Automating MCMC Algorithms, Alleviating Confounding, and Reducing Dimensions for a Class of Spatial Models

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Gaussian Random Field Models

Very widely used by statisticians and non-statisticians

- Models for spatial data
- Emulating (approximating) complex computer models
- Machine learning, nonparametric regression, classification

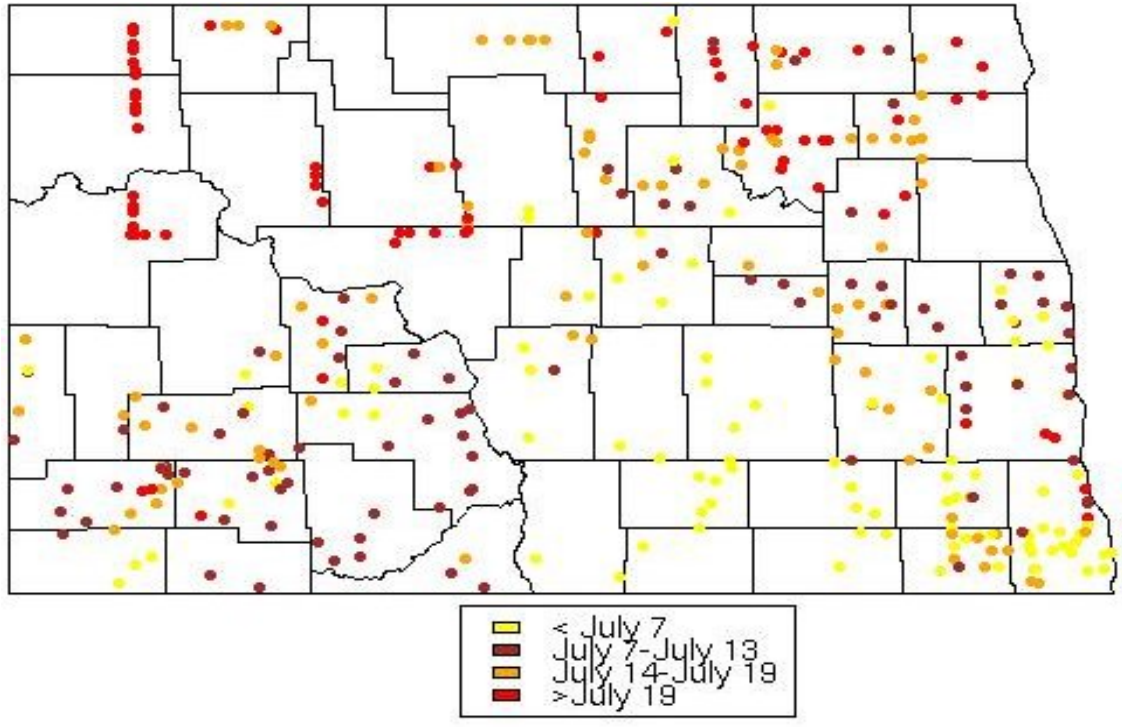
Gaussian Random Fields

Let $\mathbf{s}$ vary over index set $D \subset \mathbb{R}^d$ so the associated spatial process is $\{Z(\mathbf{s}) : \mathbf{s} \in D\}$.

- "Geostatistics": D is a subset of $\mathbb{R}^d$. Process is infinite-dimensional e.g. pollutant levels across Pennsylvania.
- "Areal/lattice data": D is a finite set of locations in $\mathbb{R}^d$, used to represent data often observed on or aggregated up to arbitrary spatial units. e.g. cancer rates by county across Minnesota.

