Spatial Generalized Linear Mixed Models

(Based on joint work with Yawen Guan and John Hughes) Social Data Analytics, Penn State, Spring 2017.

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Our Research

- Dimension-reduced spatial generalized linear mixed models (SGLMMs) for lattice data
 - Hughes, J. and Haran, M. (2013) Dimension Reduction and Alleviation of Confounding for Spatial Generalized Linear Mixed Models," *Journal of the Royal Statistical Society Series B*
- Dimension-reduced spatial generalized linear mixed models (SGLMMs) for continuous domain and lattice data Guan, Y. and Haran, M. (2016) A Computationally Efficient Projection-Based Approach for Spatial Generalized Linear Mixed Models <u>arXiv</u>

What This Talk is About

- Modeling non-Gaussian spatial data is challenging.
- Spatial generalized linear mixed models (SGLMMs) provide a general framework. They are widely used.
- Shortcomings of SGLMMs: (1) Inference presents difficult computational issues. (2) Parameter interpretation is generally misleading.
- I will describe methods that simultaneously resolve both these issues.
- ► The methods are *projection-based*.

Outline

- Spatial linear models
- Spatial generalized linear mixed models (SGLMMs)
- Both of the above for lattice and continuous-domain spatial data
- Shortcomings of SGLMMs: interpretation and computing issues
- Time permitting: Sketch of projection-based solutions to these problems.

Introduction to the ideas and computing:

Haran (2011) Gaussian random field models for spatial data, Handbook of Markov chain Monte Carlo.

Non-Gaussian Spatial Data Example #1: Lattice

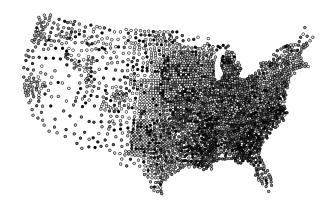
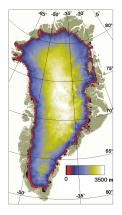


Figure: U.S. infant mortality data by county. n = 3071 Ratio of deaths to births, each averaged over 2002-2004. Darker indicates higher rate.

Non-Gaussian Spatial Data Example #2: Continuous

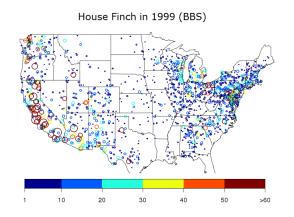
Greenland ice sheet thickness data



Bamber et al. (2001)

Non-Gaussian Spatial Data Example #3

- ▶ Data on abundance (counts) of house finch in the US
- Interested in the abundance at unsampled locations.



Pardieck et al. 2015. North American Breeding Bird Survey Dataset 1966 - 2014

Modeling Spatial Data

- Gaussian and non-Gaussian spatial data are very common and appear in a large number of disciplines.
- Common: gaussian, binary, count, zero-inflated
- Purpose of the model
 - 1. regression while adjusting for residual spatial dependence
 - 2. smoothing the spatial field and "borrowing strength"
- These models are used widely and have become particularly important in disease epidemiology and ecology.

Spatial Linear Mixed Models

- ▶ Spatial process at location **s** is $Z(\mathbf{s}) = X(\mathbf{s})\beta + W(\mathbf{s})$.
 - ▶ $X(\mathbf{s})$ are covariates at \mathbf{s} and β is a vector of coefficients.
 - Model dependence among spatial random variables by imposing it on the errors (the W(s)'s).
- Lattice: Gaussian Markov Random field (GMRF) w ⊖ the parameters for precision matrix Q(⊖).

$$\mathbf{Z}_{n\times 1}|\Theta, \beta \sim N(\mathbf{X}_{n\times p}\beta_{p\times 1}, Q^{-1}(\Theta))$$

SLMMs: Lattice Models

- ▶ $Q = \text{diag}(A\mathbf{1}) A$ where adjacency matrix A is such that $A_{ij} = 1$ if locations i and j are neighbors, 0 else
- Implications:
 - W(s) is conditionally independent of all other Ws given its neighbors
 - uncertainty about W(s) is inversely proportional to its number of neighbors.

