second derivatives are

$$\begin{aligned}\frac{\partial Q(\boldsymbol{\delta})}{\partial\boldsymbol{\delta}^{\top}} &= \mathbf{Z}^{\top}\mathbf{M} - b'(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\boldsymbol{\delta})^{\top}\mathbf{M} - \frac{1}{\sigma^2}\boldsymbol{\delta}^{\top}\\ \frac{\partial^2 Q(\boldsymbol{\delta})}{\partial\boldsymbol{\delta}\partial\boldsymbol{\delta}^{\top}} &= -\mathbf{M}^{\top}\text{diag}(b''(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\boldsymbol{\delta}))\mathbf{M} - \frac{1}{\sigma^2}\mathbf{I}.\end{aligned} \tag{3.6}$$

This is repeated until convergence (inner optimization).

Then, the Laplace approximation for the reduced-dimensional representation is

$$L(\boldsymbol{\psi}|\mathbf{Z}) = \int_{R^m}\exp\left(Q(\boldsymbol{\delta})\right)d\boldsymbol{\delta} \approx (2\pi)^{m/2}\Big|-\frac{\partial^2 Q(\widehat{\boldsymbol{\delta}})}{\partial\boldsymbol{\delta}\partial\boldsymbol{\delta}^{\top}}\Big|^{-1/2}\exp\Big(Q(\widehat{\boldsymbol{\delta}})\Big), \tag{3.7}$$

where the reduced-dimensional log-likelihood is

$$\begin{aligned}\widehat{l}(\boldsymbol{\psi}|\mathbf{Z}) &= \frac{m}{2}\log(2\pi) - \frac{1}{2}\log\Big|-\frac{\partial^2 Q(\widehat{\boldsymbol{\delta}})}{\partial\boldsymbol{\delta}\partial\boldsymbol{\delta}^{\top}}\Big| + Q(\widehat{\boldsymbol{\delta}})\\ &= \frac{m}{2}\log(2\pi) - \frac{1}{2}\log\Big|\mathbf{M}^{\top}\text{diag}(b''(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\widehat{\boldsymbol{\delta}}))\mathbf{M} + \frac{1}{\sigma^2}\mathbf{I}\Big|\\ &+ \mathbf{Z}^{\top}(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\widehat{\boldsymbol{\delta}}) - \mathbf{1}^{\top}b(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\widehat{\boldsymbol{\delta}}) + \mathbf{1}^{\top}c(\mathbf{Z}) - \frac{m}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\widehat{\boldsymbol{\delta}}^{\top}\widehat{\boldsymbol{\delta}}.\end{aligned} \tag{3.8}$$

This function is maximized over the model parameter value $\boldsymbol{\psi}$ using a numerical optimization (outer optimization). Then, the asymptotic distribution of the MLE $\widehat{\boldsymbol{\psi}}$ is $N(\boldsymbol{\psi}^{*}, \mathbf{I}^{-1}(\widehat{\boldsymbol{\psi}}))$, where $\boldsymbol{\psi}^{*}$ is the true value and $\mathbf{I}^{-1}(\widehat{\boldsymbol{\psi}})$ is the observed Fisher information.

In the lattice spatial domain, $\mathbf{W}$ follows the GMRF. Then, the $Q(\boldsymbol{\delta})$ function can be defined as

$$Q(\boldsymbol{\delta}) = \mathbf{Z}^{\top}(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\boldsymbol{\delta}) - \mathbf{1}^{\top}b(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\boldsymbol{\delta}) + \mathbf{1}^{\top}c(\mathbf{Z}) + \frac{m}{2}\log(\theta) - \frac{\theta}{2}\boldsymbol{\delta}^{\top}\mathbf{M}^{\top}\mathbf{Q}\mathbf{M}\boldsymbol{\delta}, \tag{3.9}$$

and their derivatives are

$$\begin{aligned}\frac{\partial Q(\boldsymbol{\delta})}{\partial \boldsymbol{\delta}^\intercal} &= \mathbf{Z}^\intercal\mathbf{M} - b'(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\boldsymbol{\delta})^\intercal\mathbf{M} - \theta\boldsymbol{\delta}^\intercal\mathbf{M}^\intercal\mathbf{Q}\mathbf{M} \\ \frac{\partial^2 Q(\boldsymbol{\delta})}{\partial \boldsymbol{\delta}\partial \boldsymbol{\delta}^\intercal} &= -\mathbf{M}^\intercal \mathrm{diag}(b''(\mathbf{X}\boldsymbol{\beta} + \mathbf{M}\boldsymbol{\delta}))\mathbf{M} - \theta\mathbf{M}^\intercal\mathbf{Q}\mathbf{M}.\end{aligned} \tag{3.10}$$

Similar to the continuous domain case, we can construct the Laplace approximation for the reduced-dimensional likelihood function. We optimize the logarithm of the variance parameters ($\log(\sigma^2)$, $\log(\phi)$) for numerical stability. Algorithm 1 summarizes our fast Laplace method.

Algorithm 1 A projection-based Laplace method

For $(t+1)$st update, given $\boldsymbol{\psi}_t$
Step 1. Inner optimization:
Obtain $\widehat{\boldsymbol{\delta}}$ using an iterative Newton-Raphson method as

$$\boldsymbol{\delta}^+ = \boldsymbol{\delta} - \Big(\frac{\partial^2 Q(\boldsymbol{\delta})}{\partial \boldsymbol{\delta}\partial \boldsymbol{\delta}^\intercal}\Big)^{-1}\frac{\partial Q(\boldsymbol{\delta})}{\partial \boldsymbol{\delta}}$$

Step 2. Outer optimization:
Obtain $\boldsymbol{\psi}_{t+1}$ using a numerical optimization of

$$\widehat{l}(\boldsymbol{\psi}|\mathbf{Z}) = \frac{m}{2}\log(2\pi) - \frac{1}{2}\log\Big|-\frac{\partial^2 Q(\widehat{\boldsymbol{\delta}})}{\partial \boldsymbol{\delta}\partial \boldsymbol{\delta}^\intercal}\Big| + Q(\widehat{\boldsymbol{\delta}})$$

Repeat Steps 1 and 2 until convergence, which gives MLEs $\widehat{\boldsymbol{\psi}}$.

3.3 Rank Selection

For areal data sets, Hughes and Haran (2013) suggest choosing the rank from the desired proportion of variation (e.g., 90% using the first several principal components). For point-referenced data sets over continuous domain, Guan and Haran (2019), Lee and Haran (2019) select the rank based on fitting the non-spatial GLMs as a preliminary step. Here, we adopt some of these ideas and recommend the following steps:

1. We split data into training and validation sets. For a given initial value of $\phi^{(0)}$ (e.g., first quartile of distance matrix), we can construct a synthetic spatial variable $\mathbf{U}_{\phi_{(0)}}\mathbf{D}^{1/2}_{\phi_{(0)}}$ from the eigencomponents of $\mathbf{R}_{\phi_{(0)}}$.

2. We use maximum likelihood approaches (`glm` function in `R`) to fit the standard GLM on a covariate $[\mathbf{X}, \mathbf{U}_{\phi_{(0)}}\mathbf{D}^{1/2}_{\phi_{(0)}}]$.

3. We can repeat Step 1-2 across varying ranks. Then we select the rank m that has the lowest out-of-sample cross-validated mean squared prediction error (CVMSPE).

Chapter 4

Simulation study

To validate our methods, we conduct simulation studies to count and binary data for both the continuous and the lattice spatial domains. The code for this is implemented in `R`. For our method, we only need to obtain the first m eigencomponents quickly. To implement this efficiently, we use the `RSpectra` package. The source code can be downloaded from the following repository (https://github.com/jwpark88/projLaplace). In the supplementary material, we also provide a Poisson example in a continuous domain.

4.1 Negative Binomial Example in a Continuous Domain

For the fixed model parameters $(\beta_1, \beta_2, \sigma^2, \phi) = (1, 1, 1, 0.2)$, we simulate a negative binomial data set with $n = 1,400$ observations in the $[0, 1]^2$ domain. Random effects $\mathbf{W}$ are generated from the Matérn class (Stein, 2012) covariance kernel with a smoothing parameter of 2.5. Then we use the log-link function $\log(\boldsymbol{\mu}) = \mathbf{X}\boldsymbol{\beta} + \mathbf{W}$, where $\mathbf{X}$ is the coordinate for the random effects $\mathbf{W}$. We set the true dispersion parameter ζ for the negative binomial distribution to 2. We use the first $1,000$ observations for the model fitting and 400 for the validation. We obtain the initial values for the Laplace approximation from the GLM estimates. We chose $m = 38$ by following the procedure in Chapter 3.3 (Figure 4.1).