Geostatistics

Wheat flowering in North Dakota (related to blight epidemics)

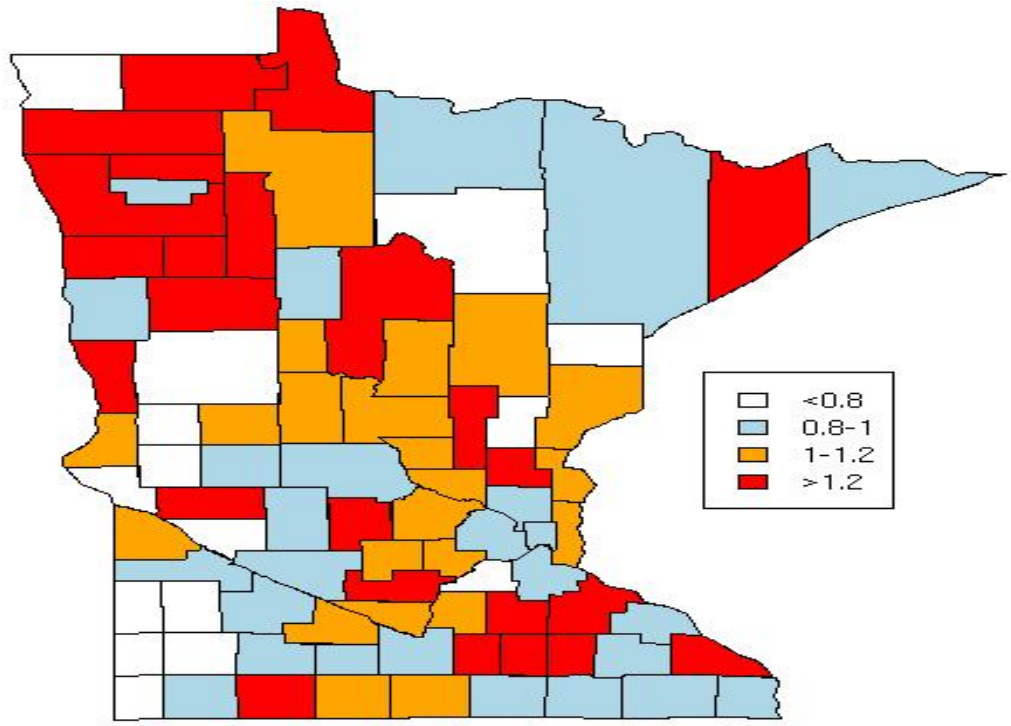


Courtesy Plant Pathology, PSU and North Dakota State.

Haran, Bhat, Molineros, DeWolf (*JABES*, 2008)

Areal Data

Minnesota cancer rates by county: $\frac{\text{observed}}{\text{expected}}$ counts

