

Introduction to Geostatistics

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- Course materials available at
<https://doserjef.github.io/CASANR23-Spatial-Modeling/>

What is spatial data?

- Any data with some geographical information (i.e., spatially indexed)
- Common sources of spatial data: agricultural, climatology, forestry, ecology, environmental health, disease epidemiology, product marketing, etc.
 - have many important predictors and response variables
 - are often presented as maps

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 - have many important predictors and response variables
 - are often presented as maps
- Other examples where spatial need not refer to space on earth:
 - Genetics (position along a chromosome)
 - Neuroimaging (data for each voxel in the brain)

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Point-referenced spatial data

- Each observation is associated with a location (point)
- Data represents a sample from a continuous spatial domain
- Also referred to as **geocoded** or **geostatistical** data

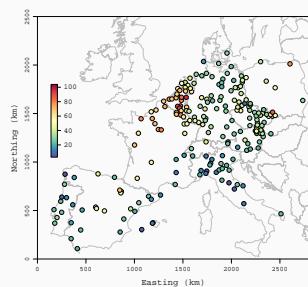


Figure: Pollutant levels in Europe in March, 2009

Point level modeling

- Point-level modeling** refers to modeling of point-referenced data collected at locations referenced by **coordinates** (e.g., lat-long, Easting-Northing).
- Data from a spatial process $\{Y(\mathbf{s}) : \mathbf{s} \in \mathcal{D}\}$, \mathcal{D} is a subset in Euclidean space.
- Example:** $Y(\mathbf{s})$ is a **pollutant level** at site \mathbf{s}
- Conceptually:** Pollutant level exists at all possible sites
- Practically:** Data will be a partial realization of a spatial process – observed at $\{\mathbf{s}_1, \dots, \mathbf{s}_n\}$
- Statistical objectives:** **Inference** about the process $Y(\mathbf{s})$; **predict** at new locations.
- Remarkable:** Can learn about entire $Y(\mathbf{s})$ surface. The **key**: Structured dependence

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Exploratory data analysis (EDA): Plotting the data

What's so special about spatial?

- A typical setup: Data observed at n locations $\{\mathbf{s}_1, \dots, \mathbf{s}_n\}$
- At each \mathbf{s}_i we observe the response $y(\mathbf{s}_i)$ and a $p \times 1$ vector of covariates $\mathbf{x}(\mathbf{s}_i)$
- Surface plots** of the data often helps to understand spatial patterns

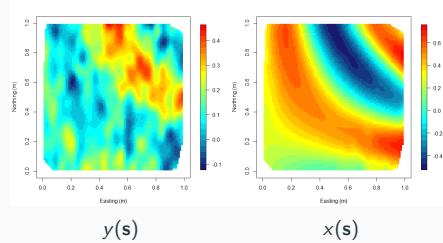


Figure: Response and covariate surface plots for Dataset 1

- Linear regression model: $y(\mathbf{s}_i) = \mathbf{x}(\mathbf{s}_i)^\top \beta + \epsilon(\mathbf{s}_i)$
- $\epsilon(\mathbf{s}_i)$ are iid $N(0, \tau^2)$ errors
- $\mathbf{y} = (y(\mathbf{s}_1), \dots, y(\mathbf{s}_n))^\top; \mathbf{X} = (\mathbf{x}(\mathbf{s}_1)^\top, \dots, \mathbf{x}(\mathbf{s}_n)^\top)^\top$
- Inference:** $\hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \sim N(\beta, \tau^2 (\mathbf{X}^\top \mathbf{X})^{-1})$
- Prediction** at new location \mathbf{s}_0 : $\widehat{y}(\mathbf{s}_0) = \mathbf{x}(\mathbf{s}_0)^\top \hat{\beta}$
- Although the data is spatial, this is an **ordinary linear regression** model

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Residual plots

Residual plots

- Surface plots of the residuals ($y(\mathbf{s}) - \widehat{y}(\mathbf{s})$) help to identify any spatial patterns left unexplained by the covariates

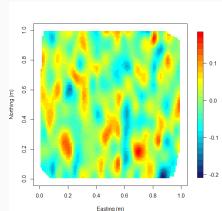


Figure: Residual plot for Dataset 1 after linear regression on $x(\mathbf{s})$

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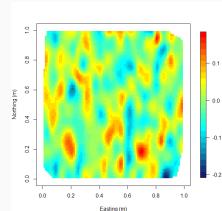


Figure: Residual plot for Dataset 1 after linear regression on $x(\mathbf{s})$

- No evident spatial pattern in plot of the residuals
- The covariate $x(\mathbf{s})$ seem to explain all spatial variation in $y(\mathbf{s})$
- Does a non-spatial regression model always suffice?**

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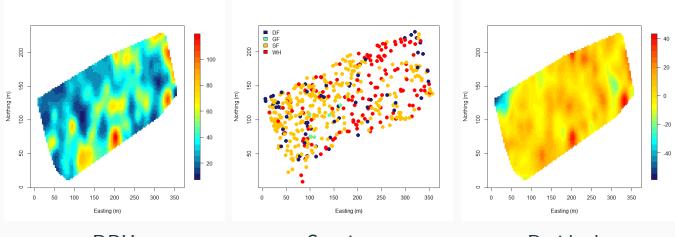
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Western Experimental Forestry (WEF) data

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- Data consist of a census of all trees in a 10 ha. stand in Oregon
- Response of interest: Diameter at breast height (DBH)
- Covariate: Tree species (Categorical variable)

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- Local spatial patterns** in the residual plot
- Simple regression on species seems to be **not sufficient**

More EDA

- Besides eyeballing residual surfaces, how to do more formal EDA to identify spatial pattern?

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First law of geography

"Everything is related to everything else, but near things are more related than distant things." – Waldo Tobler

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More EDA

- Besides eyeballing residual surfaces, how to do more formal EDA to identify spatial pattern?

First law of geography

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- In general $(Y(\mathbf{s} + \mathbf{h}) - Y(\mathbf{s}))^2$ roughly increasing with $\|\mathbf{h}\|$ will imply a spatial correlation
- Can this be formalized to identify spatial pattern?

Empirical semivariogram

- **Binning:** Make intervals $I_1 = (0, m_1)$, $I_2 = (m_1, m_2)$, and so forth, up to $I_K = (m_{K-1}, m_K)$. Representing each interval by its midpoint t_k , we define:

$$N(t_k) = \{(\mathbf{s}_i, \mathbf{s}_j) : \|\mathbf{s}_i - \mathbf{s}_j\| \in I_k\}, k = 1, \dots, K.$$

- **Empirical semivariogram:**

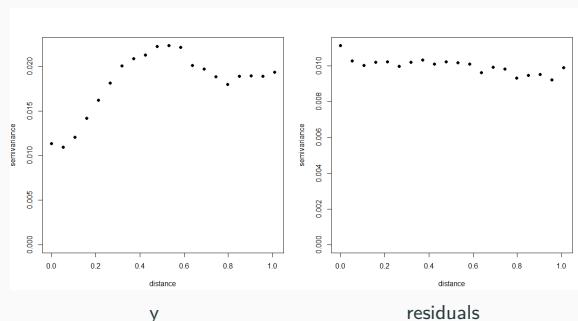
$$\gamma(t_k) = \frac{1}{2|N(t_k)|} \sum_{\mathbf{s}_i, \mathbf{s}_j \in N(t_k)} (Y(\mathbf{s}_i) - Y(\mathbf{s}_j))^2$$

- For spatial data, the $\gamma(t_k)$ is expected to roughly increase with t_k
- A flat semivariogram would suggest little spatial variation

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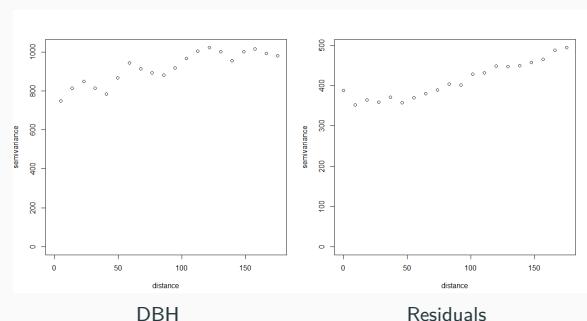
Empirical variogram: Data 1



- Residuals display little spatial variation

Empirical variograms: WEF data

- Regression model: DBH ~ Species



- Variogram of the residuals confirm unexplained spatial variation

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- When purely covariate based models does not suffice, one needs to leverage the information from locations
- General model using the locations:
 $y(\mathbf{s}) = \mathbf{x}(\mathbf{s})^\top \boldsymbol{\beta} + w(\mathbf{s}) + \epsilon(\mathbf{s})$ for all $\mathbf{s} \in \mathcal{D}$
- How to choose the function $w(\cdot)$?
- Since we want to predict at any location over the entire domain \mathcal{D} , this choice will amount to choosing a **surface** $w(\mathbf{s})$
- How should such a surface be chosen?