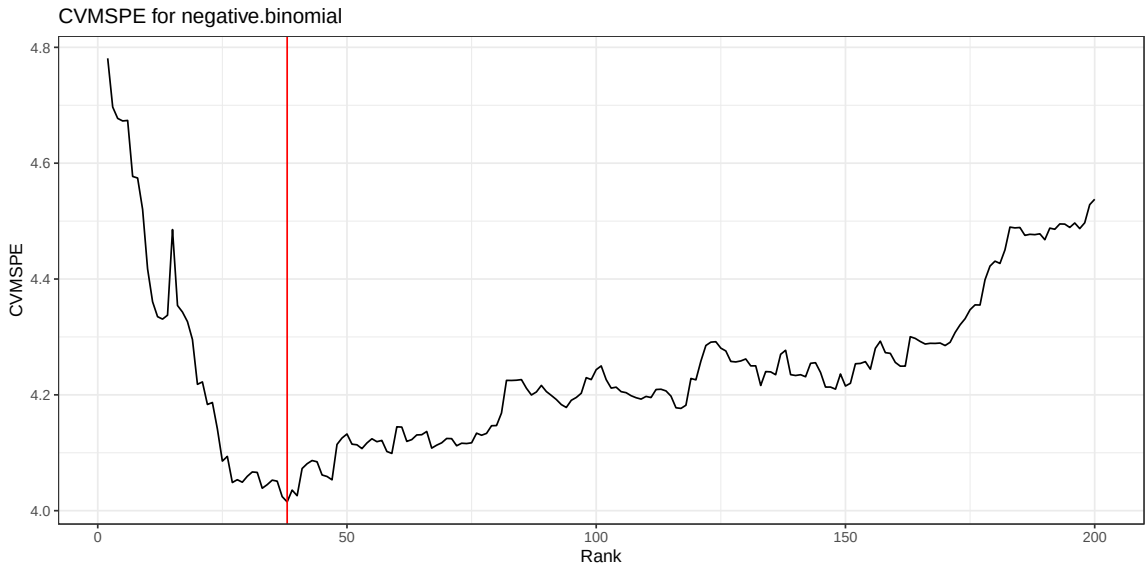

Figure 4.1: CVMSPE plot for ranks from 2 to 200. The vertical red line denotes the lowest CVMPSE (rank = 38)

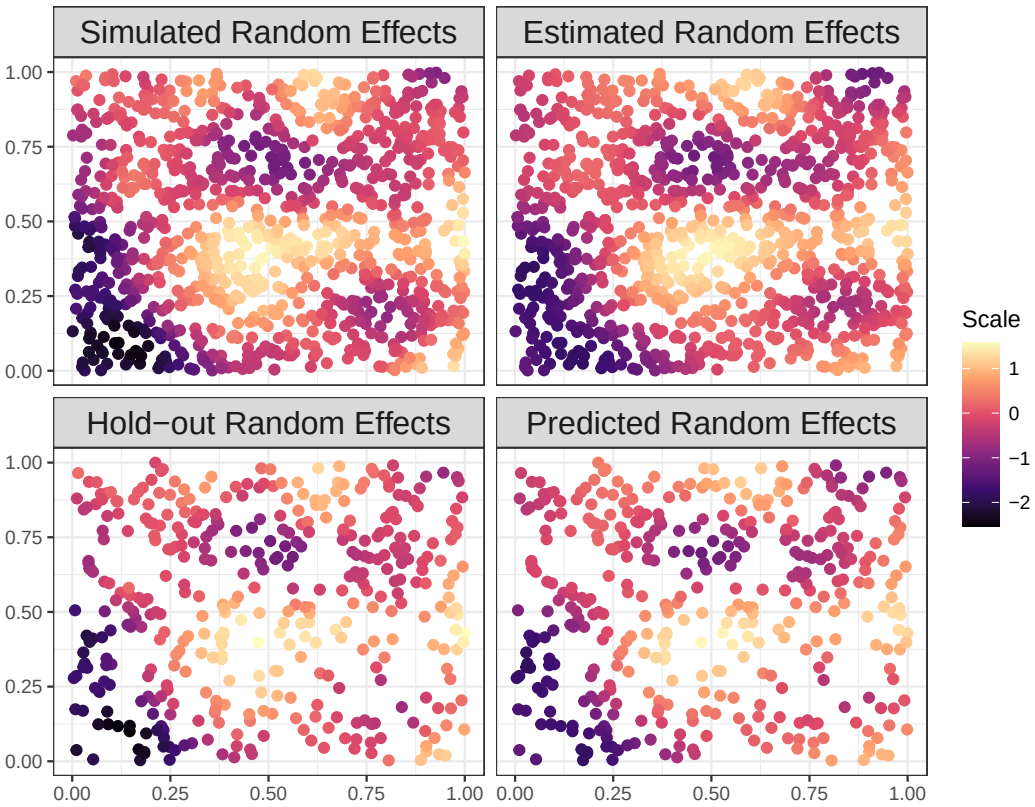

Figure 4.2: The first row represents the simulated and estimated random effects at the observed locations. The second row represents the out-of-sample cross-validated random effects and predicted random effects at the unobserved locations.

Figure 4.2 compares the simulated and the predicted random effects. The results suggest that they have similar spatial patterns. To investigate the performance of our method, we conduct simulation studies with varying n (data size) and m (rank) values. Especially, we consider $n = 1,400, 2,800, 5,600$, where $1,000, 2,000, 4,000$ observations are used for model fitting respectively. For each n, we consider three different choices of m: (1) 2% of training data, (2) recommended rank from Section 3.3, and (3) 10% of training data. This results in 9 combinations of n and m; simulation is repeated 100 times for each combination. To measure the parameter estimation accuracy, we calculate the mean square error (MSE), mean of estimates, coverage of each param-

eter. To assess prediction accuracy, we calculate the mean square prediction error (MSPE) from test data sets. Since the recommended rank is different for each simulated data set, we report the average chosen rank from 100 simulations. Since the ratio between the covariance parameters is often of interest under fixed-domain asymptotics (Zhang, 2004), we provide results for σ^2/ϕ. Note that we can easily obtain confidence intervals for covariance parameters, which is challenging under other simulation-based methods such as MCML (Park and Haran, 2020) and MCEM (Guan and Haran, 2019). For the given ϕ value, they need Monte Carlo samples of the random effects to approximate the log-likelihood (MCML) or the conditional expectation (MCEM); this makes it challenging to calculate a gradient of ϕ to obtain standard errors. Table 6.1 summarize results.

When m is at or larger than a recommended rank, our projection-based Laplace methods provide estimates accurately, and the coverages for the parameters are close to the nominal rate (95%). Furthermore, prediction accuracies from validation data sets are reasonably small. With increasing m, the amount of information loss due to the dimension reduction becomes decreased at the expense of computing time. However, diminishing returns are observed based on previous works (Hughes and Haran, 2013, Guan and Haran, 2018); increasing m beyond certain points has little benefits but increases computing time. We also observe that the proposed method provides slightly more accurate results (estimation/prediction) with increasing m. However, such differences are marginal compared to results obtained from the "recommended" rank. Therefore, the "recommended" rank can be a practical choice for fast inference. Our approach performs well in terms of estimation and prediction aspects even for large n. We can conduct accurate maximum likelihood inference within a reasonable amount of time.

4.2 Binomial Example in a Continuous Domain

We use the model parameters $(\beta_1, \beta_2, \sigma^2, \phi) = (1, 1, 1, 0.2)$ to generate a binary data set with $n = 1,400$ in the unit domain. Random effects are simulated from the Matérn covariance with a smoothing parameter of 2.5. For the given simulated $\mathbf{W}$, we use a logit link function $\text{logit}(p) = \mathbf{X}\boldsymbol{\beta} + \mathbf{W}$, where $\mathbf{X}$ is the coordinate for the random effects $\mathbf{W}$. For the model fitting, we use the first $1,000$ observations, and 400 for the prediction. Similar to the negative binomial example, we chose a rank $m = 21$ by following the procedure in Section 3.3 (Figure 4.3). We obtain the initial

values of the Laplace method from the GLM estimates.