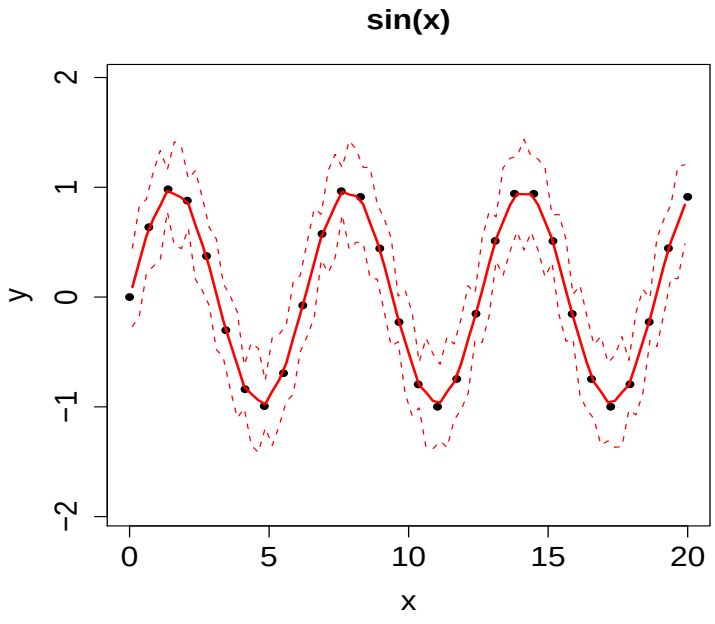


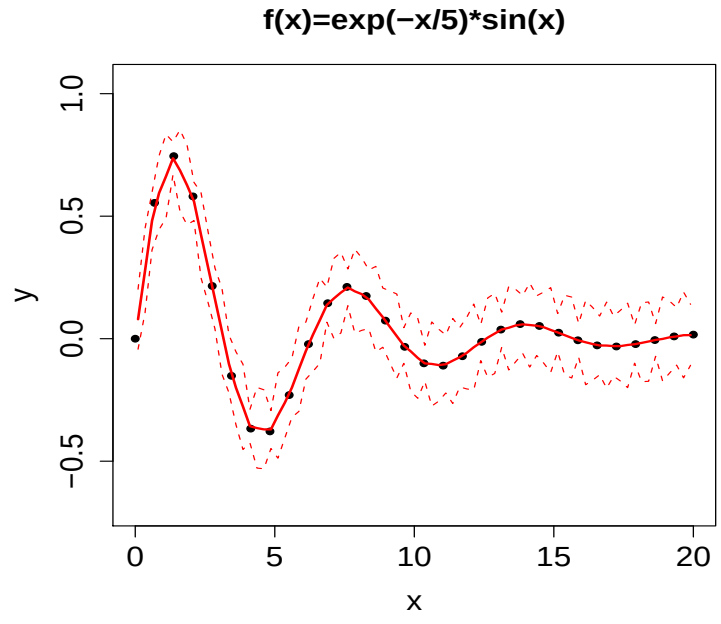
Courtesy MN Cancer Surveillance System, Dept. of Health

Haran, Hodges, Carlin (*JCGS*)

Fitting Complicated Functions

Useful for interpolating complicated functions (emulating complex computer models, machine learning).





Red curves are interpolations using *same, simple GP model*:

$y(x) = \mu + w(x)$, $\{w(x), x \in (0, 20)\}$ is a zero-mean GP.

Gaussian Random Field (Linear) Models

- Spatial process at location $\mathbf{s}$ is $Z(\mathbf{s}) = X(\mathbf{s})\beta + w(\mathbf{s})$, $X(\mathbf{s})$ are covariates at $\mathbf{s}$.
- Model dependence among spatial random variables by imposing it on random effects $\{w(\mathbf{s}), \mathbf{s} \in D\}$.
- For $\mathbf{s}_1, \ldots, \mathbf{s}_n \in D$, $\mathbf{w} = (w(\mathbf{s}_1), \ldots, w(\mathbf{s}_n))^T$ modeled via:
  - Gaussian process (GP) for continous-domain.
  - Gaussian Markov random field (GMRF) for lattice data.

Spatial Linear GP Model

- Gaussian Process (GP): Let Θ be covariance function parameters, so covariance matrix is $\Sigma(\Theta)$.
- Let $\mathbf{Z} = (Z(\mathbf{s}_1), \ldots, Z(\mathbf{s}_n))^T$

$$\mathbf{Z}|\Theta, \beta \sim N(\mathbf{X}\beta, \Sigma(\Theta))$$

Spatial Linear GMRF Model

- Gaussian Markov Random field (GMRF): Let Θ be the parameters for precision matrix $Q(\Theta)$

$$\mathbf{Z}|\Theta, \beta \sim N(\mathbf{X}\beta, Q^{-1}(\Theta))$$

  [Note: Intrinsic GMRF precision matrix is singular.]

- Specify priors for Θ, β.
- Inference based on p-dimensional posterior $\pi(\Theta, \beta \mid \mathbf{Z})$.

Typical approach for inference is Markov chain Monte Carlo (MCMC): Construct Markov chain with π as its invariant distribution.