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- One popular approach to **model** $w(\mathbf{s})$ is via Gaussian Processes (GP)
- The collection of random variables $\{w(\mathbf{s}) \mid \mathbf{s} \in \mathcal{D}\}$ is a GP if
 - it is a **valid** stochastic process
 - all finite dimensional densities $\{w(\mathbf{s}_1), \dots, w(\mathbf{s}_n)\}$ follow multivariate Gaussian distribution
- A GP is completely characterized by a mean function $m(\mathbf{s})$ and a covariance function $C(\cdot, \cdot)$
- Advantage:** **Likelihood** based inference.
 $w = (w(\mathbf{s}_1), \dots, w(\mathbf{s}_n))^\top \sim N(\mathbf{m}, \mathbf{C})$ where
 $\mathbf{m} = (m(\mathbf{s}_1), \dots, m(\mathbf{s}_n))^\top$ and $\mathbf{C} = C(\mathbf{s}_i, \mathbf{s}_j)$

Valid covariance functions and isotropy

Some common isotropic covariance functions

- $C(\cdot, \cdot)$ needs to be **valid**. For any/all $\{\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_n\}$, the resulting covariance matrix $C(\mathbf{s}_i, \mathbf{s}_j)$ for $(w(\mathbf{s}_1), w(\mathbf{s}_2), \dots, w(\mathbf{s}_n))$ must be positive definite
- So, $C(\cdot, \cdot)$ needs to be a **positive definite** function
- Simplifying assumptions:
 - Stationarity:** $C(\mathbf{s}_1, \mathbf{s}_2)$ only depends on $\mathbf{h} = \mathbf{s}_1 - \mathbf{s}_2$ (and is denoted by $C(\mathbf{h})$)
 - Isotropic:** $C(\mathbf{h}) = C(\|\mathbf{h}\|)$
 - Anisotropic:** Stationary but not isotropic
- Isotropic models are popular because of their **simplicity**, **interpretability**, and because a number of relatively **simple parametric forms** are available as candidates for C .

| Model | Covariance function, $C(t) = C(\ \mathbf{h}\)$ |
|-----------------------|---|
| Spherical | $C(t) = \begin{cases} 0 & \text{if } t \geq 1/\phi \\ \sigma^2 \left[1 - \frac{3}{2}\phi t + \frac{1}{2}(\phi t)^3 \right] & \text{if } 0 < t \leq 1/\phi \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$ |
| Exponential | $C(t) = \begin{cases} \sigma^2 \exp(-\phi t) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$ |
| Powered exponential | $C(t) = \begin{cases} \sigma^2 \exp(- \phi t ^p) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$ |
| Matérn at $\nu = 3/2$ | $C(t) = \begin{cases} \sigma^2 (1 + \phi t) \exp(-\phi t) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{otherwise} \end{cases}$ |

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Notes on exponential model

Covariance functions and semivariograms

$$C(t) = \begin{cases} \tau^2 + \sigma^2 & \text{if } t = 0 \\ \sigma^2 \exp(-\phi t) & \text{if } t > 0 \end{cases}$$

- We define the **effective range**, t_0 , as the distance at which this correlation has dropped to only 0.05. Setting $\exp(-\phi t_0)$ equal to this value we obtain $t_0 \approx 3/\phi$, since $\log(0.05) \approx -3$.
- The **nugget** τ^2 is often viewed as a “**nonspatial effect variance**.”
- The **partial sill** (σ^2) is viewed as a “**spatial effect variance**.”
- $\sigma^2 + \tau^2$ gives the maximum total variance often referred to as the **sill**
- Note **discontinuity** at 0 due to the nugget. **Intentional!** To account for measurement error or micro-scale variability.

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- Recall:** Empirical semivariogram:

$$\gamma(t_k) = \frac{1}{2|N(t_k)|} \sum_{\mathbf{s}_i, \mathbf{s}_j \in N(t_k)} (Y(\mathbf{s}_i) - Y(\mathbf{s}_j))^2$$

- For any stationary GP,
 $E(Y(\mathbf{s} + \mathbf{h}) - Y(\mathbf{s}))^2/2 = C(\mathbf{0}) - C(\mathbf{h}) = \gamma(\mathbf{h})$
- $\gamma(\mathbf{h})$ is the **semivariogram** corresponding to the covariance function $C(\mathbf{h})$

- Example:** For exponential GP,

$$\gamma(t) = \begin{cases} \tau^2 + \sigma^2(1 - \exp(-\phi t)) & \text{if } t > 0 \\ 0 & \text{if } t = 0 \end{cases}$$

, where $t = \|\mathbf{h}\|$



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The Matérn covariance function

Kriging: Spatial prediction at new locations

- The Matérn is a very versatile family:

$$C(t) = \begin{cases} \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}(2\sqrt{\nu}t\phi)^\nu K_\nu(2\sqrt{\nu}t\phi) & \text{if } t > 0 \\ \tau^2 + \sigma^2 & \text{if } t = 0 \end{cases}$$

K_ν is the modified Bessel function of order ν (computationally tractable)

- ν is a smoothness parameter controlling process smoothness.
Remarkable!
- $\nu = 1/2$ gives the exponential covariance function

- Goal:** Given observations $\mathbf{w} = (w(\mathbf{s}_1), w(\mathbf{s}_2), \dots, w(\mathbf{s}_n))^\top$, predict $w(\mathbf{s}_0)$ for a new location \mathbf{s}_0
- If $w(\mathbf{s})$ is modeled as a GP, then $(w(\mathbf{s}_0), w(\mathbf{s}_1), \dots, w(\mathbf{s}_n))^\top$ jointly follow multivariate normal distribution
- $w(\mathbf{s}_0) | \mathbf{w}$ follows a normal distribution with
 - Mean (**Kriging estimator**): $m(\mathbf{s}_0) + \mathbf{c}^\top \mathbf{C}^{-1}(\mathbf{w} - \mathbf{m})$, where $\mathbf{m} = E(\mathbf{w})$, $\mathbf{C} = \text{Cov}(\mathbf{w}, \mathbf{w})$, $\mathbf{c} = \text{Cov}(\mathbf{w}, w(\mathbf{s}_0))$
 - Variance: $\mathbf{C}(\mathbf{s}_0, \mathbf{s}_0) - \mathbf{c}^\top \mathbf{C}^{-1} \mathbf{c}$
- The GP formulation gives the **full predictive distribution** of $w(\mathbf{s}_0) | \mathbf{w}$

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Modeling with GPs

Parameter estimation

Spatial linear model

$$y(\mathbf{s}) = \mathbf{x}(\mathbf{s})^\top \boldsymbol{\beta} + w(\mathbf{s}) + \epsilon(\mathbf{s})$$

- $w(\mathbf{s})$ modeled as $GP(0, C(\cdot | \theta))$ (usually without a nugget)
- $\epsilon(\mathbf{s}) \stackrel{iid}{\sim} N(0, \tau^2)$ contributes to the nugget
- Under isotropy: $C(\mathbf{s} + \mathbf{h}, \mathbf{s}) = \sigma^2 R(|\mathbf{h}| ; \phi)$
- $\mathbf{w} = (w(\mathbf{s}_1), \dots, w(\mathbf{s}_n))^\top \sim N(\mathbf{0}, \sigma^2 \mathbf{R}(\phi))$ where $\mathbf{R}(\phi) = \sigma^2 (R(|\mathbf{s}_i - \mathbf{s}_j| ; \phi))$
- $\mathbf{y} = (y(\mathbf{s}_1), \dots, y(\mathbf{s}_n))^\top \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{R}(\phi) + \tau^2 \mathbf{I})$

- $\mathbf{y} = (y(\mathbf{s}_1), \dots, y(\mathbf{s}_n))^\top \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{R}(\phi) + \tau^2 \mathbf{I})$
- We can obtain MLEs of parameters $\boldsymbol{\beta}, \tau^2, \sigma^2, \phi$ based on the above model and use the estimates to krig at new locations
- In practice, the likelihood is often very **flat** with respect to the spatial covariance parameters and choice of **initial values** is important
- Initial values can be eyeballed from empirical semivariogram of the residuals from ordinary linear regression

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- For k total parameters and sample size n :
 - AIC: $2k - 2 \log(I(\mathbf{y} | \hat{\beta}, \hat{\theta}, \hat{\tau}^2))$
 - BIC: $\log(n)k - 2 \log(I(\mathbf{y} | \hat{\beta}, \hat{\theta}, \hat{\tau}^2))$
- Prediction based approaches using holdout data:
 - Root Mean Square Predictive Error (RMSPE):

$$\sqrt{\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} (y_i - \hat{y}_i)^2}$$
 - Coverage probability (CP): $\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} I(y_i \in (\hat{y}_{i,0.025}, \hat{y}_{i,0.975}))$
 - Width of 95% confidence interval (CIW):

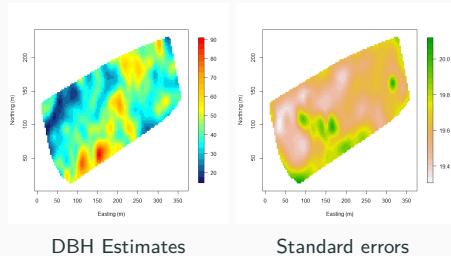
$$\frac{1}{n_{out}} \sum_{i=1}^{n_{out}} (\hat{y}_{i,0.975} - \hat{y}_{i,0.025})$$
 - The last two approaches compares the distribution of y_i instead of comparing just their point predictions

Table: Model comparison

| | Spatial | Non-spatial |
|-------|---------|-------------|
| AIC | 4419 | 4465 |
| BIC | 4448 | 4486 |
| RMSPE | 18 | 21 |
| CP | 93 | 93 |
| CIW | 77 | 82 |

WEF data: Kriged surfaces

Summary



- Geostatistics – Analysis of point-referenced spatial data
- Surface plots of data and residuals
- EDA with empirical semivariograms
- Modeling unknown surfaces with Gaussian Processes
- Kriging: Predictions at new locations
- Spatial linear regression using Gaussian Processes

Bayesian Linear Models

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Linear Regression

- Linear regression is, perhaps, *the* most widely used statistical modeling tool.
- It addresses the following question: How does a quantity of primary interest, y , vary as (depend upon) another quantity, or set of quantities, x ?
- The quantity y is called the *response* or *outcome variable*. Some people simply refer to it as the *dependent variable*.
- The variable(s) x are called *explanatory variables*, *covariates* or simply *independent variables*.
- In general, we are interested in the conditional distribution of y , given x , parametrized as $p(y | \theta, x)$.