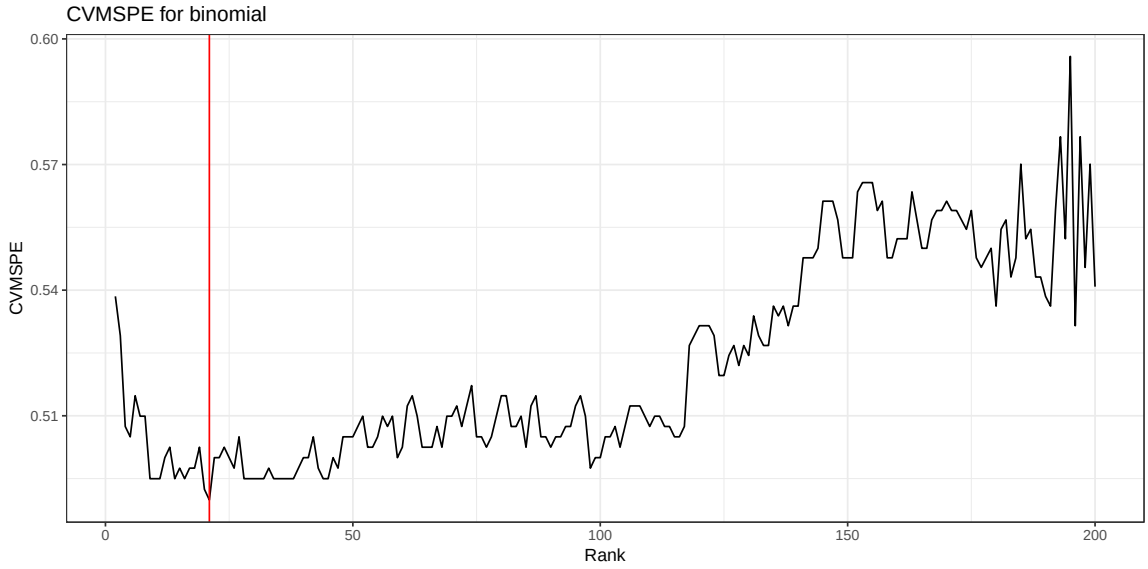

Figure 4.3: CVMSPE plot for ranks from 2 to 200. The vertical red line denotes the lowest CVMPSE (rank = 21)

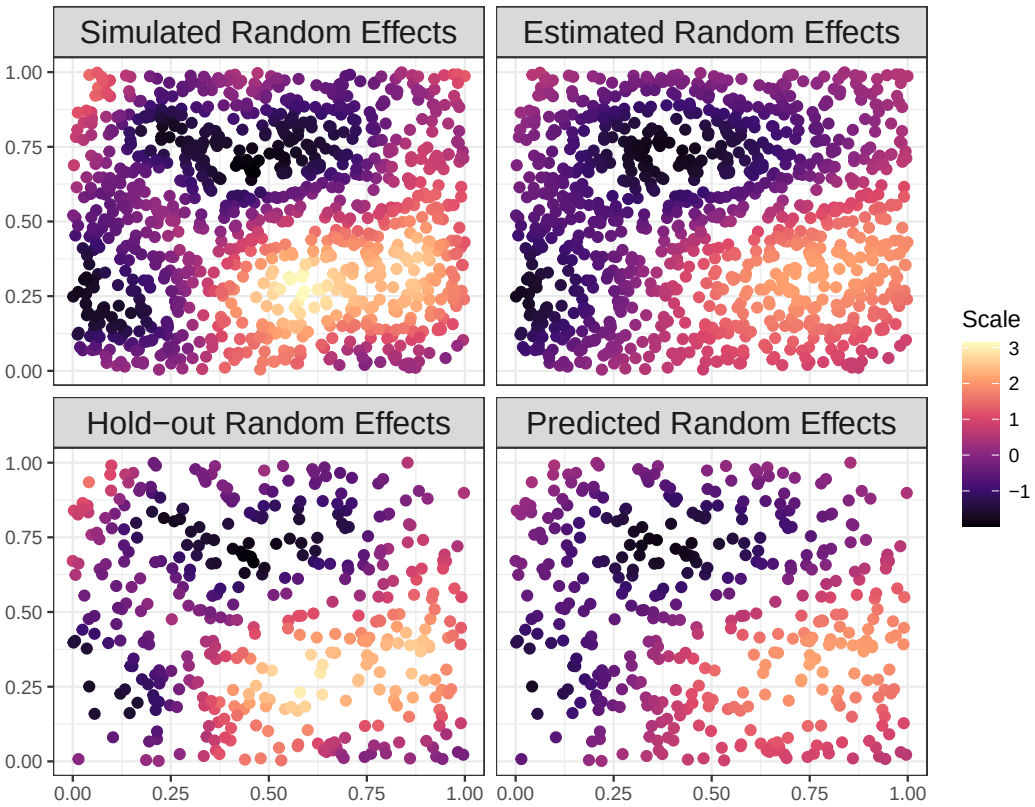

Figure 4.4: The first row represents the simulated and estimated random effects at the observed locations. The second row represents the out-of-sample cross-validated random effects and predicted random effects at the unobserved locations.

The simulated and predicted spatial random effects have similar patterns (Figure 4.4). To validate our method, we conduct simulation studies with varying n and m as in the previous section (Table 6.2). We observe that our projection-based Laplace methods provide accurate estimation, and the coverages are close to the nominal rate (95%) even with the smallest m (i.e., 2% of training data size). We observe that a recommended ranks are chosen as smaller values compared to the negative binomial cases. MSPEs from test data sets are also small for different choices of m. Similar to the negative binomial cases, we can conduct accurate maximum likelihood inference quickly for n. Especially when we use a recommended rank for $n = 5,600$, the fast Laplace method provides

accurate maximum likelihood inference within an hour.

4.3 Poisson Example in a Lattice Discrete Domain

Following the simulation settings in Hughes and Haran (2013), we show the use of our approach in a lattice domain. As in the continuous domain examples, we test the sensitivity of our method by comparing the performance across different n, m values. With the fixed parameter values $(\beta_1, \beta_2, \theta) = (1, 1, 6)$ we simulate Poisson data sets with $n = 900$ (30×30 lattice), $2,500$ (50×50 lattice), and $4,900$ (70×70 lattice). We simulate $\mathbf{W}$ from $N(0, (\theta\mathbf{M}'\mathbf{Q}\mathbf{M})^{-1})$, where $\mathbf{M}$ is obtained by taking the first k eigenvectors of the Moran operator (i.e., $\mathbf{M} \in R^{n\times k}$). We use $k = 400, 1200, 2400$ for $n = 900, 2,500, 4,900$ repectively. Then, we use the log-link function to generate a count data set. Similar to the previous simulation studies, we consider m as (1) 2% of training data, (2) recommended rank from Section 3.3 and (3) 10% of training data. Simulation is repeated 100 times for each n, m combination. Table 6.3 summarize results.

In general, our projection-based Laplace methods provide reasonably accurate estimates for regression coefficients when m is at or larger than a recommended rank. We observe that estimates are close to the simulated truth with small MSEs. However, with increasing sample size ($n \geq 2,500$), it becomes more challenging to achieve the nominal rate (95% coverage), even with m as 10% of training data. Therefore, we conduct additional experiments with m as 20% of training data and observe the improved coverages. This implies that compared to the point-referenced data examples, we need larger m to achieve the nominal rate. For researchers who want to have conservative results, we suggest choosing m as 10%-20% of training data size at the expense of computing time. Furthermore, we observe that the covariance parameter θ is slightly biased even with large m; this results in low coverage ($< 95\%$). Note that the correct estimation of θ is challenging for conditional autoregressive models, as reported by Hughes and Haran (2013).

4.4 Comparison with the Standard Laplace Method

Here, we compare the performance of our method with that of the standard Laplace method (Bonat and Ribeiro, 2016) under different numbers of data points. We use the same simulation setting as in the previous examples. Figure 4.5 shows that computing time increases dramatically for the standard Laplace algorithm (Bonat and Ribeiro, 2016), whereas our method can obtain the

maximum likelihood estimates quickly.

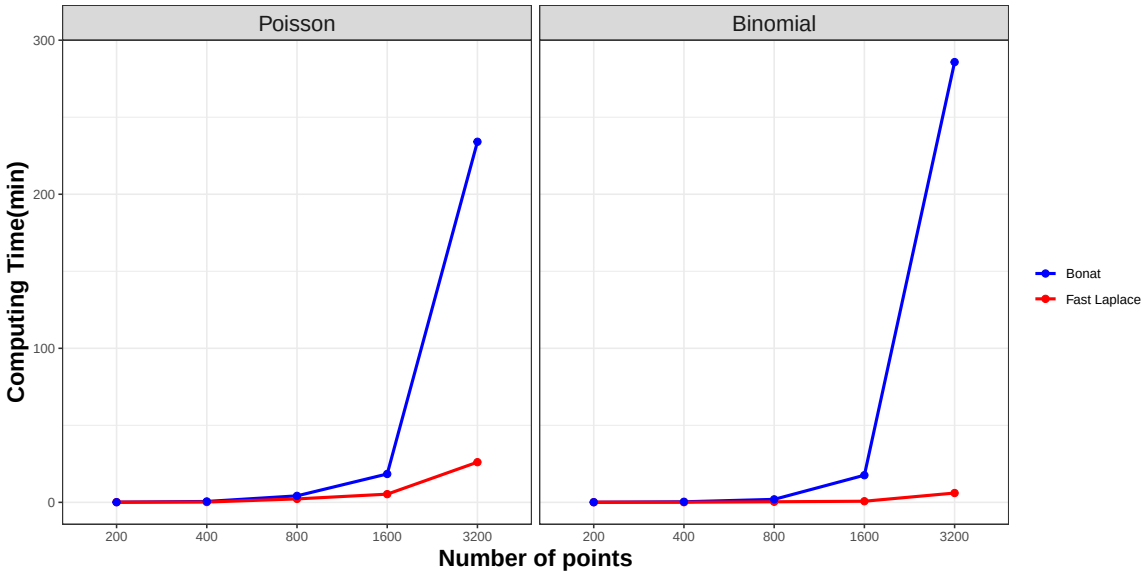

Figure 4.5: The observed computing time for the algorithms for the Poisson and binomial examples.