Spatial Generalized Linear Mixed Models (SGLMMs)

- Stage 1: Model $Z(\mathbf{s}_i)$ conditionally independent with distribution f given parameters β, Θ, spatial errors $w(\mathbf{s}_i)$

$$f(Z(\mathbf{s}_i)|\beta, \Theta, w(\mathbf{s}_i)),$$

  where $g(E(Z(\mathbf{s}_i))) = \eta(\mathbf{s}_i) = X(\mathbf{s}_i)\beta + w(\mathbf{s}_i)$, η is a canonical link function (for example the logit link).
- Stage 2: Again $\mathbf{w} = (w(\mathbf{s}_1), \ldots, w(\mathbf{s}_n))^T \sim$ GP or GMRF.
- Stage 3: Priors for Θ, β.

Besag, York, Mollié (1991), Diggle et al. (1998)

Inference/Prediction for SGLMMs

Inference is based on $(p + N)$-dimensional posterior

$$\pi(\Theta, \beta, \mathbf{w} \mid \mathbf{Z}).$$

MCMC-based inference is straightforward, but only in principle:

- Computing issues: MCMC algorithms are slow mixing, distributions are often high-dimensional.
- Modeling issues: Regression coefficients in SGLMM are not interpretable. Current interpretation and conclusions are usually wrong!

I will discuss some solutions to both problems.

MCMC basics

- Goal: estimate $E_\pi g$ for real valued functions g.

  E.g. Expected values w.r.t. posterior distribution π.
- Construct a Harris-ergodic Markov chain $X_1, X_2, \ldots$ with stationary distribution π so that if $E_\pi|g(x)| < \infty$:

$$\bar{g}_n = \sum_{i=1}^{n} g(X_i)/n \to E_\pi g$$

Careful users face several issues:

- Starting values?
- Devising/tuning the Metropolis-Hastings algorithm.
- How long to run the Markov chain?
- Accuracy of the estimator is hard to assess.

Automation of MCMC

Ideally (the holy grail):

- Automated approach for constructing algorithm. No tuning necessary.
- Generate appropriate starting values automatically.
- Have rigorous criteria for determining when to stop. Ideally one that is *directly related to inferential goals*. E.g. How accurate do you want your estimates to be?
- Some theoretical guarantees regarding all of the above.

Some Options

1. Exact sampling:
   - *Perfect* draws using a Markov chain (Propp-Wilson, 1996).
   - Make classical (old fashioned) Monte Carlo methods such as rejection sampling practical.
2. Construct Metropolis-Hastings so Markov chain sampler mixes well (e.g. uniformly or geometrically ergodic):
   - Rigorous approach for estimating Monte Carlo standard errors and stopping rules.

(1) is very difficult for SGLMMs. When achievable, less efficient than corresponding MCMC sampler.

(2) is hard to achieve, challenging analytical work.

Efficient MCMC for Spatial Linear Models

- Easier since $\pi(\Theta, \boldsymbol{\beta} \mid \mathbf{Z})$ is low-dimensional (usually 2-8 dimensions).
- Slice samplers (Agarwal, Gelfand 2005; Yan et al., 2007) or parallel multivariate slice samplers (Tibbits, Haran, Liechty (2011), *Stats and Computing*).

Efficient MCMC for SGLMMs

Computing for SGLMMs is more challenging:

- Dimensions of $\pi(\Theta, \beta, \mathbf{w} \mid \mathbf{Z})$ (more than N)
- Two-pronged problem with basic MCMC:
  - Slow mixing Markov chain.
  - Each update of Markov chain may be expensive.
- Block sampling – updating multiple components at once – can help with both issues.
- Challenges with block sampling: (1) hard to construct good block proposals, (2) matrix operations at each iteration can be expensive.

Efficient MCMC for SGLMMs

Two general routes for constructing MCMC updates:

1. Approximate SGLMM by linear spatial model.
2. Langevin-Hastings (Roberts and Tweedie, 1996; Christensen, Roberts, Sköld, 2006; Recta, Haran, Rosenberger, 2011).

In this talk I will focus on #1.