Spatial Linear Mixed Models: Inference

For both lattice and continuous-domain data:

- ▶ Maximum likelihood: maximize $\mathcal{L}(\Theta, \beta; \mathbf{Z})$ w.r.t. Θ, β .
- Bayesian inference:
 - Priors for Θ, β
 - ▶ Inference based on $\pi(\Theta, \beta \mid \mathbf{Z}) \propto \mathcal{L}(\Theta, \beta; \mathbf{Z}) p(\Theta) p(\beta)$.
- Computational challenge: primarily matrix calculations for high-dimensional matrices.

Spatial Generalized Linear Mixed Models

Model for Z at location \mathbf{s}_i

- 1. $Z(\mathbf{s}_i)|\beta, \Theta, W(\mathbf{s}_i), i = 1, ..., n$, conditionally independent E.g. $Z(\mathbf{s}_i) \mid \beta, W(\mathbf{s}_i) \sim \text{Poisson}(\mu(\mathbf{s}_i))$
- 2. Link function $g(\mu(\mathbf{s}_i)) = X(\mathbf{s}_i)\beta + W(\mathbf{s}_i)$ E.g. $\log(\mu_i) = X(\mathbf{s}_i)\beta + W(\mathbf{s}_i)$
- 3. Impose dependence: $\mathbf{W} = (W(\mathbf{s}_1), \dots, W(\mathbf{s}_n))^T$

$$p(\mathbf{W}| au) \propto au^{(n-1)/2} \exp\left(-rac{ au}{2}\mathbf{W}'Q\mathbf{W}
ight)$$

4. Priors for Θ , β

Inference based on $\pi(\Theta, \beta, \mathbf{W} \mid \mathbf{Z})$ (Besag et al. (1991), Diggle et al. (1998))

SGLMMs: Challenges

SGLMMs have become very popular even outside mainstream statistics. Flexible models but some drawbacks:

- Confounding between spatial random effects and fixed effects (covariates)
- (2) Computational challenges

Spatial Confounding in SGLMMs

- ▶ $\mathbf{P} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$, orthogonal projection onto $C(\mathbf{X})$
- $ightharpoonup \mathbf{P}^{\perp} = \mathbf{I} \mathbf{P}$, orthogonal projection onto $C(\mathbf{X})$'s orthogonal complement
- ▶ Spectral decomposition to acquire orthogonal bases, $\mathbf{K}_{n \times p}$ and $\mathbf{L}_{n \times (n-p)}$, for $C(\mathbf{X})$ and $C(\mathbf{X})^{\perp}$. Rewrite:

$$g(\mathbb{E}(Z_i | \beta, W_i)) = \mathbf{X}_i \beta + W_i = \mathbf{X}_i \beta + \mathbf{K}_i \gamma + \mathbf{L}_i \delta.$$

K is collinear with X.

This is the source of confounding. Appears to cause variance inflation.

Computing for SGLMMs

MCMC algorithms for SGLMMs are challenging to construct:

- Spatial random effects: one random effect for each data point. n+p+1 dimensions where n=size of data, p=number of predictors. MCMC is slow per iteration due to high dimensionality
- Markov chain is slow mixing due to strong cross-correlations among the spatial random effects.

Several attempts to address these issues: Rue and Held (2005), Haran et al. (2003), Haran and Tierney (2010)

Observations

- Spatial random effects W are the cause of confounding issues as well as computational challenges.
- W are just a device to induce dependence. Not intrinsically important.
- ► Idea: reparameterize and reduce dimensions of W.