Furthermore, we compare our method with competitors (standard Laplace (Bonat and Ribeiro, 2016), projection-based MCML (Park and Haran, 2020), MCMC (Guan and Haran, 2018)) in the supplementary material (Section D). We compare different algorithms in large binomial data sets with $n = 2,800, 5,600$ using the same simulation settings in Section 4.2. In summary, our algorithm provides comparable estimations and predictions to competitors within a shorter time. We observe that the projection-based Laplace method is about 6 times faster than the standard Laplace method. In addition, our method can achieve the nominal rate (95% coverage) for covariance parameters as well, which is challenging to projection-based MCML (see the supplementary material for more details).

Note that the reported computing time is obtained from our simulation settings; therefore, it is not absolute but relative scales. Both Laplace methods update model parameters from outer optimization (Step 2 in Algorithm 1), which has order p complexity. Therefore, both algorithms will take longer with an increasing number of spatial covariates.

Chapter 5

Real data analysis

We apply our methods to two real data examples with a large number of observations: (1) COVID-19 count data from US counties and (2) binary patterns of Antarctic ice sheets over the continuous domain. In both cases, our approach provides MLEs and predictions quickly.

5.1 US COVID-19 Data

Caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) coronavirus disease 2019 (COVID-19) was first reported in Wuhan, Hubei providence, China in December 2019 (WHO, 2020). As of March 2021, there have been more than 100 million confirmed cases, with more than 2 million deaths worldwide. The disease has spread rapidly through contact with infected people (CDC, 2020), which has led to significant societal challenges. Understanding the spatial patterns of confirmed cases is valuable not only for scientific reasons but also for public health, such as developing vaccination and intervention strategies to control epidemics. Furthermore, investigating the relationship between spatial covariates can provide useful insights into the mechanism of disease spread. The estimated regression coefficients tell us whether there is a positive (or negative) relation between each spatial covariate and the confirmed cases (count response). Our method provides accurate maximum likelihood inference for thousands of observations quickly.

Here, we study COVID-19 confirmed cases data set collected from the Centers for Disease Control and Prevention(CDC) and the Census Bureau. The data set provides a cumulative number of confirmed cases from 3,108 US counties between January 1, 2020, and July 11, 2020. As co-

variates, we use the percentage of white residents, the percentage of black residents, the percentage of male, and the percentage of older people ($\geq$ 65). We use the population of each county as an offset. We obtain the initial values of the model parameters from the Poisson GLM estimates. We use a reduced rank $m = 207$, which has the lowest CVMSPE (Figure 5.2). The projection-based Laplace method takes about 45 minutes. Regular Laplace methods (Bonat and Ribeiro, 2016) are computationally expensive because they have to deal with a 3,108-dimensional optimization to find a mode of the Laplace approximation for the fixed model parameter value.

Table 6.4 shows the parameter estimates and their confidence intervals. We observe that the black proportion and the male proportion show a positive relationship, while the white proportion and the old people proportion have a negative relationship with the COVID-19 risk. Note that our study is county-level; we cannot interpret this result at the individual level. For instance, we do not imply that older people have a low COVID-19 risk, but rather that the county with a high population of older people has a low risk. This is reasonable because counties with a higher proportion of older people would have less economic/daily activities; this results in a low COVID-19 risk. Figure 5.1 shows that there are similar spatial patterns between the observed and fitted number of confirmed cases. We detect three high-intensity regions near California, Florida, and eastern United States (New York City, New Jersey), suggesting these areas could be disease hotspots. The prediction standard errors are larger at larger predicted values, which is natural as more extreme values tend to be more difficult to predict.

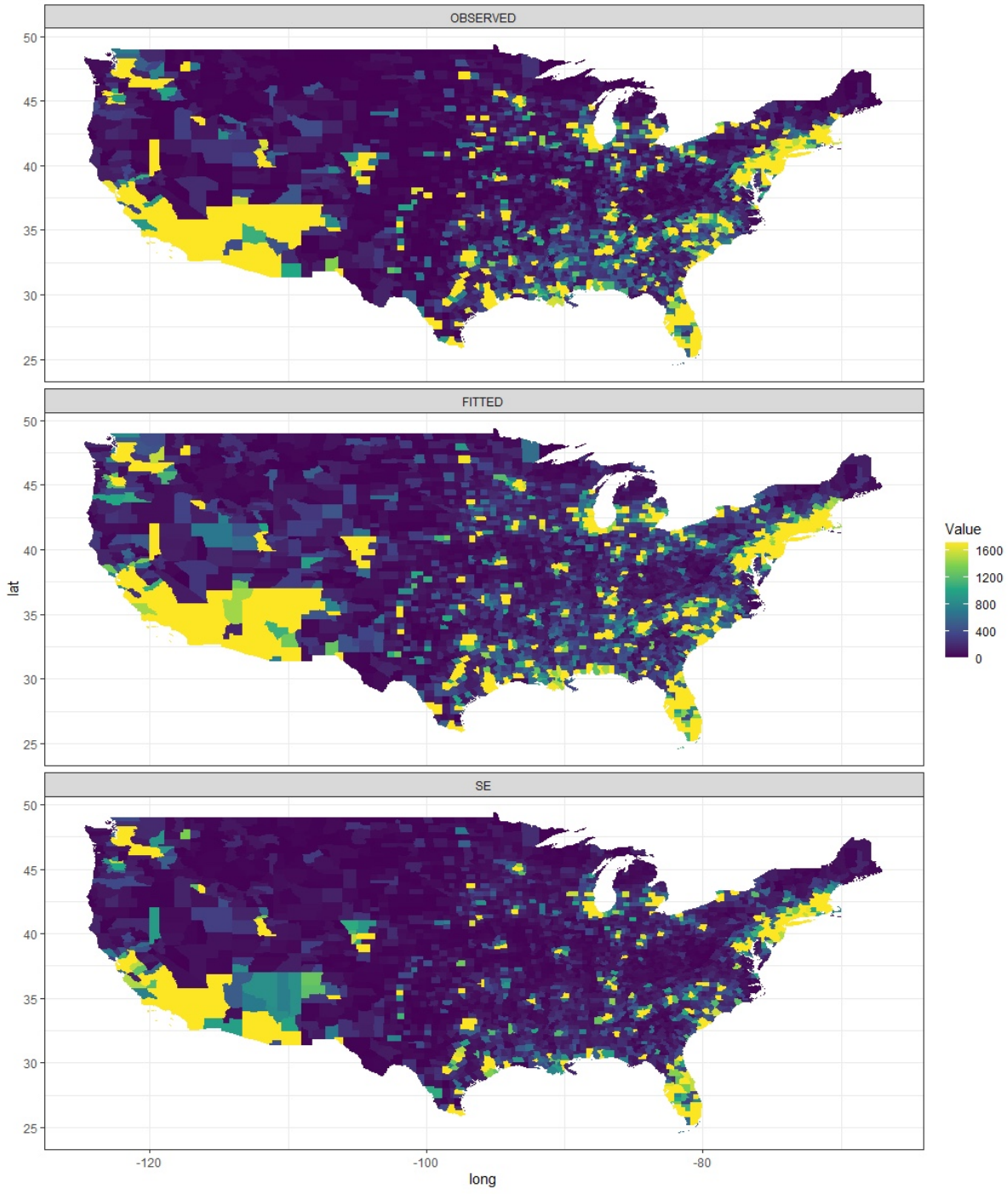

Figure 5.1: The upper panel shows the observed number of confirmed cases by county. The middle panel shows the estimated mean of confirmed cases by county. The lower panel is the corresponding standard error of estimates.