Linearization of an SGLMM

- Target posterior of SGLMM is $\pi(\Theta, \boldsymbol{\beta}, \mathbf{w} \mid \mathbf{Z})$.
- Approximate the SGLMM by a linear spatial model:
  - Transform data $\mathbf{Z}$ to $\mathbf{Y}$ and use approximation of form:

$$\mathbf{Y} \mid \Theta, \boldsymbol{\beta}, \mathbf{w} \sim N(\mathbf{X}\boldsymbol{\beta} + \mathbf{w}, C).$$

    Let posterior for this approximate model be $S(\Theta, \boldsymbol{\beta}, \mathbf{w})$.

- Analytically integrate: $S_1(\Theta, \boldsymbol{\beta}) = \int S(\Theta, \boldsymbol{\beta}, \mathbf{w}) d\mathbf{w}$. Can rewrite approximate joint distribution as:

$$S(\Theta, \boldsymbol{\beta}, \mathbf{w}) = S_1(\Theta, \boldsymbol{\beta}) S_2(\mathbf{w} \mid \Theta, \boldsymbol{\beta}),$$

with $S_2(\mathbf{w} \mid \Theta, \boldsymbol{\beta})$ multivariate normal.

Approximation

Construct heavy-tailed approximation $\hat{\pi}(\Theta, \beta, \mathbf{w})$:

- We have: $S_1(\Theta, \beta) S_2(\mathbf{w} \mid \Theta, \beta) \approx \pi(\Theta, \beta, \mathbf{w}|Y)$.
- Find heavy-tailed approximation to $S_1(\Theta, \beta)$: $\hat{\pi}_1(\Theta, \beta)$.
- Find heavy-tailed (multi-t) approximation to $S_2(\mathbf{w}|\Theta, \beta)$, $\hat{\pi}_2(\mathbf{w}|\Theta, \beta)$.

Haran and Tierney (2011); Haran (2011)

A Joint Proposal Distribution

- $\hat{\pi}(\Theta, \boldsymbol{\beta}, \mathbf{w})$: proposal for Monte Carlo algorithms.
- Can sample sequentially from $\hat{\pi}$:
  1. Sample $\Theta, \boldsymbol{\beta} \sim \hat{\pi}_1(\Theta, \boldsymbol{\beta})$.
  2. Sample $\mathbf{w} \mid \Theta, \boldsymbol{\beta} \sim \hat{\pi}_2(\mathbf{w} \mid \Theta, \boldsymbol{\beta})$.

Stopping Rules, Estimating Standard Errors

MCMC using $\hat{\pi}$:

- Under mild moment conditions, CLT holds for estimate of expectations (cf. Roberts and Rosenthal, 2004).
- Can calculate a *consistent* estimate of MCMC standard error: **consistent batch means** (Jones et al., 2006).
- **'Fixed width' stopping rule**: When estimated standard error is below a desired level, stop the sampler.

Justifications:

- Theoretical: Jones, Haran, Caffo, Neath (2006), *JASA*
- Examples: Flegal, Haran, Jones (2008), *Stat Science*. More reliable and intuitive than Gelman-Rubin diagnostic.

Automated MCMC

1. Generate starting values from $\hat{\pi}$: genuinely overdispersed with respect to π (cf. Gelman and Rubin, 1992).
2. Construct a Metropolis-Hastings 'independence sampler' (cf. Tierney, 1994): propose every M-H update from $\hat{\pi}$.
   - Can prove that the resulting sampler is uniformly ergodic. (Haran and Tierney, 2010).
   - The sampler is "embarrassingly parallel."
3. Stop Markov chain when desired MCMC standard errors are attained (estimated using consistent batch means).

Implications for MCMC for SGLMMs

In practice: Works well for popular Besag, York, Mollié (1991) model, even for $\approx$ 1000 dimensions.

This is like iid Monte Carlo !

- CLT holds (generally not true for MCMC) under similar conditions to iid Monte Carlo. Have easy to compute, consistent standard error estimates.
- Easy to determine starting values.
- Automated, rigorous stopping rule.