Spatial Confounding: Reparameterization Solution

- Reich, Hodges and Zadnik (2006) propose solution: since K have no scientific meaning, delete them from the model.
- ▶ $g(\mathbb{E}(Z_i | \beta, \delta)) = \mathbf{X}_i \beta + \mathbf{L}_i \delta$. Prior for random effects δ now

$$\label{eq:posterior} p(\boldsymbol{\delta} \,|\, \boldsymbol{\tau}) \propto \boldsymbol{\tau}^{(n-p)/2} \exp\left(-\frac{\tau}{2} \boldsymbol{\delta}' \mathbf{Q}^* \boldsymbol{\delta}\right),$$

where $\mathbf{Q}^* = \mathbf{L}'\mathbf{Q}\mathbf{L}$.

- Corrects issues due to confounding
- # of parameters reduced (only slightly) from n + p + 1 to n + 1. Computational challenge remains.
- RHZ approach does not fully account for underlying graph

Our Sparse Reparameterization

- Represent graph G = (V, E) using A, n × n adjacency matrix with entries diag(A) = 0 and A_{ij} = 1{(i, j) ∈ E, i ≠ j}, with 1{·} an indicator function
- ▶ Basic idea inspired by Griffith (2003): augment a generalized linear model with selected eigenvectors of (I – 11'/n)A(I – 11'/n). This appears in Moran's / statistic (nonparametric measure of spatial dependence),

$$I(\mathbf{A}) \propto rac{\mathbf{Z}'(\mathbf{I} - \mathbf{11}'/n)\mathbf{A}(\mathbf{I} - \mathbf{11}'/n)\mathbf{Z}}{\mathbf{Z}'(\mathbf{I} - \mathbf{11}'/n)\mathbf{Z}},$$

Background for Sparse Reparameterization

- ► Griffith's goal: reveal the structure of missing spatial covariates. Our goal: smoothing orthogonal to **X**
- ▶ Hence, we replace I 11'/n with P^{\perp}
- ▶ $\mathbf{M}_{\mathbf{X}}(\mathbf{A}) = \mathbf{P}^{\perp} \mathbf{A} \mathbf{P}^{\perp}$, Moran operator for \mathbf{X} with respect to the graph G, appears in numerator of generalized Moran's I:

$$\emph{I}_{X}(A) \propto \frac{Z'P^{\perp}AP^{\perp}Z}{Z'P^{\perp}Z}.$$

Applying the Sparse Reparameterization

Replacing L with M in the RHZ model gives

$$g(\mathbb{E}(Z_i | \beta, \delta)) = \mathbf{X}_i \beta + \mathbf{M}_i \delta.$$

And the prior for the random effects is now

$$p(\delta \mid \tau) \propto \tau^{q/2} \exp\left(-\frac{\tau}{2} \delta' \mathbf{Q}^{**} \delta\right),$$

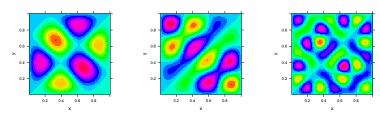
where $\mathbf{Q}^{**} = \mathbf{M}'\mathbf{Q}\mathbf{M}$.

- Corrects issues due to confounding
- Potential for dimension reduction: if we reduce dimensions of \mathbf{M}_i to q, the # parameters is reduced from n + p + 1 to q + p + 1 (q can be small)

Interpreting the Resulting Reparameterization

► "Tailored" to **X** and *G*: eigenvectors comprise all possible patterns of clustering residual to **X** and accounting for *G*

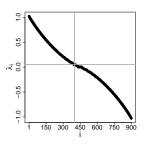
Some selected basis vectors for the 30 \times 30 lattice.



Interpreting the Resulting Reparameterization

 Positive (negative) eigenvalues correspond to varying degrees of positive (negative) spatial dependence (Boots and Tiefelsdorf, 2000)

The standardized eigenvalues for the 30×30 lattice.