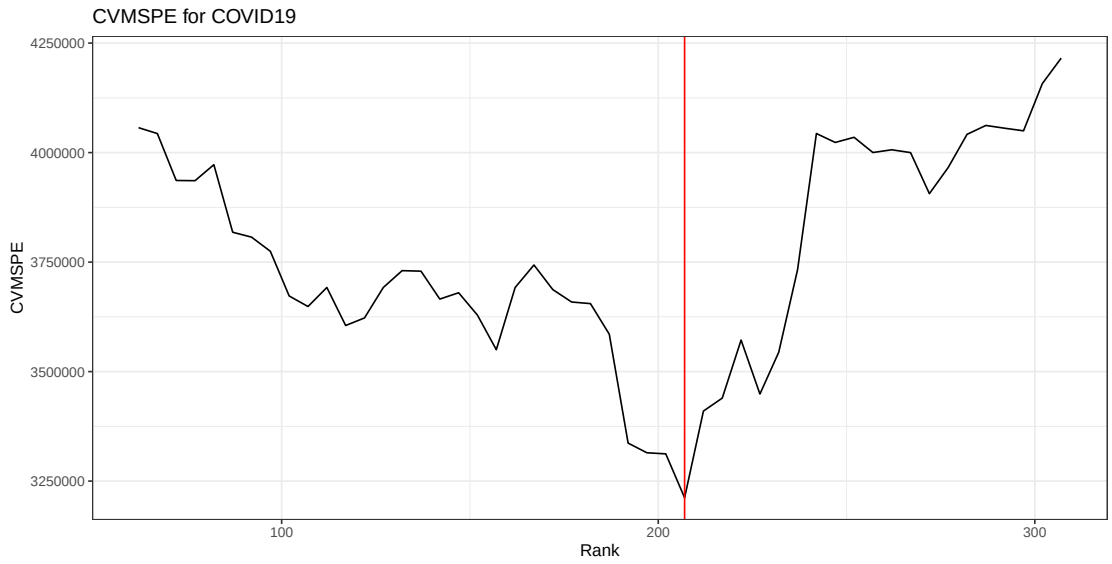

Figure 5.2: CVMSPE plot for US COVID-19 data. The vertical red line denotes the lowest CVMPSE (rank = 207)

5.2 Antarctic Ice Sheet Data

The mass loss from ice sheets may cause a global sea-level rise (Deschamps et al., 2012). Especially, the Antarctic ice sheet contains 30 million cubic kilometers of ice; this is sufficient ice to contribute up to 60 meters to sea-level rise if they were to melt completely (White et al., 2019). Several recent studies (Zhang, 2007, Serreze and Barry, 2011) indicate that some fraction of this ice may melt within the next few hundred years due to global climate change. A significant proportion of the world's population lives within a low-elevation coastal zone (Greve et al., 2011), and sea-level rise poses increased risk for their life. Considering that ice thickness is an important indicator of climate change, understanding the spatial pattern of ice thickness is crucial for future sea-level rise. Despite its importance, providing accurate estimation/prediction of ice thickness is challenging because it is a high-dimensional and non-Gaussian spatial variable. For this study, our method provides accurate interpolation of ice thickness within a reasonable amount of time.

We apply our method to the Antarctic ice sheet data set (Pollard et al., 2015). This data set represents a binary spatial pattern of ice thickness (the binary ice-no ice patterns are derived from

these data). The ice sheet data set is observed with a fine 20 km resolution over 171×171 grid points, centered on the South Pole, and it spans the whole Antarctic continent (see Pollard et al. (2015) for more details). We randomly select 6,000 locations. Then, 4,900 locations are used for training and the remaining 1,100 locations are used for model prediction. As in the simulated examples, we use the initial values for the model parameters taken from the binomial GLM estimates. We choose a reduced rank of 50, which has the lowest CVMSPE.

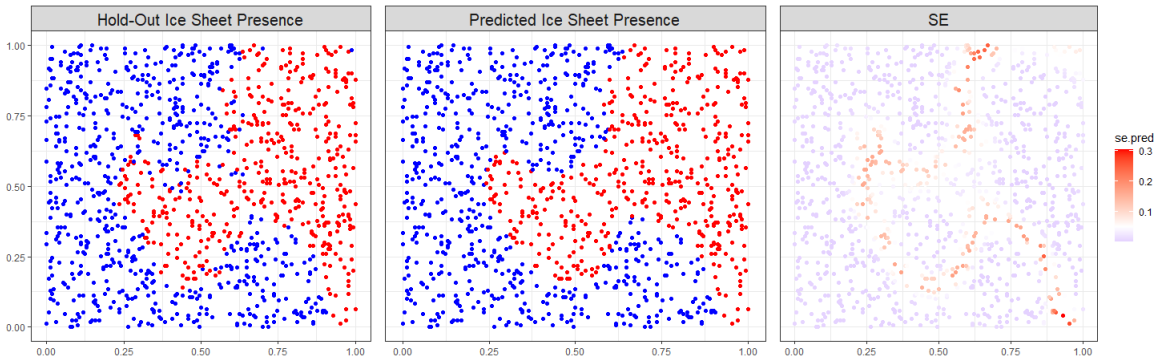

Figure 5.3: The left panel shows the observed ice thickness and the middle panel shows the predicted ice thickness. Red and blue points indicate ice-no ice patterns. The right panel shows the corresponding standard error of estimates.

Our fast Laplace approximation only takes about 50 minutes. Because of the high-dimensional 4,900 optimization for the latent variables, the regular Laplace method (Bonat and Ribeiro, 2016) is infeasible. Projection-based MCEM approaches (Guan and Haran, 2019) and MCML approaches (Park and Haran, 2020) can provide similar computing costs to our method. However, both require numerous components to be tuned, which can lead to practical implementation issues for users. Furthermore, we can obtain standard errors for the range parameter easily from the numerical optimization. Table 6.5 reports the parameter estimates and their confidence intervals. Based on the regression coefficient estimates, we verify that, on average, ice becomes thicker in northeastern directions, which can also be checked from observed ice sheet presence (Figure 5.3). The predictions of the ice thickness patterns are the main interest of this analysis. To classify ice-no ice pattern, we dichotomize the predicted probabilities at 0.5. Figure 5.3 shows that the similar binary spatial

patterns between the observed and predicted locations with accuracy 0.96. We observe that the prediction standard errors are larger at the boundaries of the ice sheet. Predicting the boundary regions are more difficult because of the mixed binary patterns.

Chapter 6

Conclusion

In this manuscript, we develop a projection-based Laplace method for high-dimensional spatial latent variable models. Based on novel projection approaches, we replace a high-dimensional optimization problem with a much lower-dimensional optimization problem to obtain the Laplace approximation of the integrand. We show that our approaches provide accurate maximum likelihood estimations and predictions quickly for both continuous and lattice domains. Compared with simulation-based methods such as MCEM (Guan and Haran, 2019) and MCML (Park and Haran, 2020), our method is automatic in that users can avoid tuning of the algorithm, including the convergence diagnostic of MCMC chains. Therefore, our fast Laplace method may be an useful alternative for maximum likelihood inference. Furthermore, our algorithm can provide accurate standard errors for the estimates, which can be challenging for the MCEM and MCML approaches.

We apply our methods to environmental and epidemiological data sets, providing accurate interpolation. Furthermore, we could obtain scientific insights into the spatial patterns of non-Gaussian responses from regression coefficients. For instance, we observe that the percentage of black residents and male residents have positive relationships with COVID-19 cases. On the other hand, the percentage of white residents and old residents have negative relationships with COVID-19 cases. For the Antarctic ice sheet example, we found that, on average, ice becomes thicker in northeastern directions.

The main contribution of this study is to develop a practical Laplace method for maximum likelihood inference for large non-Gaussian spatial data sets, which frequently arise in environmental sciences. Developing extensions of the projection-based Laplace approach to the high-dimensional

spatio-temporal model may be an interesting direction for future research. Considering that the Laplace approximation is convenient for maximum likelihood inference for latent variable models, the methods and ideas described here in could be applicable to a broader class of problems. Examples include generalized linear latent variable models (Bianconcini and Cagnone, 2012), longitudinal data analysis (Molenberghs and Verbeke, 2005), and stochastic volatility models in finance (Jacquier et al., 2007).

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Table 6.1: Inference results for simulated negative binomial data sets in a continuous domain. For different combinations of n and m, average computing time (minutes), MSPE, mean of estimates, MSE, and coverage are calculated from 100 simulations. Asterisk symbols indicate a recommended rank.

n	m	Time	MSPE	Parameter	True	Mean	MSE	Coverage
1,400	20	1	0.154	β_1	1	1.065	0.057	0.66
				β_2	1	1.043	0.057	0.71
				$\log\zeta$	0.693	0.505	0.062	0.37
				$\log(\sigma^2/\phi)$	1.609	1.727	0.314	0.87
	56$*$	4	0.075	β_1	1	1.005	0.013	0.94
				β_2	1	1.001	0.017	0.89
				$\log\zeta$	0.693	0.664	0.010	0.91
				$\log(\sigma^2/\phi)$	1.609	1.585	0.096	0.95
	100	7	0.063	β_1	1	1.003	0.011	0.95
				β_2	1	1.001	0.013	0.91
				$\log\zeta$	0.693	0.699	0.008	0.97
				$\log(\sigma^2/\phi)$	1.609	1.552	0.100	0.93
2,800	40	18	0.051	β_1	1	1.018	0.007	0.91
				β_2	1	1.001	0.006	0.97
				$\log\zeta$	0.693	0.649	0.006	0.82
				$\log(\sigma^2/\phi)$	1.609	1.555	0.066	0.97
	82$*$	22	0.040	β_1	1	1.016	0.005	0.97
				β_2	1	1.003	0.005	0.98
				$\log\zeta$	0.693	0.683	0.004	0.95
				$\log(\sigma^2/\phi)$	1.609	1.531	0.055	0.95
	200	76	0.039	β_1	1	1.019	0.007	0.94
				β_2	1	1.007	0.007	0.98
				$\log\zeta$	0.693	0.686	0.032	0.96
				$\log(\sigma^2/\phi)$	1.609	1.514	0.056	0.94
5,600	80	58	0.024	β_1	1	1.006	0.003	0.95
				β_2	1	1.001	0.004	0.91
				$\log\zeta$	0.693	0.680	0.002	0.93
				$\log(\sigma^2/\phi)$	1.609	1.492	0.052	0.97
	120$*$	97	0.023	β_1	1	1.007	0.003	0.95
				β_2	1	1.001	0.004	0.93
				$\log\zeta$	0.693	0.686	0.002	0.93
				$\log(\sigma^2/\phi)$	1.609	1.496	0.053	0.96
	400	430	0.023	β_1	1	1.006	0.003	0.96
				β_2	1	0.999	0.004	0.94
				$\log\zeta$	0.693	0.695	0.002	0.93
				$\log(\sigma^2/\phi)$	1.609	1.486	0.053	0.95