Observations

General MCMC recipe, even when approximation/theory is too hard:

1. Construct a good MCMC sampler.
2. Run the sampler until MCMC standard errors are small enough. Calculate MCMC standard errors using **consistent batch means**: $<$ 10 lines of `R` code available on my website.

Not a panacea (and none exists): should still run from multiple starting values, very long chains, etc. No guarantees when distribution is multi-modal.

General (non SGLMM) Uses

The fixed-width strategy can be used as a diagnostic for *any* MCMC algorithm.

- Simulation studies, nested Monte Carlo. E.g. posterior expected values across randomly generated data sets. Need (automatically) shorter or longer runs for different data sets to obtain comparable estimates.
- Automatically runs longer when Markov chain mixes poorly, or expectation is challenging (e.g. tail probabilities). Shorter for less accuracy or if chain is fast mixing.
- More reliable than some popular convergence diagnostics (examples in Flegal, Haran, Jones, 2008).

“Halftime” Summary

Possible to construct efficient automated MCMC algorithms for SGLMMs using approximations and theoretical developments:

- Consistent estimate of standard errors.
- Known mixing properties of Markov chain.
- Automatically generate starting values.
- **Simple, rigorous stopping rule (‘fixed width’): when desired accuracy is attained, stop.**
- Useful to take advantage of sparsity, parallel computing when possible.

Now: Interpretability of spatial random effects...

SGLMM Random Effects

- Spatial random effects ($\mathbf{w}$) are introduced as a device for modeling dependence.
- Inferential issues: confounding between β and $\mathbf{w}$ leading to variance inflation for (β) inference.
- Computational issues: at least one random effect for each data point so high-dimensional posterior distribution ($n + p$) with a lot of dependence among random effects.
  Two-pronged computing issues.

Why Are There Inferential Issues?

- Let $\mathbf{P}$ be orthogonal projection onto $\text{span}(\mathbf{X})$, $\mathbf{P} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$.
- Let $\mathbf{P}^{\perp}$ be orthogonal projection onto $\text{span}(\mathbf{X})$'s orthogonal complement, $\mathbf{P}^{\perp} = \mathbf{I} - \mathbf{P}$.
- Spectral decomposition to acquire orthogonal bases, $\mathbf{K}_{n\times p}$ and $\mathbf{L}_{n\times(n-p)}$, for $\text{span}(\mathbf{X})$ and $\text{span}(\mathbf{X})^{\perp}$, respectively. These bases allow us to write:

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

which exposes the source of the spatial confounding: $\mathbf{K}$ is collinear with $\mathbf{X}$.

A Reparameterization

- **K** have no scientific meaning, so delete them

$$g(\mathbb{E}(Z_i \mid \boldsymbol{\beta}, \boldsymbol{\delta})) = \mathbf{X}_i\boldsymbol{\beta} + \mathbf{L}_i\boldsymbol{\delta}.$$

  Prior for random effects $\boldsymbol{\delta}$,
  $p(\boldsymbol{\delta} \mid \tau) \propto \tau^{(n-p)/2} \exp\left(-\frac{\tau}{2}\boldsymbol{\delta}'\mathbf{Q}^*\boldsymbol{\delta}\right)$, where $\mathbf{Q}^* = \mathbf{L}'\mathbf{Q}\mathbf{L}$.

- Corrects issues due to confounding.
- Slight reduction in dimensions: $n + p$ to n.
- *Reparameterization ignores underlying graph/spatial dependence structure.*

Reich, Hodges and Zadnik (2006)