Exploiting the New Parameterization

- If we assume positive spatial dependence, eigenvectors corresponding to negative spatial dependence (negative eigenvalues) should be removed.
- Small eigenvalues may not be meaningful. Remove corresponding eigenvectors.
- Result: much reduced dimensions

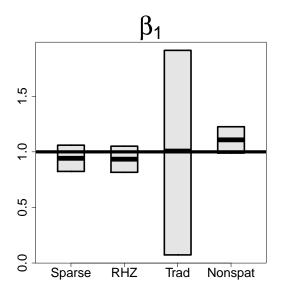
Study: Inference for Spatial Binary

 30×30 lattice simulated from RHZ model with $\beta_1 = \beta_2 = 1$. Predictors are the coordinates of unit square.

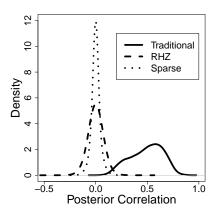
Model	\hat{eta}_1 CI(eta_1)	$\hat{eta}_2 \; CI(eta_2)$
Sparse	1.080 (0.613, 1.556)	1.130 (0.644, 1.635)
RHZ	1.120 (0.637, 1.606)	1.192 (0.679, 1.713)
Traditional	0.500 (-2.655, 3.616)	-0.605 (-3.698, 2.577)

- Point and interval estimates for Traditional are very poor:
 95% interval includes 0
- Sparse and RHZ produce similar (good) results
 Similar results for Gaussian (linear) and Poisson

Spatial Count Data: Simulation Results



De-correlated Random Effects



Greatly improves efficiency of simple MCMC. No need for elaborate proposals (cf. Held and Rue (2005), Haran et al. (2003), Haran and Tierney (2010)).

Spatial Binary: Computational Efficiency

Model	Dimension	Running Time
Sparse	228	2.5 hours
RHZ	901	18.5 hours
Traditional	903	38.5 hours

- MCMC algorithm is
 - faster per iteration (far fewer random effects)
 - mixes faster (random effects are "decorrelated")
- ► Far greater speed-ups with much smaller *q*, e.g. 25-50 is adequate for our examples (we are also being *extremely* careful by running very long chains!)

Real data example: 14 days (traditional) versus 2-8 hours

Summary for Lattice Models

- SGLMMs provide a very general approach for modeling non-Gaussian spatial data
- Our sparse approach results in more interpretable regression coefficients
- We allow for only meaningful spatial dependence and a natural approach to dimension reduction
- Automated MCMC is computationally efficient, allowing for routine analysis of large data sets

Continuous-domain Data

What do we do when the data are continuous-domain?

Model dependence via a Gaussian process:

$$p(\mathbf{W} \mid \sigma^2, \phi) \sim N(\mathbf{0}, \sigma^2 \Sigma_{\phi}),$$

where
$$\Sigma_{ij} = Cov(W(\mathbf{s}_i), W(\mathbf{s}_j)) = C(||\mathbf{s}_i - \mathbf{s}_j||)$$

- Spatial linear mixed models
 - Lattice models: can take advantage of sparse matrices. Computing is more difficult for continuous domain (dense matrices): reduced rank/other approaches.
- Spatial generalized linear mixed models
 - Projections have to be done differently than for lattice models, but idea is similar.

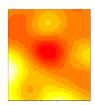
Gaussian Process for Dependence and Interpolation

- A Gaussian process is an infinite-dimensional random process, any finite-dimension of which is a multivariate normal.
- Matérn covariance function describes dependence, e.g.

$$\begin{array}{ll} \nu=0.5, & \textit{C(h)}=\sigma^2\exp(-\frac{|h|}{\phi}) \text{ (Exponential)} \\ \nu=2.5, & \textit{C(h)}=\sigma^2\left(1+\frac{\sqrt{5}|h|}{\phi}+\frac{5|h|^2}{3\phi^2}\right)\exp(-\frac{\sqrt{5}|h|}{\phi}) \\ \nu=\infty, & \textit{C(h)}=\sigma^2\exp(-\frac{|h|^2}{2\phi^2}) \text{ (Square exponential)} \end{array}$$







Spatial Generalized Linear Mixed Models

Example model for count data $Z(\mathbf{s}), s \in \mathcal{D} \subset \mathcal{R}^d$.