- Typically, we have a set of *units* or *experimental subjects*
 $i = 1, 2, \dots, n$.
- For each of these units we have measured an outcome y_i and a set of explanatory variables $\mathbf{x}_i^\top = (1, x_{i1}, x_{i2}, \dots, x_{ip})$.
- The first element of \mathbf{x}_i^\top is often taken as 1 to signify the presence of an “intercept.”
- We collect the outcome and explanatory variables into an $n \times 1$ vector and an $n \times (p+1)$ matrix:

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}; \quad \mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \dots & x_{1p} \\ 1 & x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix}.$$

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- The linear model is the most fundamental of all serious statistical models underpinning:
 - ANOVA: y_i is continuous, x_{ij} 's are *all* categorical
 - REGRESSION: y_i is continuous, x_{ij} 's are continuous
 - ANCOVA: y_i is continuous, x_{ij} 's are continuous for some j and categorical for others.

Conjugate Bayesian Linear Regression

- A conjugate Bayesian linear model is given by:
 $y_i | \beta, \sigma^2, \mathbf{x}_i \stackrel{\text{ind}}{\sim} N(\mu_i, \sigma^2); \quad i = 1, 2, \dots, n;$
 $\mu_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip} = \mathbf{x}_i^\top \beta; \quad \beta = (\beta_0, \beta_1, \dots, \beta_p)^\top;$
 $\beta | \sigma^2 \sim N(\boldsymbol{\mu}_\beta, \sigma^2 \mathbf{V}_\beta); \quad \sigma^2 \sim IG(a, b).$
- Unknown parameters include the regression parameters and the variance, i.e. $\theta = \{\beta, \sigma^2\}$.
- We assume \mathbf{X} is observed without error and all inference is conditional on \mathbf{X} .
- The above model is often written in terms of the posterior density $p(\theta | \mathbf{y}) \propto p(\theta, \mathbf{y})$:

$$IG(\sigma^2 | a, b) \times N(\beta | \boldsymbol{\mu}_\beta, \sigma^2 \mathbf{V}_\beta) \times \prod_{i=1}^n N(y_i | \mathbf{x}_i^\top \beta, \sigma^2).$$

Conjugate Bayesian (General) Linear Regression

- A more general conjugate Bayesian linear model is given by:
 $\mathbf{y} | \beta, \sigma^2, \mathbf{X} \sim N(\mathbf{X}\beta, \sigma^2 \mathbf{V}_y)$
 $\beta | \sigma^2 \sim N(\boldsymbol{\mu}_\beta, \sigma^2 \mathbf{V}_\beta);$
 $\sigma^2 \sim IG(a, b).$
- \mathbf{V}_y , \mathbf{V}_β and $\boldsymbol{\mu}_\beta$ are assumed fixed.
- Unknown parameters include the regression parameters and the variance, i.e. $\theta = \{\beta, \sigma^2\}$.
- We assume \mathbf{X} is observed without error and all inference is conditional on \mathbf{X} .
- The posterior density $p(\theta | \mathbf{y}) \propto p(\theta, \mathbf{y})$:

$$IG(\sigma^2 | a, b) \times N(\beta | \boldsymbol{\mu}_\beta, \sigma^2 \mathbf{V}_\beta) \times N(\mathbf{y} | \mathbf{X}\beta, \sigma^2 \mathbf{V}_y)$$

- The model on the previous slide is a special case with $\mathbf{V}_y = \mathbf{I}_n$ ($n \times n$ identity matrix).

Conjugate Bayesian (General) Linear Regression

- The joint posterior density can be written as

$$p(\beta, \sigma^2 | \mathbf{y}) \propto \underbrace{IG(\sigma^2 | a^*, b^*)}_{p(\sigma^2 | \mathbf{y})} \times \underbrace{N(\beta | \mathbf{Mm}, \sigma^2 \mathbf{M})}_{p(\beta | \sigma^2, \mathbf{y})},$$

where

$$a^* = a + \frac{n}{2}; \quad b^* = b + \frac{1}{2} \left(\boldsymbol{\mu}_\beta^\top \mathbf{V}_\beta^{-1} \boldsymbol{\mu}_\beta + \mathbf{y}^\top \mathbf{V}_y^{-1} \mathbf{y} - \mathbf{m}^\top \mathbf{M} \mathbf{m} \right);$$

$$\mathbf{m} = \mathbf{V}_\beta^{-1} \boldsymbol{\mu}_\beta + \mathbf{X}^\top \mathbf{V}_y^{-1} \mathbf{y}; \quad \mathbf{M}^{-1} = \mathbf{V}_\beta^{-1} + \mathbf{X}^\top \mathbf{V}_y^{-1} \mathbf{X}.$$

- Exact posterior sampling from $p(\beta, \sigma^2 | \mathbf{y})$ will automatically yield samples from $p(\beta | \mathbf{y})$ and $p(\sigma^2 | \mathbf{y})$.
- For each $j = 1, 2, \dots, N$ do the following:
 - Draw $\sigma_{(j)}^2 \sim IG(a^*, b^*)$
 - Draw $\beta_{(j)} \sim N(\mathbf{Mm}, \sigma_{(j)}^2 \mathbf{M})$
- The above is sometimes referred to as *composition sampling*.

Exact sampling from joint posterior distributions

- Suppose we wish to draw samples from a joint posterior:
 $p(\theta_1, \theta_2 | \mathbf{y}) = p(\theta_1 | \mathbf{y}) \times p(\theta_2 | \theta_1, \mathbf{y}).$
- In conjugate models, it is often easy to draw samples from $p(\theta_1 | \mathbf{y})$ and from $p(\theta_2 | \theta_1, \mathbf{y})$.
- We can draw N samples from $p(\theta_1, \theta_2 | \mathbf{y})$ as follows.
- For each $j = 1, 2, \dots, N$ do the following:
 - Draw $\theta_{1(j)} \sim p(\theta_1 | \mathbf{y})$
 - Draw $\theta_{2(j)} \sim p(\theta_2 | \theta_{1(j)}, \mathbf{y})$
- Remarkably, the $\theta_{2(j)}$'s drawn above have marginal distribution $p(\theta_2 | \mathbf{y})$ (see, Gelfand and Smith 1990).
- “Automatic Marginalization” we draw samples $p(\theta_1, \theta_2 | \mathbf{y})$ and automatically get samples from $p(\theta_1 | \mathbf{y})$ and $p(\theta_2 | \mathbf{y})$.

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Bayesian predictions from linear regression

- Let $\tilde{\mathbf{y}}$ denote an $m \times 1$ vector of outcomes we seek to predict based upon predictors $\tilde{\mathbf{X}}$.

- We seek the posterior predictive density:

$$p(\tilde{\mathbf{y}} | \mathbf{y}) = \int p(\tilde{\mathbf{y}} | \theta, \mathbf{y}) p(\theta | \mathbf{y}) d\theta.$$

- Posterior predictive inference: sample from $p(\tilde{\mathbf{y}} | \mathbf{y})$.

- For each $j = 1, 2, \dots, N$ do the following:

- Draw $\theta_{(j)} \sim p(\theta | \mathbf{y})$
- Draw $\tilde{\mathbf{y}}_{(j)} \sim p(\tilde{\mathbf{y}} | \theta_{(j)}, \mathbf{y})$

Bayesian predictions from linear regression (cont'd)

- For legitimate probabilistic predictions (forecasting), the conditional distribution $p(\tilde{\mathbf{y}} | \theta, \mathbf{y})$ must be well-defined.
- For example, consider the case with $\mathbf{V}_y = \mathbf{I}_n$. Specify the linear model:

$$\begin{bmatrix} \mathbf{y} \\ \tilde{\mathbf{y}} \end{bmatrix} = \begin{bmatrix} \mathbf{X} \\ \tilde{\mathbf{X}} \end{bmatrix} \beta + \begin{bmatrix} \epsilon \\ \tilde{\epsilon} \end{bmatrix}; \quad \begin{bmatrix} \epsilon \\ \tilde{\epsilon} \end{bmatrix} \sim N \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \sigma^2 \begin{bmatrix} \mathbf{I}_n & \mathbf{O} \\ \mathbf{O} & \mathbf{I}_m \end{bmatrix} \right).$$

- Easy to derive the conditional density:

$$p(\tilde{\mathbf{y}} | \theta, \mathbf{y}) = p(\tilde{\mathbf{y}} | \theta) = N(\tilde{\mathbf{y}} | \tilde{\mathbf{X}}\beta, \sigma^2 \mathbf{I}_m)$$

- Posterior predictive density:

$$p(\tilde{\mathbf{y}} | \mathbf{y}) = \int N(\tilde{\mathbf{y}} | \tilde{\mathbf{X}}\beta, \sigma^2 \mathbf{I}_m) p(\beta, \sigma^2 | \mathbf{y}) d\beta d\sigma^2.$$

- For each $j = 1, 2, \dots, N$ do the following:

- Draw $\{\beta_{(j)}, \sigma_{(j)}^2\} \sim p(\beta, \sigma^2 | \mathbf{y})$
- Draw $\tilde{\mathbf{y}}_{(j)} \sim N(\tilde{\mathbf{X}}\beta_{(j)}, \sigma_{(j)}^2 \mathbf{I}_m)$

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Bayesian predictions from general linear regression

- For example, consider the case with general \mathbf{V}_y . Specify:

$$\begin{bmatrix} \mathbf{y} \\ \tilde{\mathbf{y}} \end{bmatrix} = \begin{bmatrix} \mathbf{X} \\ \tilde{\mathbf{X}} \end{bmatrix} \beta + \begin{bmatrix} \epsilon \\ \tilde{\epsilon} \end{bmatrix}; \quad \begin{bmatrix} \epsilon \\ \tilde{\epsilon} \end{bmatrix} \sim N \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \sigma^2 \begin{bmatrix} \mathbf{V}_y & \mathbf{V}_{y\tilde{y}} \\ \mathbf{V}_{y\tilde{y}}^\top & \mathbf{V}_{\tilde{y}} \end{bmatrix} \right).$$

- Derive the conditional density

$$p(\tilde{\mathbf{y}} | \theta, \mathbf{y}) = N(\tilde{\mathbf{y}} | \mu_{\tilde{y}|y}, \sigma^2 \mathbf{V}_{\tilde{y}|y}):$$

$$\mu_{\tilde{y}|y} = \tilde{\mathbf{X}}\beta + \mathbf{V}_{y\tilde{y}}^\top \mathbf{V}_y^{-1}(\mathbf{y} - \mathbf{X}\beta); \quad \mathbf{V}_{\tilde{y}|y} = \mathbf{V}_{\tilde{y}} - \mathbf{V}_{y\tilde{y}}^\top \mathbf{V}_y^{-1} \mathbf{V}_{y\tilde{y}}.$$

- Posterior predictive density:

$$p(\tilde{\mathbf{y}} | \mathbf{y}) = \int N(\tilde{\mathbf{y}} | \mu_{\tilde{y}|y}, \sigma^2 \mathbf{V}_{\tilde{y}|y}) p(\beta, \sigma^2 | \mathbf{y}) d\beta d\sigma^2.$$

- For each $j = 1, 2, \dots, N$ do the following:

- Draw $\{\beta_{(j)}, \sigma_{(j)}^2\} \sim p(\beta, \sigma^2 | \mathbf{y})$
- Compute $\mu_{\tilde{y}|y}$ using $\beta_{(j)}$ and draw $\tilde{\mathbf{y}}_{(j)} \sim N(\mu_{\tilde{y}|y}, \sigma_{(j)}^2 \mathbf{V}_{\tilde{y}})$

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Application to Bayesian Geostatistics

- Consider the spatial regression model

$$y(s_i) = \mathbf{x}^\top(s_i)\beta + w(s_i) + \epsilon(s_i),$$

where $w(s_i)$'s are spatial random effects and $\epsilon(s_i)$'s are unstructured errors ("white noise").

- $\mathbf{w} = (w(s_1), w(s_2), \dots, w(s_n))^\top \sim N(\mathbf{0}, \sigma^2 \mathbf{R}(\phi))$

- $\epsilon = (\epsilon(s_1), \epsilon(s_2), \dots, \epsilon(s_n))^\top \sim N(\mathbf{0}, \tau^2 \mathbf{I}_n)$

- Integrating out random effects leads to a Bayesian model:

$$IG(\sigma^2 | a, b) \times N(\beta | \mu_\beta, \sigma^2 \mathbf{V}_\beta) \times N(\mathbf{y} | \mathbf{X}\beta, \sigma^2 \mathbf{V}_y)$$

where $\mathbf{V}_y = \mathbf{R}(\phi) + \alpha \mathbf{I}_n$ and $\alpha = \tau^2 / \sigma^2$.

- Fixing ϕ and α (e.g., from variogram or other EDA) yields a conjugate Bayesian model (see `bayesGeostatExact()` in `spBayes` package).

- Exact posterior sampling is easily achieved as before!

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Inference on spatial random effects

- Rewrite the model in terms of \mathbf{w} as:

$$\begin{aligned} IG(\sigma^2 | a, b) \times N(\beta | \mu_\beta, \sigma^2 \mathbf{V}_\beta) \times N(\mathbf{w} | \mathbf{0}, \sigma^2 \mathbf{R}(\phi)) \\ \times N(\mathbf{y} | \mathbf{X}\beta + \mathbf{w}, \tau^2 \mathbf{I}_n). \end{aligned}$$

- Posterior distribution of spatial random effects \mathbf{w} :

$$p(\mathbf{w} | \mathbf{y}) = \int N(\mathbf{w} | \mathbf{M}\mathbf{m}, \sigma^2 \mathbf{M}) \times p(\beta, \sigma^2 | \mathbf{y}) d\beta d\sigma^2,$$

where $\mathbf{m} = (1/\alpha)(\mathbf{y} - \mathbf{X}\beta)$ and $\mathbf{M}^{-1} = \mathbf{R}^{-1}(\phi) + (1/\alpha)\mathbf{I}_n$.

- For each $j = 1, 2, \dots, N$ do the following:

- Draw $\{\beta_{(j)}, \sigma_{(j)}^2\} \sim p(\beta, \sigma^2 | \mathbf{y})$
- Compute \mathbf{m} from $\beta_{(j)}$ and draw $\mathbf{w}_{(j)} \sim N(\mathbf{M}\mathbf{m}, \sigma_{(j)}^2 \mathbf{M})$

Inference on the process

- Posterior distribution of $w(s_0)$ at new location s_0 :

$$p(w(s_0) | \mathbf{y}) = \int N(w(s_0) | \mu_{w(s_0)|w}, \sigma_{w(s_0)|w}^2) \times p(\sigma^2, \mathbf{w} | \mathbf{y}) d\sigma^2 d\mathbf{w},$$

where

$$\mu_{w(s_0)|w} = \mathbf{r}^\top(s_0; \phi) \mathbf{R}^{-1}(\phi) \mathbf{w};$$

$$\sigma_{w(s_0)|w}^2 = \sigma^2 \{1 - \mathbf{r}^\top(s_0; \phi) \mathbf{R}^{-1}(\phi) \mathbf{r}(s_0, \phi)\}$$

- For each $j = 1, 2, \dots, N$ do the following:

- Compute $\mu_{w(s_0)|w}$ and $\sigma_{w(s_0)|w}^2$ from $\mathbf{w}_{(j)}$ and $\sigma_{(j)}^2$.
- Draw $w_{(j)}(s_0) \sim N(\mu_{w(s_0)|w}, \sigma_{w(s_0)|w}^2)$.

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Bayesian “kriging” or prediction

Non-conjugate models: The Gibbs Sampler

- Posterior predictive distribution at new location s_0 is $p(y(s_0) | \mathbf{y})$:

$$\int N(y(s_0) | \mathbf{x}^\top(s_0)\beta + w(s_0), \alpha\sigma^2) \times p(\beta, \sigma^2, \mathbf{w} | \mathbf{y}) d\beta d\sigma^2 d\mathbf{w},$$

- For each $j = 1, 2, \dots, N$ do the following:

1. Draw $y_{(j)}(s_0) \sim N(\mathbf{x}^\top(s_0)\beta_{(j)} + w_{(j)}(s_0), \alpha\sigma_{(j)}^2)$.

- Let $\theta = (\theta_1, \dots, \theta_p)$ be the parameters in our model.

- Initialize with starting values $\theta^{(0)} = (\theta_1^{(0)}, \dots, \theta_p^{(0)})$

- For $j = 1, \dots, N$, update successively using the *full conditional distributions*:

$$\begin{aligned}\theta_1^{(j)} &\sim p(\theta_1^{(j)} | \theta_2^{(j-1)}, \dots, \theta_p^{(j-1)}, \mathbf{y}) \\ \theta_2^{(j)} &\sim p(\theta_2^{(j)} | \theta_1^{(j)}, \theta_3^{(j-1)}, \dots, \theta_p^{(j-1)}, \mathbf{y})\end{aligned}$$

⋮

$$\begin{aligned}&(\text{the generic } k^{\text{th}} \text{ element}) \\ \theta_k^{(j)} &\sim p(\theta_k | \theta_1^{(j)}, \dots, \theta_{k-1}^{(j)}, \theta_{k+1}^{(j-1)}, \dots, \theta_p^{(j-1)}, \mathbf{y})\end{aligned}$$

⋮

$$\theta_p^{(j)} \sim p(\theta_p | \theta_1^{(j)}, \dots, \theta_{p-1}^{(j)}, \mathbf{y})$$

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- In principle, the Gibbs sampler will work for extremely complex hierarchical models. The only issue is sampling from the full conditionals. They may not be amenable to easy sampling – when these are not in closed form. A more general and extremely powerful - and often easier to code - algorithm is the Metropolis-Hastings (MH) algorithm.
- This algorithm also constructs a Markov chain, but does not necessarily care about full conditionals.
- Popular approach: Embed Metropolis steps within Gibbs to draw from full conditionals that are not accessible to directly generate from.