A Sparse Reparameterization

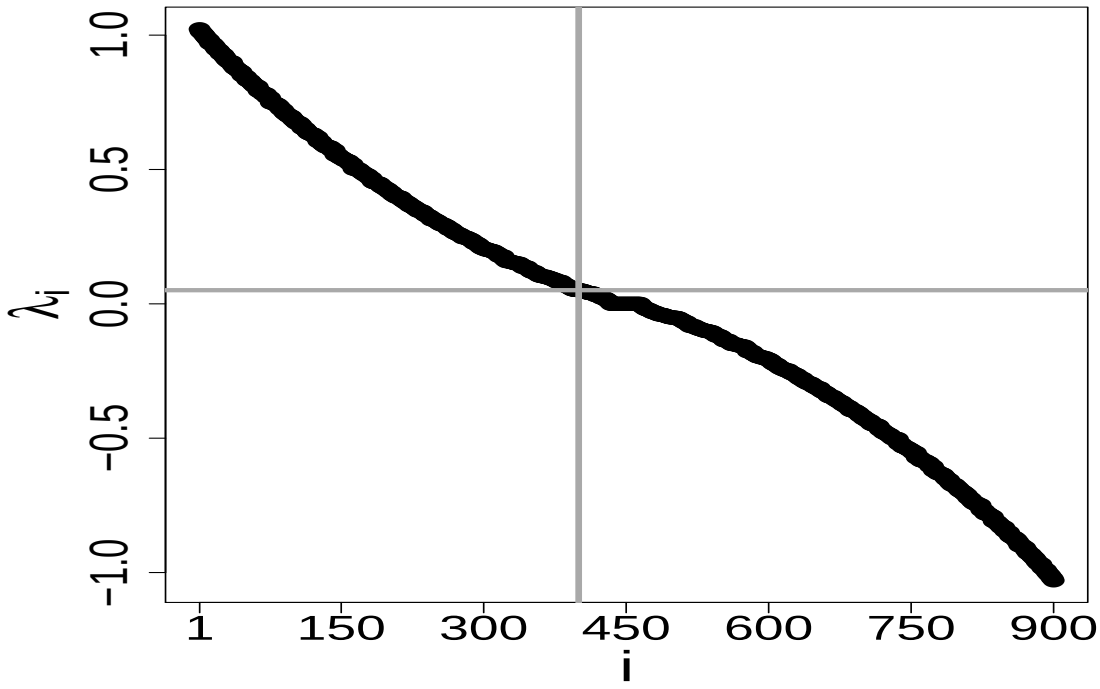
- Represent the graph/lattice $G = (V, E)$ using its adjacency matrix, $\mathbf{A}$, which is the $n \times n$ matrix with entries given by $\text{diag}(\mathbf{A}) = \mathbf{0}$ and $\mathbf{A}_{ij} = 1\{(i, j) \in E, i \neq j\}$, where $1\{\cdot\}$ denotes the indicator function.
- Our approach is inspired by Griffith (2003). Griffith's goal: reveal structure of missing spatial covariates. Our goal: smoothing orthogonal to $\mathbf{X}$.

$$\mathbf{M}(\mathbf{A}) = \mathbf{P}^{\perp}\mathbf{A}\mathbf{P}^{\perp}$$

- Eigenvectors comprise all possible patterns of clustering residual to $\mathbf{X}$ and accounting for G.

Eigenvalues

Infant mortality data example:



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

A Sparse Reparameterization

- Replacing **L** with **M** in the RHZ model gives

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

  And the prior for the random effects is now

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

- Corrects issues due to confounding.
- Disallows negative dependence (so long as $\lambda_q > 0$)
- Dimension reduction
  - Traditional: $n + p$. RHZ reparameterization: n.
  - Sparse/graph-based reparamaterization: $q + p$ (where q is $n/4$ in examples that follow but could be much smaller).

"However beautiful the strategy, you should occasionally look at the results." - Winston Churchill

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.