1. Data model:

$$Z(\mathbf{s}_i) \mid eta, W(\mathbf{s}_i) \stackrel{Indep.}{\sim} \mathsf{Poisson}(\mu(\mathbf{s}_i)), i = 1, \dots, n$$
 $\log (\mu(\mathbf{s}_i)) = X(\mathbf{s}_i)eta + W(\mathbf{s}_i),$

2. Process model: impose dependence via Gaussian process

$$\mathbf{W} \mid \sigma^2, \phi \sim \mathcal{N}\left(\mathbf{0}, \sigma^2 \Sigma_{\phi}\right)$$

3. Priors for β , σ^2 , ϕ

MCMC Inference based on posterior, $\pi(\beta, \sigma^2, \phi, \mathbf{W} \mid \mathbf{Z})$ Reference: [Diggle et al., 1998]

Challenges

Inference for SGLMMs is based on:

$$\pi(\boldsymbol{\beta}, \sigma^2, \phi, \mathbf{W} \mid \mathbf{Z}) \propto \prod_{i}^{n} f(\mathbf{Z}(\mathbf{s}_i) \mid \boldsymbol{\beta}, \mathbf{W}(\mathbf{s}_i)) |\sigma^2 \Sigma_{\phi}|^{-\frac{1}{2}} \exp\left(-\frac{\mathbf{W}' \Sigma_{\phi}^{-1} \mathbf{W}}{2\sigma^2}\right) p(\boldsymbol{\beta}, \sigma^2, \phi)$$

- Dimensionality and computational cost:
 - Dimension of W increases as number of observation increases
 - ► Evaluation involves Cholesky decompostion of $Σ_φ$, cost $O(n^3)$.
 - ► For bird data (n = 1257), it takes 2 days for 10⁵ iteration
- Cross-correlations and confounding:
 - ► Strong cross-correlations among random effects (**W**) result

Outline of Projection-based Approach

- 1. Fast approximation to the principal components of Σ_{ϕ} :
 - 1.1 Low-distortion embedding of Σ_{ϕ} ,
 - 1.2 Approximate first m eigenvectors $U = \mathbf{s}(u_1, \ldots, u_m)$ and eigenvalues $D_m = \operatorname{diag}(\lambda_1, \ldots, \lambda_m)$ via Nyström method. [Banerjee et al., 2012] used a similar algorithm to approximate Σ_{ϕ} in Gaussian process regression
- 2. Replace n-dimensional **W** with $UD_m^{1/2}$ **s** δ , **s** δ has smaller dimension and its components are approximately independent.
- 3. Project $UD_m^{1/2}$ **s** δ to $C^{\perp}(X)$
 - Makes random effects orthogonal to fixed effects
- 4. Fit the reduced model under Bayesian framework.

Step 1: Approximate Eigenvectors by Nyström's Method

- ▶ Partition the positive semi-definite $K = \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix}$
- $ightharpoonup K_{11} = \Phi^T K \Phi$, where $\Phi = [I_{m \times m}; 0_{m \times (n-m)}]^T$
- Denote V and Λ the eigen vectors and values, respectively.
- ▶ Compute exact decomposition for the small $m \times m$ matrix

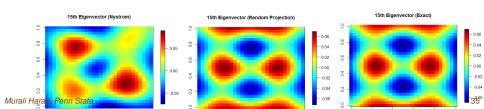
$$K_{11} = V(K_{11})\Lambda(K_{11})V(K_{11})^T$$

► Approximate V(K) by scaling $V(K_{11})$ up to high dimension [Williams and Seeger, 2001]

$$\tilde{V}(K) = \sqrt{\frac{m}{n}} \begin{bmatrix} K_{11} \\ K_{21} \end{bmatrix} V(K_{11}) \Lambda(K_{11})^{-1},$$