When we don't want to fix ϕ and $\alpha = \tau^2/\sigma^2$

Latent Bayesian Model

$$\begin{aligned}N(\mathbf{y} | \mathbf{X}\beta + \mathbf{w}, \tau^2 \mathbf{I}) \times N(\mathbf{w} | \mathbf{0}, \sigma^2 \mathbf{R}(\phi)) \times N(\beta | \boldsymbol{\mu}_\beta, \mathbf{V}_\beta) \\ \times IG(\tau^2 | a_\tau, b_\tau) \times IG(\sigma^2 | a_\sigma, b_\sigma) \times Unif(\phi | a_\phi, b_\phi)\end{aligned}$$

Sampler:

- Full conditionals for β , τ^2 , σ^2 and $w(s_i)$'s
- Metropolis step for updating ϕ
- **Pros:** Full conditional distributions for all parameters except ϕ , easy to code up
- **Cons:** High-dimensional parameter space can mean slow convergence

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When we don't want to fix ϕ and $\alpha = \tau^2/\sigma^2$ (cont'd)

Collapsed Bayesian Model

$$\begin{aligned}N(\mathbf{y} | \mathbf{X}\beta, \sigma^2 \mathbf{R}(\phi) + \tau^2 \mathbf{I}) \times N(\beta | \boldsymbol{\mu}_\beta, \mathbf{V}_\beta) \\ \times IG(\tau^2 | a_\tau, b_\tau) \times IG(\sigma^2 | a_\sigma, b_\sigma) \times Unif(\phi | a_\phi, b_\phi)\end{aligned}$$

Sampler:

- Full conditional for β
- Metropolis step for updating τ^2 , σ^2 , ϕ
- **Pros:** Low-dimensional parameter space
- “Recover” $w(s_i)$'s in a posterior predictive fashion

We can also integrate out β ! See Finley et al. (2015) for details
<https://www.jstatsoft.org/article/view/v063i13> and implementation in the spBayes package.

The Metropolis-Hastings Algorithm

- The Metropolis-Hastings algorithm: Start with a initial value for $\theta = \theta^{(0)}$. Select a *candidate* or *proposal* distribution from which to propose a value of θ at the j -th iteration: $\theta^{(j)} \sim q(\theta^{(j-1)}, \nu)$. For example, $q(\theta^{(j-1)}, \nu) = N(\theta^{(j-1)}, \nu)$ with ν fixed.
- Compute
$$r = \frac{p(\theta^* | \mathbf{y})q(\theta^{(j-1)} | \theta^*, \nu)}{p(\theta^{(j-1)} | \mathbf{y})q(\theta^* | \theta^{(j-1)}, \nu)}$$
- If $r \geq 1$ then set $\theta^{(j)} = \theta^*$. If $r \leq 1$ then draw $U \sim (0, 1)$. If $U \leq r$ then $\theta^{(j)} = \theta^*$. Otherwise, $\theta^{(j)} = \theta^{(j-1)}$.
- Repeat for $j = 1, \dots, N$. This yields $\theta^{(1)}, \dots, \theta^{(N)}$, which, after a burn-in period, will be samples from the true posterior distribution. It is important to monitor the acceptance ratio r of the sampler through the iterations. Rough recommendations: for vector updates $r \approx 20\%$., for scalar updates $r \approx 40\%$. This can be controlled by “tuning” ν .
- Popular approach: Embed Metropolis steps within Gibbs to draw from full conditionals that are not accessible to directly generate from.

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- Example: For the linear model, our parameters are (β, σ^2) . We write $\theta = (\beta, \log(\sigma^2))$ and, at the j -th iteration, propose $\theta^* \sim N(\theta^{(j-1)}, \Sigma)$. The log transformation on σ^2 ensures that all components of θ have support on the entire real line and can have meaningful proposed values from the multivariate normal. But we need to transform our prior to $p(\beta, \log(\sigma^2))$.
- Let $z = \log(\sigma^2)$ and assume $p(\beta, z) = p(\beta)p(z)$. Let us derive $p(z)$.
REMEMBER: we need to adjust for the jacobian. Then $p(z) = p(\sigma^2)|d\sigma^2/dz| = p(e^z)e^z$. The jacobian here is $e^z = \sigma^2$.
- Let $p(\beta) = 1$ and an $p(\sigma^2) = IG(\sigma^2 | a, b)$. Then log-posterior is:

$$-(a + n/2 + 1)z + z - \frac{1}{e^z} \{b + \frac{1}{2}(Y - X\beta)^T(Y - X\beta)\}.$$

- A symmetric proposal distribution, say $q(\theta^* | \theta^{(j-1)}, \Sigma) = N(\theta^{(j-1)}, \Sigma)$, cancels out in r . In practice it is better to compute $\log(r)$: $\log(r) = \log(p(\theta^* | y)) - \log(p(\theta^{(j-1)} | y))$. For the proposal, $N(\theta^{(j-1)}, \Sigma)$, Σ is a $d \times d$ variance-covariance matrix, and $d = \dim(\theta) = p + 1$.
- If $\log r \geq 0$ then set $\theta^{(j)} = \theta^*$. If $\log r \leq 0$ then draw $U \sim (0, 1)$. If $U \leq r$ (or $\log U \leq \log r$) then $\theta^{(j)} = \theta^*$. Otherwise, $\theta^{(j)} = \theta^{(j-1)}$.
- Repeat the above procedure for $j = 1, \dots, N$ to obtain samples $\theta^{(1)}, \dots, \theta^{(N)}$.

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Consider again the spatially-varying intercept model for generic location s

$$y(s) = x(s)^\top \beta + w(s) + \epsilon(s), \quad s \in \mathcal{D} \subseteq \mathbb{R}^d,$$

where

$y(s)$ is the outcome,

$x(s)$ is $p \times 1$ set of predictors including an intercept,

β is a vector of p regression parameters,

$w(s)$ is a spatial random effect,

$\epsilon(s)$ is the independent noise process with variance τ^2 .

Computation issues

- Storage: n^2 pairwise distances to compute \mathbf{K}_θ
- \mathbf{K}_θ is dense; Need to solve $\mathbf{K}_\theta \mathbf{x} = \mathbf{b}$ and need $\det(\mathbf{K}_\theta)$
- This is best achieved using $\text{chol}(\mathbf{K}_\theta) = \mathbf{LDL}^\top$
- Complexity: roughly $O(n^3)$ flops

Computationally infeasible for large datasets

Nearest Neighbor Gaussian Processes for Large Spatial Data

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May 15, 2023

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Likelihood from (full rank) GP models

- Assuming $w(s) \sim GP(0, K_\theta(\cdot, \cdot))$ implies that for a set of n locations¹

$$\mathbf{w} = (w(s_1), w(s_2), \dots, w(s_n))^\top \sim MVN(\mathbf{0}, \mathbf{K}_\theta)$$

- Estimating process parameters from the likelihood involves:

$$p(\mathbf{w}) \propto -\frac{1}{2} \log(\det(\mathbf{K}_\theta)) - \frac{1}{2} \mathbf{w}^\top \mathbf{K}_\theta^{-1} \mathbf{w}$$

- Bayesian inference: priors on θ and many Markov chain Monte Carlo (MCMC) iterations

¹ $K_\theta(\cdot, \cdot)$ is any valid spatial covariance function, e.g., $\sigma^2 R(\cdot, \cdot; \phi)$, with $\theta = (\sigma^2, \phi)$.

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Burgeoning literature on spatial big data

- Low-rank models:** (Wahba, 1990; Higdon, 2002; Rasmussen and Williams, 2006; Cressie and Johannesson, 2008; Banerjee et al., 2008, 2010; Gramacy and Lee, 2008; Finley et al., 2009; Lemos and Sansó, 2009; Sang et al., 2011; Sang and Huang, 2012; Guhaniyogi et al., 2011; Katzfuss and Hammerling, 2017)
- Spectral approximations and composite likelihoods:** (Fuentes, 2007; Paciorek, 2007; Eidsvik et al., 2014)
- Multi-resolution approaches:** (Nyckha et al., 2015; Johannesson et al., 2007; Katzfuss, 2017; Guhaniyogi and Sansó, 2020)
- Sparsity:** (Solve $\mathbf{Ax} = \mathbf{b}$ by (i) sparse \mathbf{A} , or (ii) sparse \mathbf{A}^{-1})
 - Covariance tapering (Furrer et al., 2006; Du et al., 2009; Kaufman et al., 2008; Stein, 2013; Shaby and Ruppert, 2012)
 - GMRFs to GPs: INLA (Rue et al., 2009; Lindgren et al., 2011)
 - LAGP Gramacy et al., 2014; Gramacy and Apley, 2015)
 - Nearest-neighbor Gaussian Process (NNGP)** models (Datta et al., 2016a,c,b; Finley et al., 2019a) builds on Vecchia (1988).

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Reduced (Low) rank models

- $\mathbf{K}_\theta \approx \mathbf{J}_\theta \mathbf{K}_\theta^* \mathbf{J}_\theta^\top + \mathbf{D}_\theta$
- \mathbf{J}_θ is $n \times r$ matrix of spatial basis functions, $r \ll n$
- \mathbf{K}_θ^* is $r \times r$ spatial covariance matrix
- \mathbf{D}_θ is either diagonal or sparse
- Examples: Kernel projections, Splines, Predictive process, FRK, spectral basis ...
- Computations exploit above structure: roughly $O(nr^2) \ll O(n^3)$ flops

Reduced (Low) rank models (cont'd)

Low-rank models: hierarchical approach

$$N(\mathbf{w}^* | \mathbf{0}, \mathbf{K}_\theta^*) \times N(\mathbf{w} | \mathbf{J}_\theta \mathbf{w}^*, \mathbf{D})$$

- \mathbf{w} is $n \times 1$ and n is large
- \mathbf{w}^* is $r \times 1$, where $r \ll n$, defined over a user-defined set of locations, or knots, $\mathcal{S}^* = \{\mathbf{s}_1^*, \mathbf{s}_2^*, \dots, \mathbf{s}_r^*\}$.
- \mathbf{J}_θ is $n \times r$ is a matrix of “basis” functions
- \mathbf{D} is $n \times n$, but easy to invert (e.g., diagonal)
- Derive $\text{var}(\mathbf{w})$ (or $\text{var}(\mathbf{w}^* | \mathbf{y})$) in alternate ways to obtain $(\mathbf{J}_\theta \mathbf{K}_\theta^* \mathbf{J}_\theta^\top + \mathbf{D})^{-1} = \mathbf{D}^{-1} - \mathbf{D}^{-1} \mathbf{J}_\theta (\mathbf{K}_\theta^{*-1} + \mathbf{J}_\theta^\top \mathbf{D}^{-1} \mathbf{J}_\theta)^{-1} \mathbf{J}_\theta^\top \mathbf{D}^{-1}$.