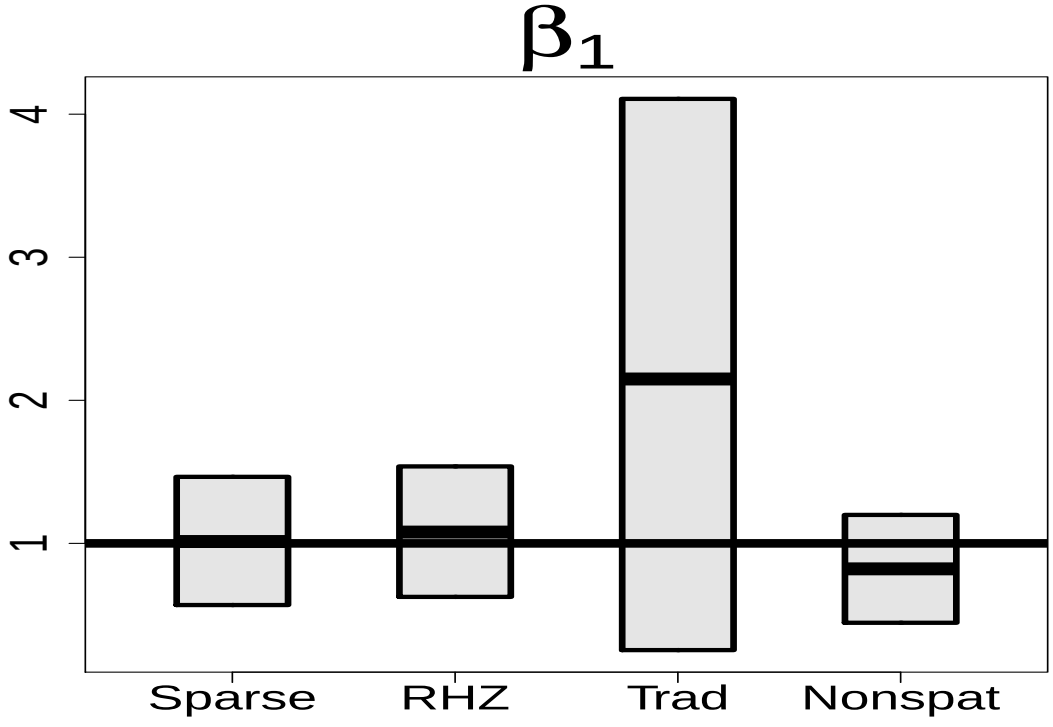
Model	$\hat{\beta}_1$ CI(β_1)	$\hat{\beta}_2$ CI(β_2)
Sparse	1.080 (0.613, 1.556)	1.130 (0.644, 1.635)
RHZ	1.120 (0.637, 1.606)	1.192 (0.679, 1.713)
Traditional	0.500 (-2.655, 3.616)	-0.605 (-3.698, 2.577)

- Traditional model CIs for β_1, β_2 include 0, i.e., they claim non-significance.
- Similar results for other SGLMMs including for Poisson and Gaussian (linear).

Simulation 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.



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 and mixes faster.
- Can potentially obtain greater speed-ups by further reducing dimensionality.

Summary

SGLMMs are a flexible, useful class of models.

- Modeling concerns: our reparameterization results in
  - interpretable regression coefficients, sensible spatial dependence.
  - natural approach to dimension reduction. MCMC faster per iteration and Markov chains mix better.
- Computational concerns: possible to construct MCMC algorithms using heavy-tailed approximations for SGLMM posteriors
  - Approximation specifies algorithm completely.
  - Rigorous estimates of standard errors.
  - Theoretically justified stopping rule.

More Generally ...

- Need to be careful when interpreting parameters in hierarchical models, particularly in the presence of random effects with dependence.
- Challenging open problem: Reparameterization/dimension reduction for Gaussian process-based SGLMMs.
- General principle for MCMC-based inference: construct good algorithms, run chains for as long as possible, and use fixed-width approach – *always monitor MCMC standard errors of posterior expectations*.

Collaborators

- J. Hughes, U. of Minnesota Biostatistics
- M.M. Tibbits
- J.M. Flegal, U.C. Riverside
- G.L. Jones, U. Minnesota
- J.C. Liechty, Penn State
- L. Tierney, U. of Iowa

Select References

- R code for MCMC standard errors:
  `http://www.stat.psu.edu/~mharan/cbm.R`
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