Table 6.2: Inference results for simulated binary data sets in a continuous domain. For different combinations of n and m, average computing time (minutes), MSPE, mean of estimates, MSE, and coverage are calculated from 100 simulations. Asterisk symbols indicate a recommended rank.

n	m	Time	MSPE	Parameter	True	Mean	MSE	Coverage
1,400	20	1	0.254	β_1	1	0.993	0.093	0.91
				β_2	1	0.994	0.089	0.90
				$\log(\sigma^2/\phi)$	1.609	1.307	0.534	0.94
	30$*$	1	0.223	β_1	1	1.009	0.090	0.92
				β_2	1	1.012	0.075	0.91
				$\log(\sigma^2/\phi)$	1.609	1.411	0.432	0.91
	100	4	0.211	β_1	1	1.021	0.087	0.96
				β_2	1	1.034	0.075	0.94
				$\log(\sigma^2/\phi)$	1.609	1.520	0.206	0.97
2,800	40	6	0.142	β_1	1	1.008	0.047	0.89
				β_2	1	0.991	0.036	0.95
				$\log(\sigma^2/\phi)$	1.609	1.490	0.170	0.94
	47$*$	7	0.139	β_1	1	1.000	0.046	0.93
				β_2	1	0.985	0.032	0.96
				$\log(\sigma^2/\phi)$	1.609	1.494	0.188	0.92
	200	37	0.136	β_1	1	1.003	0.044	0.91
				β_2	1	0.991	0.032	0.97
				$\log(\sigma^2/\phi)$	1.609	1.503	0.159	0.93
5,600	80	55	0.084	β_1	1	0.990	0.018	0.95
				β_2	1	0.988	0.018	0.97
				$\log(\sigma^2/\phi)$	1.609	1.538	0.108	0.94
	85$*$	56	0.084	β_1	1	0.990	0.018	0.96
				β_2	1	0.987	0.018	0.97
				$\log(\sigma^2/\phi)$	1.609	1.535	0.111	0.93
	400	445	0.084	β_1	1	0.992	0.018	0.95
				β_2	1	0.989	0.018	0.97
				$\log(\sigma^2/\phi)$	1.609	1.540	0.111	0.94

Table 6.3: Inference results for simulated Poisson data sets in a lattice domain. For different combinations of n and m, average computing time (minutes), mean of estimates, MSE, and coverage are calculated from 100 simulations. Asterisk symbols indicate a recommended rank.

n	m	Time	Parameter	True	Mean	MSE	Coverage
900	18	<1	β_1	1	1.026	0.003	0.90
			β_2	1	1.025	0.003	0.94
			$\log\theta$	1.792	1.451	0.341	0.81
	45$*$	<1	β_1	1	1.018	0.003	0.94
			β_2	1	1.017	0.002	0.96
			$\log\theta$	1.792	1.438	0.265	0.70
	90	1	β_1	1	1.014	0.003	0.96
			β_2	1	1.012	0.002	0.99
			$\log\theta$	1.792	1.577	0.138	0.81
2,500	50	2	β_1	1	1.028	0.002	0.80
			β_2	1	1.028	0.002	0.85
			$\log\theta$	1.792	1.430	0.210	0.65
	110$*$	5	β_1	1	1.021	0.001	0.89
			β_2	1	1.019	0.001	0.94
			$\log\theta$	1.792	1.440	0.164	0.52
	250	7	β_1	1	1.016	0.001	0.91
			β_2	1	1.013	0.001	0.96
			$\log\theta$	1.792	1.570	0.074	0.68
	500	34	β_1	1	1.011	0.001	0.94
			β_2	1	1.007	0.001	0.98
			$\log\theta$	1.792	1.663	0.040	0.78
4,900	98	16	β_1	1	1.025	0.001	0.74
			β_2	1	1.025	0.001	0.73
			$\log\theta$	1.792	1.451	0.153	0.47
	203$*$	38	β_1	1	1.018	0.001	0.81
			β_2	1	1.013	0.001	0.80
			$\log\theta$	1.792	1.487	0.118	0.38
	490	123	β_1	1	1.012	0.001	0.87
			β_2	1	1.013	0.001	0.85
			$\log\theta$	1.792	1.607	0.049	0.57
	980	649	β_1	1	1.006	0.001	0.91
			β_2	1	1.007	0.001	0.89
			$\log\theta$	1.792	1.681	0.023	0.81

Table 6.4: Inference results for the US COVID-19 data.

Parameter	Estimate	95% CI
Intercept	-6.996	(-7.011,-6.081)
White	-1.485	(-1.503,-1.466)
Black	0.178	(0.159,0.197)
Male	7.363	(7.327,7.399)
Old	-2.705	(-2.752,-2.658)
$\log \theta$	-0.751	(-0.944,-0.558)

Table 6.5: Inference results for the Antarctic ice sheet data.

Parameter	Estimate	95% CI
Intercept	-4.661	(-7.102,-2.219)
x-coordinate	1.535	(-1.793,4.862)
y-coordinate	5.812	(2.050 ,9.574)
$\log \sigma^2$	1.824	(1.409 ,2.239)
$\log \phi$	-2.238	(-2.436,-2.040)

Chapter 7

Appendix

Supplementary Material for A Projection-based Laplace Approximation for Spatial Latent Variable Models

7.1 Projection Methods for a Continuous Spatial Domain

Here, we describe the random projection methods for a continuous domain. Assume that we want to reduce the dimension of the latent variables from n to m. Consider $\mathbf{\Phi} = [\mathbf{I}_{m\times m}, \mathbf{0}_{m\times(n-m)}]'$, an $n \times m$ truncation matrix. The $n \times n$ positive semi-definite matrix $\mathbf{R}$ is partitioned as $\begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \mathbf{R}_{21} & \mathbf{R}_{22} \end{bmatrix}$, where $\mathbf{R}_{11} = \mathbf{\Phi}'\mathbf{R}\mathbf{\Phi}$ from Nyström's method (Williams and Seeger, 2001). Then, this deterministic approach conducts an eigendecomposition of $\mathbf{R}_{11}$, where $\mathbf{V}_{11}$ is its eigenvectors and $\mathbf{\Lambda_{11}}$ is the diagonal matrix with their eigenvalues. Finally, the deterministic Nyström method constructs the $n \times m$ projection matrix using $\sqrt{\frac{m}{n}}[\mathbf{R}\mathbf{\Phi}][\mathbf{V}_{11}{\mathbf{\Lambda_{11}}}^{-1}]$.

Banerjee et al. (2012), Guan and Haran (2018) develop the probabilistic version of constructing the projection matrix. Now, the truncation matrix is $\mathbf{\Phi} = \mathbf{R}\mathbf{\Omega}$, where $\mathbf{\Omega}$ is an $n \times 2m$ random matrix with $\Omega_{ij} \sim N(0, 1/\sqrt{2m})$. They use $2m$ instead of m to improve the approximation (Halko et al., 2011), and we follow this in our study. Guan and Haran (2018) uses a variant of Nyström's method to guarantee orthogonality between the eigenvectors. For the final approximation to the eigenvectors, Guan and Haran (2018) use the first m columns of the left singular vectors of $[\mathbf{R}\mathbf{\Phi}][\mathbf{V}_{11}{\mathbf{\Lambda_{11}}}^{-1/2}]$. Algorithm 2 summarizes the random projection methods.

Algorithm 2 Random projection methods

For the $n \times n$ positive semi-definite matrix $\mathbf{R}$.