This is the famous Sherman-Woodbury-Morrison formula.

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See, e.g., Finley et al. (2017) for implantation details and software for the Gaussian predictive process (GPP) model.

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Simulation experiment

- 2500 locations on a unit square
- $y(\mathbf{s}) = \beta_0 + \beta_1 x(\mathbf{s}) + w(\mathbf{s}) + \epsilon(\mathbf{s})$
- Single covariate $x(\mathbf{s})$ generated as iid $N(0, 1)$
- Spatial effects generated from $GP(0, \sigma^2 R(\cdot, \cdot | \phi))$
- $R(\cdot, \cdot | \phi)$ is exponential correlation function with decay ϕ
- Candidate models: Full GP and Gaussian Predictive Process (GPP) with 64 knots

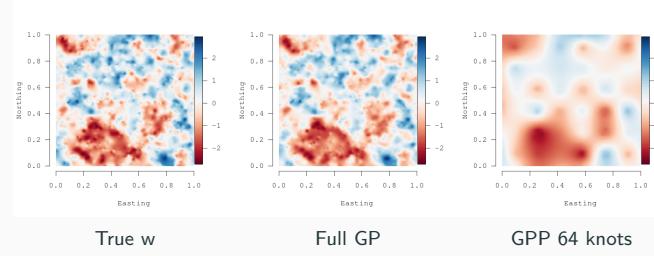


Figure: Comparing full GP vs low-rank GPP with 2500 locations. Figure (c) exhibits oversmoothing by a low-rank process (predictive process with 64 knots)

See Stein (2014) for very good reasons NOT to use reduced-rank spatial models.

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Low rank Gaussian Predictive Process

Pros

- Proper Gaussian process
- Allows for coherent spatial interpolation at arbitrary resolution
- Can be used as prior for spatial random effects in any hierarchical setup for spatial data
- Computationally tractable

Low rank Gaussian Predictive Process

Cons

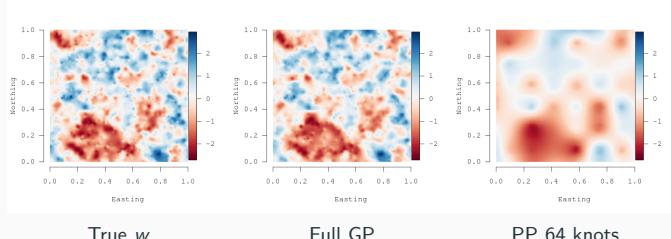


Figure: Comparing full GP vs low-rank GP with 2500 locations

- Low rank models, like the GPP, tend to oversmooth
- Increasing the number of knots can fix this but will lead to heavy computation

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Sparse matrices

Cholesky factors

- Idea: Use a **sparse** matrix instead of a low rank matrix to approximate the dense full GP covariance matrix
- Goals:
 - Scalability: Both in terms of **storage** and computing **inverse** and **determinant**
 - Closely approximate full GP inference
 - Proper Gaussian process model like the GPP

- Write a joint density $p(\mathbf{w}) = p(w_1, w_2, \dots, w_n)$ as:

$$p(w_1)p(w_2 | w_1)p(w_3 | w_1, w_2) \cdots p(w_n | w_1, w_2, \dots, w_{n-1})$$

- For Gaussian distribution $\mathbf{w} \sim N(\mathbf{0}, \mathbf{K}_\theta)$ this \Rightarrow

$$w_1 = 0 + \eta_1;$$

$$w_2 = a_{21}w_1 + \eta_2;$$

$$\dots \quad \dots \quad \dots$$

$$w_n = a_{n1}w_1 + a_{n2}w_2 + \cdots + a_{n,n-1}w_{n-1} + \eta_n;$$

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Cholesky factors

Cholesky factors

- Write a joint density $p(\mathbf{w}) = p(w_1, w_2, \dots, w_n)$ as:

$$p(w_1)p(w_2 | w_1)p(w_3 | w_1, w_2) \cdots p(w_n | w_1, w_2, \dots, w_{n-1})$$

- For Gaussian distribution $\mathbf{w} \sim N(\mathbf{0}, \mathbf{K}_\theta)$ this \Rightarrow

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 \\ a_{21} & 0 & 0 & \dots & 0 & 0 \\ a_{31} & a_{32} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{n,n-1} & 0 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_n \end{bmatrix} + \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \vdots \\ \eta_n \end{bmatrix}$$

$$\Rightarrow \mathbf{w} = \mathbf{Aw} + \boldsymbol{\eta}; \quad \boldsymbol{\eta} \sim N(\mathbf{0}, \mathbf{D}).$$

- Write a joint density $p(\mathbf{w}) = p(w_1, w_2, \dots, w_n)$ as:

$$p(w_1)p(w_2 | w_1)p(w_3 | w_1, w_2) \cdots p(w_n | w_1, w_2, \dots, w_{n-1})$$

- For Gaussian distribution $\mathbf{w} \sim N(\mathbf{0}, \mathbf{K}_\theta)$ this \Rightarrow

$$\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 \\ a_{21} & 0 & 0 & \dots & 0 & 0 \\ a_{31} & a_{32} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{n,n-1} & 0 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_n \end{bmatrix} + \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \vdots \\ \eta_n \end{bmatrix}$$

$$\Rightarrow \mathbf{w} = \mathbf{Aw} + \boldsymbol{\eta}; \quad \boldsymbol{\eta} \sim N(\mathbf{0}, \mathbf{D}).$$

- Cholesky factorization:

$$\mathbf{K}_\theta = (\mathbf{I} - \mathbf{A})^{-1} \mathbf{D} (\mathbf{I} - \mathbf{A})^{-\top}, \text{ where } \mathbf{D} = \text{diag}(\text{var}\{w_i | w_{\{j < i\}}\})$$

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Cholesky factors

Cholesky Factors and Directed Acyclic Graphs (DAGs)

- For Gaussian distribution $N(\mathbf{w} | \mathbf{0}, \mathbf{K}_\theta)$,
$$\mathbf{K}_\theta = (\mathbf{I} - \mathbf{A})^{-1} \mathbf{D} (\mathbf{I} - \mathbf{A})^{-\top}; \quad \mathbf{D} = \text{diag}(\text{var}\{w_i | w_{\{j < i\}}\})$$
- If \mathbf{L} is from $\text{chol}(\mathbf{K}_\theta) = \mathbf{LDL}^\top$, then $\mathbf{L}^{-1} = \mathbf{I} - \mathbf{A}$.
- a_{ij} 's obtained from $n - 1$ linear systems by comparing coefficients of w_j 's in

$$\sum_{j < i} a_{ij} w_j = E[w_i | w_{\{j < i\}}] \quad i = 2, \dots, n$$

- Non-zero elements of \mathbf{A} and \mathbf{D} are computed:

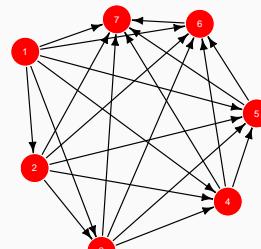
$\mathbf{D}[1,1] = \mathbf{K}[1,1]$ and first row of \mathbf{A} is zero.

```
for(i in 1:(n-1)) {
  A[i+1,1:i] = solve(K[1:i,1:i], K[1:i,i+1])
  D[i+1,i+1] = K[i+1,i+1] - dot(K[i+1,1:i], A[i+1,1:i])
```

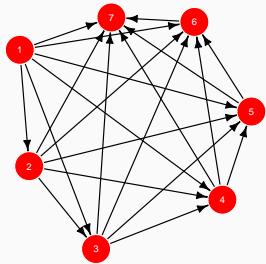
}

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- Number of non-zero entries (**sparsity**) of \mathbf{A} equals number of arrows in the graph
- In particular: Sparsity of the i^{th} row of \mathbf{A} is same as the number of arrows towards i in the DAG

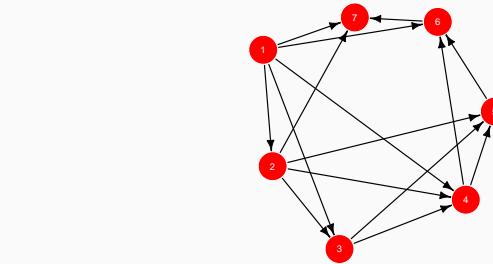


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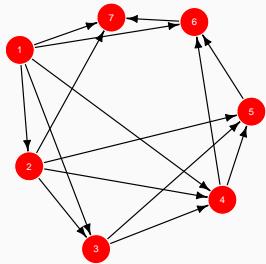
$$\begin{aligned} p(y_1)p(y_2|y_1)p(y_3|y_1,y_2)p(y_4|y_1,y_2,y_3) \\ \times p(y_5|y_1,y_2,y_3,y_4)p(y_6|y_1,y_2,\dots,y_5)p(y_7|y_1,y_2,\dots,y_6). \end{aligned}$$