Step 1: Approximation using Random Projection

- Originally used to approximate large matrices [Sarló, 2006]
- ► Efficient Gaussian process regression by approximating the covariance matrix [Banerjee et al., 2012]
- We use random projection to improve approximation of eigen components of Σ_Φ
- ► Replace truncation matrix with a random matrix $Φ = Ω_{n \times m}$, with $Ω_{ii} \sim N(0, 1/\sqrt{m})$
- $K_{11} = \Phi^T K \Phi$, and $\tilde{V}(K) = [K \Phi] V(K_{11}) \Lambda(K_{11})^{-1}$



Step 2: Random Projection Algorithm Details

Approximates the leading m eigencomponents of the covariance matrix $K = \Sigma_{\phi}$.

Algorithm 1 Random projection algorithm:

- 1. Low dimensional projection from $R^{n \times n}$ to $R^{n \times k}$, m < k << n: Form random matrix $\Phi = \Omega_{n \times k}$, or take $\Phi = K^{\alpha}\Omega_{n \times k}$ detail on α
- 2. Nyström's method to approximate eigendecomposition: Form $K_{11} = \Phi^T K \Phi$ SVD for K_{11} : $V(K_{11}) \Lambda(K_{11}) V(K_{11})^T$ Form Nyström extension $C = [K \Phi][V(K_{11}) \Lambda(K_{11})^{-1/2}]$ SVD for $C: UDV^T$
- Take the first m columns of U, and the first m diagonal elements of D² as our approximation to the leading m eigencomponents of K

(Recall) Outline of Projection-based Approach

- 1. Fast approximation to the principal components of Σ_{ϕ} :
 - 1.1 Low-distortion embedding of Σ_{ϕ} ,
 - 1.2 Approximate first *m* eigen-components via Nyström method.
 - [Banerjee et al., 2012] used a similar algorithm to approximate Σ_{ϕ} in Gaussian process regression
- 2. Replace n-dimensional **W** with $UD_m^{1/2}$ **s** δ , **s** δ has smaller dimension and its components are approximately independent.
- 3. Project $UD_m^{1/2}$ **s** δ to $C^{\perp}(X)$
 - Makes random effects orthogonal to fixed effects
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Step 3: Orthogonal Projection

- ▶ Let $P_{[X]} = X(X^TX)^{-1}X^T$, and $P_{[X]}^{\perp} = I P_{[X]}$.
- Source of confounding:

$$g\{E(\mathbf{Z}\mid\boldsymbol{\beta},\mathbf{W},\sigma^2,\phi)\} = X\boldsymbol{\beta} + \mathbf{W} = X\boldsymbol{\beta} + P_{[X]}(\mathbf{W}) + P_{[X]}^{\perp}(\mathbf{W})$$

- ▶ Restricted spatial regression: $P_{[X]}(\mathbf{W})$ is in the span of X, so remove this part to eliminate confounding [Reich et al., 2006].
- Need adjustment to obtain valid inference [Hanks et al., 2015]

$$\boldsymbol{\beta}^{(k)} = \tilde{\boldsymbol{\beta}}^{(k)} - (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \mathbf{W}^{(k)}$$

Problem: $P_{[X]}^{\perp}(\mathbf{W}) \sim N(\mathbf{0}, P_{[X]}^{\perp} \Sigma P_{[X]}^{\perp})$ is still high-dim. If X is nxp input matrix, then $P_{[X]}^{\perp} \Sigma P_{[X]}^{\perp}$ has rank n-p. Murali Haran, Penn State

Step 4: Inference Based on Reparameterizaion

Spatial generalized linear mixed models:

$$g\{E(Z_i \mid \beta, W_i)\} = X_i\beta + W_i$$
$$\mathbf{W} \mid \sigma^2, \phi \sim N_n(\mathbf{0}, \sigma^2 \Sigma_{\phi})$$