1. Construct the $n \times 2m$ random truncation matrix: $\mathbf{\Phi} = \mathbf{R\Omega}$, where $\Omega_{ij} \sim N(0, 1/\sqrt{2m})$.
2. Conduct Nyström's approximation for the eigendecomposition:
   - Form $\mathbf{R}_{11} = \mathbf{\Phi}'\mathbf{R}\mathbf{\Phi}$
   - SVD for $\mathbf{R}_{11} = \mathbf{V}_{11}\mathbf{\Lambda_{11}}\mathbf{V}'_{11}$
   - Form Nyström's approximation $\mathbf{C} = [\mathbf{R\Phi}][\mathbf{V}_{11}{\mathbf{\Lambda_{11}}}^{-1/2}]$
   - SVD for $\mathbf{C} = \mathbf{UDV}'$

The first m columns of $\mathbf{U}$ and the first m diagonal elements of $\mathbf{D}^2$ are used as the eigencomponents of $\mathbf{R}$.

7.2 Comparison with the Projection-based Monte Carlo Maximum Likelihood Approach

Monte Carlo maximum likelihood (MCML) (Geyer and Thompson, 1992, Christensen, 2004) is a flexible approach for obtaining MLEs. Park and Haran (2020) develops a fast MCML. Our fast Laplace method is similar to that of Park and Haran (2020), Guan and Haran (2019) in that we use projection approaches to reduce the dimension of the spatial latent variables. However, our approach requires fewer components to be tuned as well as provides uncertainties for the parameters easily. Based on the projection methods, Park and Haran (2020) represent the likelihood function as

$$\begin{aligned} L(\psi|\mathbf{Z}) &= \int_{R^m} f_{\mathbf{Z}|\delta}(\mathbf{Z}|\beta, \mathbf{M}, \delta) f_\delta(\delta|\theta) d\delta = \int_{R^m} f_{\mathbf{Z},\delta}(\mathbf{Z}, \delta|\psi) d\delta \\ &\propto \int_{R^m} \frac{f_{\mathbf{Z},\delta}(\mathbf{Z}, \delta|\psi)}{f_{\mathbf{Z},\delta}(\mathbf{Z}, \delta|\widetilde{\psi})} f_{\delta|\mathbf{Z}}(\delta|\mathbf{Z}, \widetilde{\psi}) d\delta. \end{aligned} \tag{7.1}$$

Then, they obtain the MLE by maximizing the Monte Carlo approximation of the log-likelihood as

$$\widehat{l(\psi)} = \log\left(\frac{1}{K}\sum_{k=1}^{K} \frac{f_{\mathbf{Z},\delta}(\mathbf{Z}, \delta^{(k)}|\psi)}{f_{\mathbf{Z},\delta}(\mathbf{Z}, \delta^{(k)}|\widetilde{\psi})}\right), \tag{7.2}$$

where $f_{\delta|\mathbf{Z}}(\delta|\mathbf{Z}, \widetilde{\psi}) \propto f_{\mathbf{Z}|\delta}(\mathbf{Z}|\widetilde{\beta}, \mathbf{M}, \delta) f_\delta(\delta|\widetilde{\theta})$ is called the importance function. Park and Haran (2020) generates MCMC samples of $\delta^{(1)}, \ldots, \delta^{(K)}$, which have a much smaller dimension ($m << n$) than that in the original method (Christensen, 2004). Here, we compare our fast Laplace method with the fast MCML method (Park and Haran, 2020) in the simulated Poisson and binary data examples. Table 7.1 and 7.2 show that our Laplace method is faster than MCML and provide comparable estimates.

Table 7.1: Parameter estimates from the projection-based MCML and projection-based Laplace method for the simulated Poisson data in a continuous domain.

Method	$\beta_1 = 1$	$\beta_2 = 1$	$\log \sigma^2 = 0$	$\log \phi = -1.609$	Time(min)
Fast MCML	1.046	0.927	0.368	-1.388	25.741
Fast Laplace	1.058	0.914	0.161	-1.511	4.030

Table 7.2: Parameter estimates from the projection-based MCML and projection-based Laplace method for the simulated binary data in a continuous domain.

Method	$\beta_1 = 1$	$\beta_2 = 1$	$\log \sigma^2 = 0$	$\log \phi = -1.609$	Time(min)
Fast MCML	0.707	1.315	0.059	-1.219	23.340
Fast Laplace	0.792	1.396	0.397	-1.346	2.131

7.3 Simulation Study for the Poisson Example in a Continuous Domain

Using $(\beta_1, \beta_2, \sigma^2, \phi) = (1, 1, 1, 0.2)$, we generate a Poisson data set with $n = 1,400$ observations in the unit domain. We simulate the random effects from the Matérn covariance and use the log-link function $\log(\boldsymbol{\lambda}) = \mathbf{X}\boldsymbol{\beta}+\mathbf{W}$. Here, $\mathbf{X}$ is the coordinate for the random effects. Similar to the examples in the main manuscript, we conduct cross validation for 400 points. We choose the reduced rank of $m = 100$, which can explain more than 99% of the variation.

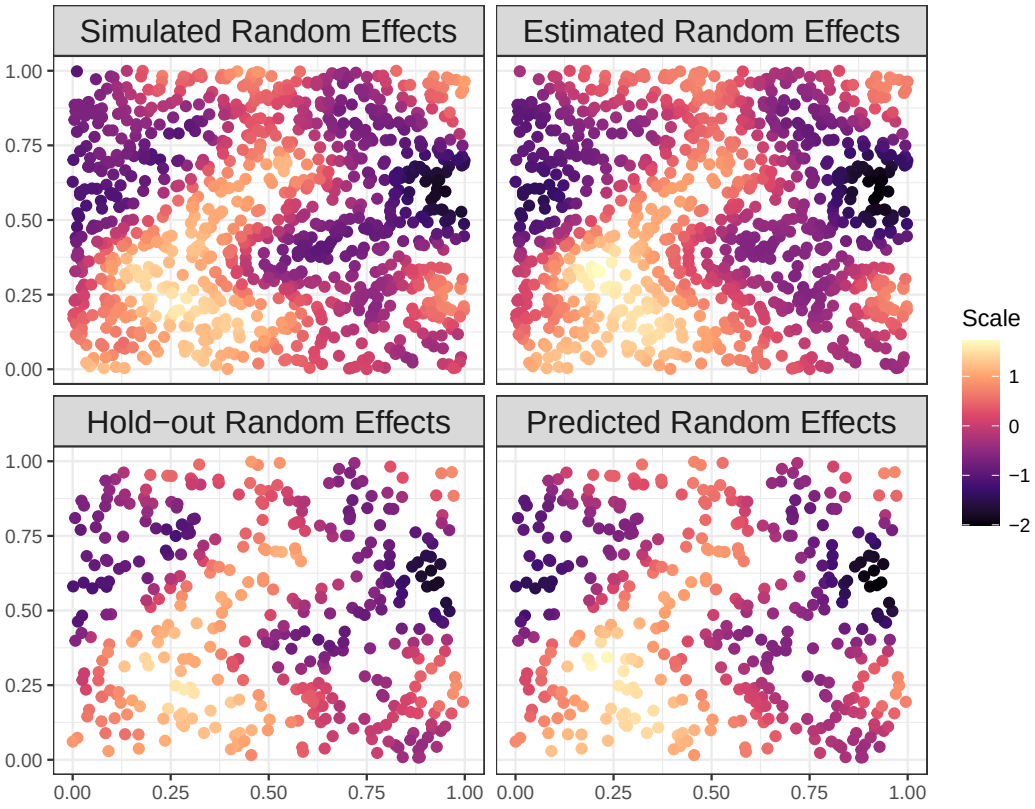

Figure 7.1: The first row represents the simulated and estimated random effects at the observed locations. The second row represents the out-of-sample cross-validated random effects and predicted random effects at the unobserved locations.

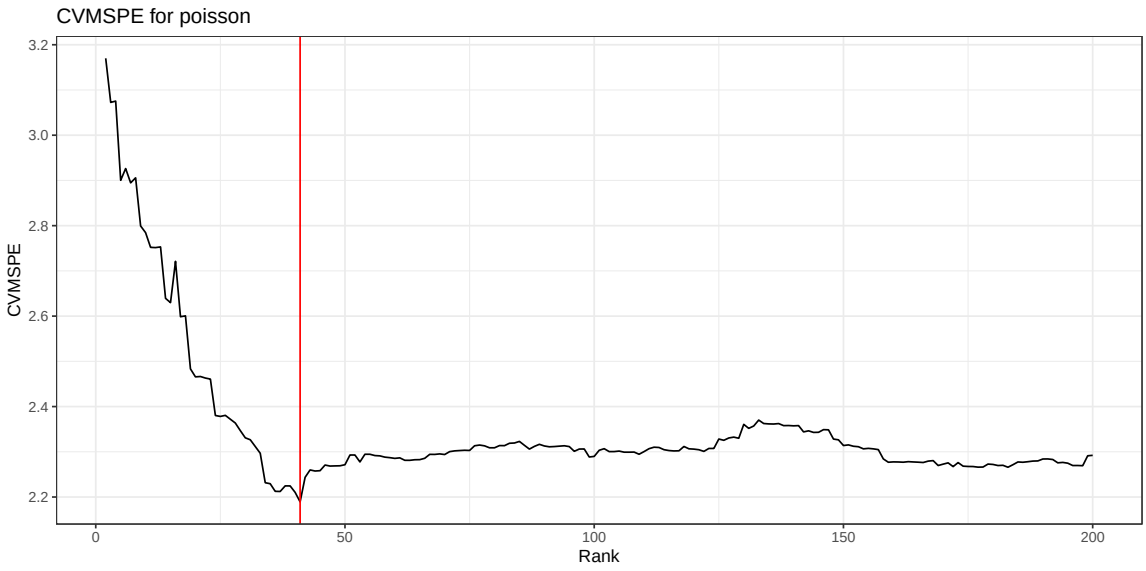

Figure 7.2: VMSPE plot for ranks 2-200. The vertical red line denotes lowest CVMPSE (rank = 41)

Figure 7.1 shows that the simulated and predicted random effects have similar spatial patterns. Table 7.3 indicates that our method is robust across different m values; the parameter estimates are reasonably close to the true values. We thus conduct simulation studies 100 times under the same parameter settings. Based on CVMSPE plot (Figure 7.2), we choose the reduced rank as 41.