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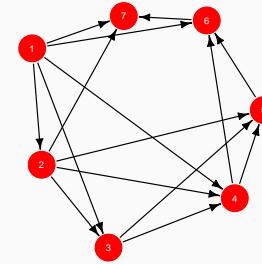
$$\begin{aligned} p(y_1)p(y_2|y_1)p(y_3|y_1,y_2)p(y_4|y_1,y_2,y_3) \\ p(y_5|y_1,y_2,y_3,y_4)p(y_6|y_1,y_2,y_3,y_4,y_5)p(y_7|y_1,y_2,y_3,y_4,y_5,y_6) \end{aligned}$$

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- Create a **sparse** DAG by keeping at most m arrows pointing to each node
- Set $a_{ij} = 0$ for all i,j which has no arrow between them
- Fixing $a_{ij} = 0$ introduces **conditional independence** and w_j drops out from the conditional set in $p(w_i | \{w_k : k < i\})$

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- $N(i)$ denote **neighbor set** of i , i.e., the set of nodes from which there are arrows to i
 - $a_{ij} = 0$ for $j \notin N(i)$ and nonzero a_{ij} 's obtained by solving:
- $$E[w_i | w_{N(i)}] = \sum_{j \in N(i)} a_{ij} w_j$$
- The above linear system is only $m \times m$

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- Non-zero elements of sparse \mathbf{A} and \mathbf{D} are computed:
- ```
D[1,1] = K[1,1] and first row of A is zero.
for(i in 1:(n-1)) {
 Pa = N[i+1] # neighbors of i+1
 A[i+1,Pa] = solve(K[Pa,Pa], K[i+1,Pa])
 D[i+1,i+1] = K[i+1,i+1] - dot(K[i+1,Pa], A[i+1,Pa])
}

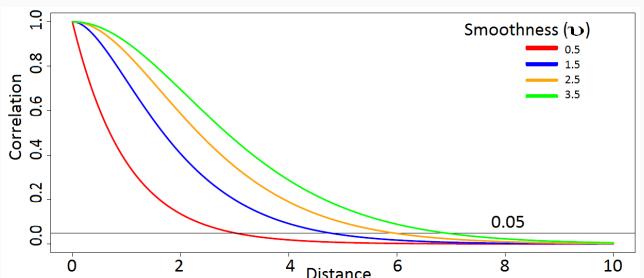
```
- We need to solve  $n - 1$  linear systems of size at most  $m \times m$ .
  - We effectively model a (sparse) Cholesky factor instead of computing it.

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### Choosing neighbor sets

Matern Covariance Function:

$$K(\mathbf{s}_i, \mathbf{s}_j) = \frac{1}{2^{\nu-1}\Gamma(\nu)} (\|\mathbf{s}_i - \mathbf{s}_j\|/\phi)^{\nu} \mathcal{H}_{\nu}(\|\mathbf{s}_i - \mathbf{s}_j\|/\phi); \phi > 0, \nu > 0,$$



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## Choosing neighbor sets

## Nearest neighbors

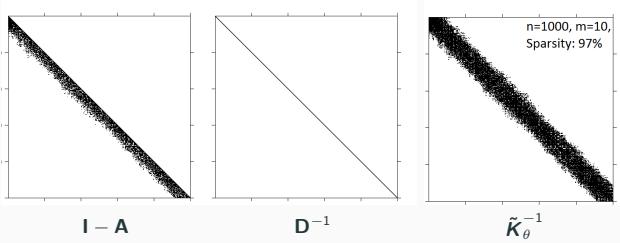
- Spatial covariance functions decay with distance
- Vecchia (1988):  $N(\mathbf{s}_i) = m\text{-nearest neighbors}$  of  $\mathbf{s}_i$  in  $\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_{i-1}$ 
  - Nearest points have highest correlations
  - Theory: "Screening effect" – Stein, 2002
- We use Vecchia's choice of  $m$ -nearest neighbor
- Other choices proposed in Stein et al. (2004); Gramacy and Apley (2015); Guinness (2018) can also be used, with additional discussion in Finley et al. (2019) and Katzfuzz and Guinness (2021)

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## Sparse precision matrices

- The neighbor sets and the covariance function  $K(\cdot, \cdot)$  define a sparse Cholesky factor  $\mathbf{A}$
- $N(\mathbf{w} | \mathbf{0}, \mathbf{K}_\theta) \approx N(\mathbf{w} | \mathbf{0}, \tilde{\mathbf{K}}_\theta)$ ;  $\tilde{\mathbf{K}}_\theta^{-1} = (\mathbf{I} - \mathbf{A})^\top \mathbf{D}^{-1} (\mathbf{I} - \mathbf{A})$



- $\det(\tilde{\mathbf{K}}_\theta) = \prod_{i=1}^n D_i$ ,
- $\tilde{\mathbf{K}}_\theta^{-1}$  is sparse with  $O(nm^2)$  entries

Explore some  $\mathbf{A}$  and  $\tilde{\mathbf{K}}_\theta^{-1}$  sparsity patterns [https://github.com/finleya/NNGP\\_LDL](https://github.com/finleya/NNGP_LDL)

## Extension to a Process

- We have defined  $\mathbf{w} \sim N(\mathbf{0}, \tilde{\mathbf{K}}_\theta)$  over the set of data locations  $S = \{\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_n\}$
- For  $\mathbf{s} \notin S$ , define  $N(\mathbf{s})$  as set of  $m$ -nearest neighbors of  $\mathbf{s}$  in  $S$
- Define  $w(\mathbf{s}) = \sum_{i: \mathbf{s}_i \in N(\mathbf{s})} a_i(\mathbf{s}) w(\mathbf{s}_i) + \eta(\mathbf{s})$  where  $\eta(\mathbf{s}) \stackrel{iid}{\sim} N(0, d(\mathbf{s}))$ 
  - $a_i(\mathbf{s})$  and  $d(\mathbf{s})$  are once again obtained by solving  $m \times m$  system
- Well-defined GP over entire domain
  - Nearest Neighbor GP (NNGP) – Datta et al., JASA, (2016)

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## Hierarchical spatial regression with NNGP

## Hierarchical spatial regression with NNGP

### Spatial linear model

$$y(\mathbf{s}) = \mathbf{x}(\mathbf{s})^\top \boldsymbol{\beta} + w(\mathbf{s}) + \epsilon(\mathbf{s})$$

- $w(\mathbf{s})$  modeled as NNGP derived from a  $GP(0, (\cdot, \cdot, |\sigma^2, \phi))$
- $\epsilon(\mathbf{s}) \stackrel{iid}{\sim} N(0, \tau^2)$  contributes to the nugget
- Priors for the parameters  $\boldsymbol{\beta}$ ,  $\sigma^2$ ,  $\tau^2$  and  $\phi$
- Only difference from a full GP model is the NNGP prior  $w(\mathbf{s})$

### Full Bayesian Model

$$\begin{aligned} N(\mathbf{y} | \mathbf{X}\boldsymbol{\beta} + \mathbf{w}, \tau^2 \mathbf{I}) &\times N(\mathbf{w} | \mathbf{0}, \tilde{\mathbf{K}}_\theta) \times N(\boldsymbol{\beta} | \boldsymbol{\mu}_\beta, \mathbf{V}_\beta) \\ &\times IG(\tau^2 | a_\tau, b_\tau) \times IG(\sigma^2 | a_\sigma, b_\sigma) \times Unif(\phi | a_\phi, b_\phi) \end{aligned}$$

Gibbs sampler:

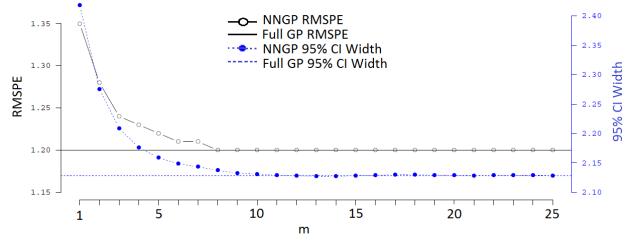
- Full conditionals for  $\boldsymbol{\beta}$ ,  $\tau^2$ ,  $\sigma^2$  and  $w(\mathbf{s}_i)$ 's
- Metropolis step for updating  $\phi$
- Posterior predictive distribution at any location using composition sampling

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## Choosing $m$

## Storage and computation



- Run NNGP in parallel for few values of  $m$
- Choose  $m$  based on model evaluation metrics
- Our results suggested that typically  $m \approx 20$  yielded excellent approximations to the full GP

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### Storage:

- Never needs to store  $n \times n$  distance matrix
- Stores smaller  $m \times m$  matrices
- Total storage requirements  $O(nm^2)$

### Computation:

- Only involves inverting small  $m \times m$  matrices
- Total flop count per iteration of Gibbs sampler is  $O(nm^3)$
- Since  $m \ll n$ , NNGP offers great scalability for large datasets

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## Simulation experiment

## Fitted Surfaces

- 2500 locations on a unit square
- $y(\mathbf{s}) = \beta_0 + \beta_1 x(\mathbf{s}) + w(\mathbf{s}) + \epsilon(\mathbf{s})$
- Single covariate  $x(\mathbf{s})$  generated as iid  $N(0, 1)$
- Spatial effects generated from  $GP(0, \sigma^2 R(\cdot, \cdot | \phi))$
- $R(\cdot, \cdot | \phi)$  is exponential correlation function with decay  $\phi$
- Candidate models: Full GP, Gaussian Predictive Process (GPP) with 64 knots and NNGP