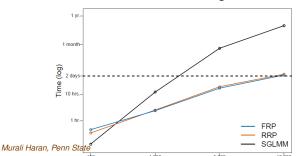
Usual: inference based on $\pi(\beta, \sigma^2, \phi, \mathbf{W} \mid \mathbf{Z})$

- ▶ Obtain U, D_m of Σ_{ϕ}
- ▶ D_m is m-dim diagonal matrix with $D_{ii} = i^{th}$ eigenvalue
- ► FRP: replace \boldsymbol{W} with $UD_m^{1/2}\delta$ to approximate SGLMM or RRP: replace \boldsymbol{W} with $P_{[X]}^{\perp}UD_m^{1/2}\delta$ to approximate restricted spatial model
- Reduced Model:

$$g\left\{E(Z_i\mid\beta,U,D_m,\delta)\right\}=X_i\beta+(P_{[X]}^\perp UD_m^{1/2})_i\delta$$

Computational Advantages: Reduced Random Effects

- ▶ Reduced dimension of random effects δ to m << n, e.g. m = 50, n = 1000.
- Restricted spatial generalized linear mixed model with random projections takes about 4 hrs
- ► Complexity: $O(n^2m)$ for reparameterization vs $O(n^3)$
- Our approach can fit large data sets within a reasonable amount of time, but fitting the traditional model is infeasible.



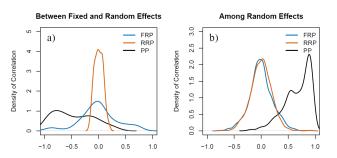
FRP = full model with random projection

RRP = restricted model with random projection

SGLMM = traditional model

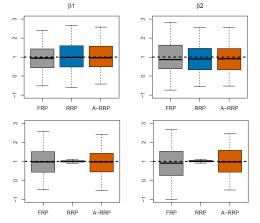
Computational Advantages: Improved MCMC Mixing

- Alleviate confounding between fixed and random effects.
- ▶ Reparameterized δ are approximately independent.
- De-correlating random effects results in better MCMC mixing.



Poisson Model Simulation Study: Point Estimation

► Simulate: $\beta = (1,1)^T$, and Matérn $(\nu, \phi, \sigma^2) = (2.5, 0.2, 1)$



FRP: full model

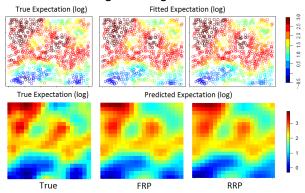
RRP: restricted model (orthogonalized random effects)

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DRP State of inforces.

Poisson Model Prediction Performance

- Simulate n = 1000 spatial count data
- Prediction on 20 x 20 grid using rank = 50

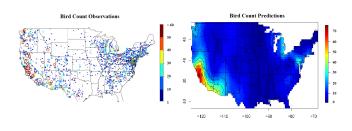


FRP: full model

RRP: restricted model (orthogonalized random effects)

Interpolated Bird Counts

- Approximate the SGLMM with only the intercept term.
- Computation time is about 7 hours,
- Small bird counts in the center and most of the East Coast
- Large counts centered near New York area and the West



Pardieck et al. 2015. North American Breeding Bird Survey Dataset 1966 - 2014

Summary

- Projection-based approach for non-Gaussian spatial data
- The approach has the following advantages:
 - 1. reduces the dimensions of the posterior distribution
 - 2. reparameterization improves mixing of the MCMC algorithm
 - 3. able to adjust for spatial confounding
 - 4. principled method for determining rank select rank
- We recommend fitting restricted model with random projections.
- If concern about confounding, we recommend adjusting the fixed effects a posteriori to recover the inference
- Simulations: good inference and prediction performance
- ► Caveats: our approach is faster than existing approaches but does not scale to larger data (n > 5,000 may be