Table 7.3: Simulated Poisson data in a continuous domain. 95% confidence intervals are constructed based on the observed Fisher information.

Rank	$\beta_1 = 1$	$\beta_2 = 1$	$\log \sigma^2 = 0$	$\log \phi = -1.609$	$\log(\sigma^2/\phi) = 1.609$	Time(sec)
m=25	0.887	0.901	-0.722	-1.755	1.033	29.711
	(0.776, 0.998)	(0.791, 1.011)	(-1.201, -0.243)	(-1.947, -1.563)	(0.565, 1.500)	
m=50	0.944	0.954	-0.415	-1.820	1.405	48.152
	(0.832,1.056)	(0.842,1.066)	(-1.040,0.210)	(-2.227,-1.413)	(0.971,1.839)	
m=75	0.948	0.954	-0.180	-1.591	1.410	85.033
	(0.835,1.061)	(0.840,1.068)	(-0.881,0.521)	(-1.869,-1.313)	(0.909,1.911)	
m=100	0.927	0.951	-0.371	-1.717	1.346	111.169
	(0.814,1.040)	(0.837,1.065)	(-0.974,0.232)	(-1.981,-1.453)	(0.911,1.782)	

Table 7.4: Results from the fast Laplace approximation on 100 simulated Poisson data sets in a continuous domain.

Parameter	True	Mean	SD	MSE	Coverage
β_1	1	1.003	0.063	0.004	0.92
β_2	1	1.006	0.059	0.003	0.94
$\log \sigma^2$	0	-0.064	0.310	0.099	0.94
$\log \phi$	-1.609	-1.621	0.117	0.014	0.98
$\log (\sigma^2/\phi)$	1.609	1.558	0.240	0.060	0.95

7.4 Comparisons with Competitors

We compare the performance of the proposed method with competitors (standard Laplace, reduced-rank MCMC, reduced-rank MCML) in binomial example with $n = 2,800, 5,600$. Each of the algorithms is implemented using the source code provided in the original articles. For maximum likelihood algorithms (standard Laplace, reduced-rank Laplace, reduced-rank MCML), simulation is repeated 100 times. We report the result from the reduced-rank MCMC for a single simulated data set due to high computational costs. We use the same simulation settings as in Section 4.2.

For both $n = 2,800$ (Table 7.5), and $n = 5,600$ (Table 7.6) cases, we observe that the projection-based maximum likelihood algorithms are faster than the standard Laplace but provide comparable estimation and prediction accuracies. Especially, the projection-based Laplace method is about 6 times faster than the standard Laplace method. Compared to the projection-based MCML, the projection-based Laplace provides more accurate parameter estimations (better coverage with lower MSE) and predictions (lower MSPE). Furthermore, the projection-based Laplace can obtain confidence intervals for covariance parameters, while MCML (Park and Haran, 2020) cannot. This is because calculating a gradient of ϕ to obtain standard errors is challenging for MCML (Park and Haran, 2020).

Comparing Bayesian and frequentist algorithms is challenging because they have a different point of view. In general, frequentist methods can be faster than Bayes methods because they can avoid the repeated simulations from MCMC. On the other hand, Bayes approaches have the advantage that they are flexible for constructing hierarchical models or can easily incorporate prior knowledge into the posterior distribution. Naturally, in terms of computing time, we observe that frequentist alternatives are faster than the Bayes algorithm (Guan and Haran, 2018).

Table 7.5: Inference results for the simulated binary data ($n = 2,800$) in a continuous domain. For each maximum likelihood algorithm (Laplace, fast Laplace, fast MCML), average computing time (minutes), mean of estimates, MSE, and coverage are calculated from 100 simulations. Fast MCMC was run for 30,000 iterations from a single simulation. For all projection-based algorithms, the recommended rank is used.

Method	Time	MSPE	Parameter	True	Mean	MSE	Coverage
Laplace	39	0.135	β_1	1	1.003	0.044	0.93
			β_2	1	0.990	0.031	0.97
			$\log(\sigma^2/\phi)$	1.609	1.511	0.161	0.91
Fast Laplace	7	0.139	β_1	1	1.000	0.046	0.93
			β_2	1	0.985	0.032	0.96
			$\log(\sigma^2/\phi)$	1.609	1.494	0.188	0.92
Fast MCML	25	0.228	β_1	1	0.989	0.053	0.82
			β_2	1	0.978	0.030	0.94
			$\log(\sigma^2/\phi)$	1.609	1.639	0.251	NA
Fast MCMC	956	0.128	β_1	1	0.922		
			β_2	1	0.869		
			$\log(\sigma^2/\phi)$	1.609	1.482		

Table 7.6: Inference results for the simulated binary data ($n = 5,600$) in a continuous domain. For each maximum likelihood algorithm (Laplace, fast Laplace, fast MCML), average computing time (minutes), mean of estimates, MSE, and coverage are calculated from 100 simulations. Fast MCMC was run for 30,000 iterations from a single simulation. For all projection-based algorithms, the recommended rank is used.

Method	Time	MSPE	Parameter	True	Mean	MSE	Coverage
Laplace	351	0.082	β_1	1	1.005	0.018	0.96
			β_2	1	0.991	0.018	0.97
			$\log(\sigma^2/\phi)$	1.609	1.546	0.110	0.90
Fast Laplace	56	0.139	β_1	1	0.990	0.018	0.96
			β_2	1	0.987	0.018	0.97
			$\log(\sigma^2/\phi)$	1.609	1.535	0.111	0.93
Fast MCML	145	0.148	β_1	1	1.009	0.018	0.91
			β_2	1	0.990	0.016	0.92
			$\log(\sigma^2/\phi)$	1.609	1.628	0.162	NA
Fast MCMC	9754	0.093	β_1	1	1.059		
			β_2	1	1.061		
			$\log(\sigma^2/\phi)$	1.609	1.745		

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국문 초록

공간적 잠재 변수 모델을 위한 차원축소 기반의 라플라스 근사 방법론

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라플라스 방법은 다양한 잠재 변수 모델에서 최대 우도 추정량을 얻을 수 있는 실용적인 방법이다. 해당 방법의 핵심적인 아이디어는 주변 가능도의 적분을 적분을 정규분포로 근사시키는 것이다. 상관성이 있는 잠재변수의 차원이 늘어나고, 따라서 라플라스 근사에 사용되는 최적화 기법이 고차원 공간에서 이루어짐에 따라 계산에 어려움이 생긴다. 이러한 문제가 발생하는 한 가지 예로는 생태학, 역학, 사회학 등에서 널리 사용되는 공간적 잠재 변수 모델을 들 수 있다. 따라서 본 논문에서는 차원축소 기법에 기반하여 라플라스 근사법을 더 빠르게 수행할 수 있는 방법론을 제안한다. 새롭게 제안하는 방법론은 시뮬레이션 기반의 마르코프 체인 몬테카를로 (Markov Chain Monte Carlo, MCMC) 방법론 보다 잠재적으로 더 빠르며, 초모수(Hyper Parameter)의 조정을 필요로하지 않는다. 또한, 환경 과학에서 자주 쓰이는 다양한 비가우시안 공간 데이터에 활용될 수 있을 것이다. 특히 미국 COVID-19 확진자 수와 남극 지방 얼음의 두께에 관한 데이터에서 나타나는 공간적 패턴들을 탐구해볼 것이다. 또한, 여러 시나리오를 가정한 시뮬레이션 연구를 통해 새롭게 제안된 방법론이 정확하고 빠른 최대우도추정이 가능하다는 점을 조사할 것이다. 더 나아가 제시된 방법론은 다양한 고차원 랜덤효과 모형의 최대 우도 추정을 함에 있어서 더 넓게 이용될 수 있을 것이다.

핵심단어: 라플라스 방법; 수치해석적 최적화; 차원축소; 공간보간기법; 일반화된 공간 선형 혼합 모형