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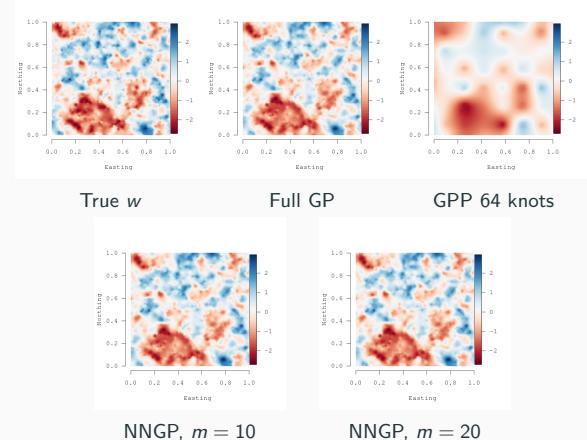


Figure: Univariate synthetic data analysis

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## Parameter estimates

## Model evaluation

| True       | NNGP     |                     | Predictive Process  | Full              |
|------------|----------|---------------------|---------------------|-------------------|
|            | $m = 10$ | $m = 20$            | 64 knots            | Gaussian Process  |
| $\beta_0$  | 1        | 1.00 (0.62, 1.31)   | 1.03 (0.65, 1.34)   | 1.30 (0.54, 2.03) |
| $\beta_1$  | 5        | 5.01 (4.99, 5.03)   | 5.01 (4.99, 5.03)   | 5.03 (4.99, 5.06) |
| $\sigma^2$ | 1        | 0.96 (0.78, 1.23)   | 0.94 (0.77, 1.20)   | 1.29 (0.96, 2.00) |
| $\tau^2$   | 0.1      | 0.10 (0.08, 0.13)   | 0.10 (0.08, 0.13)   | 0.08 (0.04, 0.13) |
| $\phi$     | 12       | 12.93 (9.70, 16.77) | 13.36 (9.99, 17.15) | 5.61 (3.48, 8.09) |

|                    | NNGP         |          | Predictive Process | Full             |
|--------------------|--------------|----------|--------------------|------------------|
|                    | $m = 10$     | $m = 20$ | 64 knots           | Gaussian Process |
| DIC score          | 2390         | 2377     | <b>13678</b>       | 2364             |
| RMSPE              | 1.2          | 1.2      | <b>1.68</b>        | 1.2              |
| Run time (Minutes) | <b>14.40</b> | 46.47    | 43.36              | <b>560.31</b>    |

- NNGP performs at par with Full GP
- GPP oversmooths and performs much worse both in terms of parameter estimation and model comparison
- NNGP yields huge computational gains

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## Multivariate spatial linear model

## Multivariate GPs

- Spatial linear model for  $q$ -variate spatial data:  
 $y_i(s) = \mathbf{x}_i^\top(s)\beta_i + w_i(s) + \epsilon_i(s)$  for  $i = 1, 2, \dots, q$
- $\epsilon(s) = (\epsilon_1(s), \epsilon_2(s), \dots, \epsilon_q(s))^\top \sim N(0, E)$  where  $E$  is the  $q \times q$  noise matrix
- $w(s) = (w_1(s), w_2(s), \dots, w_q(s))^\top$  is modeled as a  $q$ -variate Gaussian process

- $\text{Cov}(w(s_i), w(s_j)) = K(s_i, s_j | \theta)$  – a  $q \times q$  cross-covariance matrix
- Choices for the function  $K(\cdot, \cdot | \theta)$ 
  - Multivariate Matérn
  - Linear model of co-regionalization
- For data observed at  $n$  locations, all choices lead to a dense  $nq \times nq$  matrix  $\mathbf{K}_\theta = \text{Cov}(w(s_1), w(s_2), \dots, w(s_n))$
- Not scalable when  $nq$  is large

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## Multivariate NNGPs

## U.S. Forest biomass data

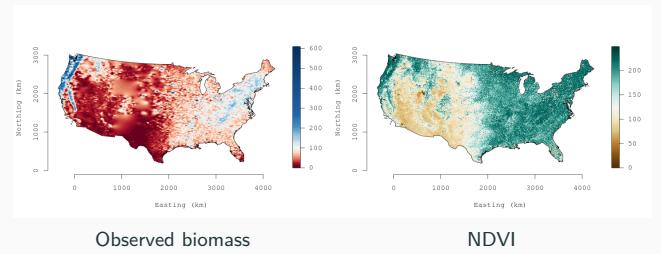
- Cholesky factor approach similar to the univariate case

$$\begin{bmatrix} \mathbf{w}(s_1) \\ \mathbf{w}(s_2) \\ \mathbf{w}(s_3) \\ \vdots \\ \mathbf{w}(s_n) \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 \\ \mathbf{A}_{21} & 0 & 0 & \dots & 0 & 0 \\ \mathbf{A}_{31} & \mathbf{A}_{32} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{A}_{n1} & \mathbf{A}_{n2} & \mathbf{A}_{n3} & \dots & \mathbf{A}_{n,n-1} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{w}(s_1) \\ \mathbf{w}(s_2) \\ \mathbf{w}(s_3) \\ \vdots \\ \mathbf{w}(s_n) \end{bmatrix} + \begin{bmatrix} \eta(s_1) \\ \eta(s_2) \\ \eta(s_3) \\ \vdots \\ \eta(s_n) \end{bmatrix}$$

$\implies \mathbf{w} = \mathbf{Aw} + \eta; \quad \eta \sim N(\mathbf{0}, \mathbf{D}), \quad \mathbf{D} = \text{diag}(\mathbf{D}_1, \mathbf{D}_2, \dots, \mathbf{D}_n).$

Only differences:

- $\mathbf{w}(s_i)$  and  $\eta(s_i)$ 's are  $q \times 1$  vectors and  $\mathbf{A}_{ij}$  and  $\mathbf{D}_i$ 's are  $q \times q$  matrix
- we must solve  $n - 1$  at most  $mq \times mq$  linear systems (challenging when  $q$  gets large, e.g.,  $q > 5$ ).



- Forest biomass data from measurements at 114,371 plots
- NDVI (greenness) is used to predict forest biomass

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## U.S. Forest biomass data

## Forest biomass dataset

### Non Spatial Model

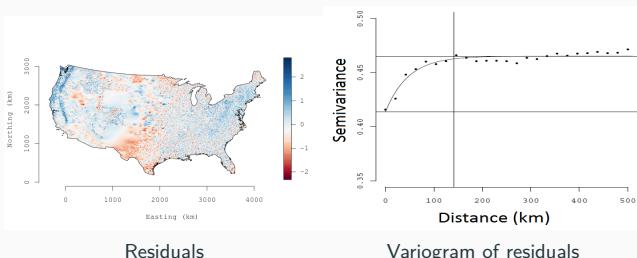
$$\text{Biomass} = \beta_0 + \beta_1 \text{NDVI} + \text{error}, \quad \hat{\beta}_0 = 1.043, \quad \hat{\beta}_1 = 0.0093$$

- $n \approx 10^5$  (Forest Biomass)  $\Rightarrow$  full GP requires storage  $\approx 40 \text{Gb}$  and time  $\approx 140 \text{ hrs}$  per iteration.

- We use a spatially varying coefficients NNGP model

### Model

- $\text{Biomass}(s) = \beta_0(s) + \beta_1(s) \text{NDVI}(s) + \epsilon(s)$
- $\mathbf{w}(s) = (\beta_0(s), \beta_1(s))^\top \sim \text{Bivariate NNGP}(0, \tilde{K}(\cdot, \cdot | \theta)), \quad m = 5$
- Time  $\approx 6 \text{ seconds}$  per iteration
- Full inferential output: 41 hours (25000 MCMC iterations)



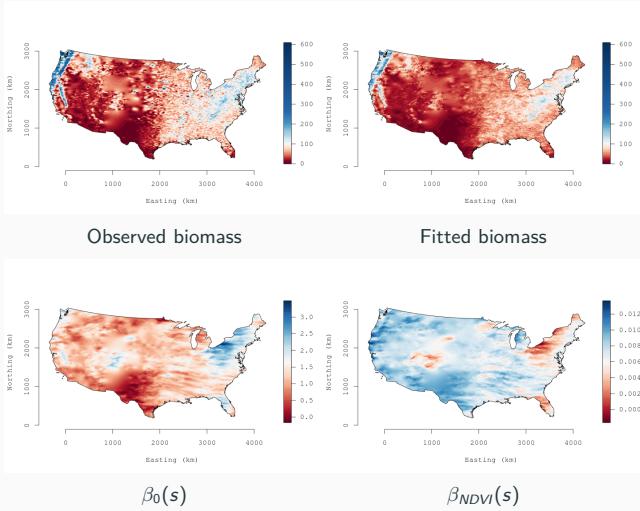
Strong spatial pattern among residuals

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## Forest biomass data

## Reducing parameter dimensionality



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- The Gibbs sampler algorithm for the NNGP updates  $w(\mathbf{s}_1), w(\mathbf{s}_2), \dots, w(\mathbf{s}_n)$  sequentially
- Dimension of the MCMC for this sequential algorithm is  $O(n)$
- If the number of data locations  $n$  is very large, this high-dimensional MCMC can converge slowly
- Although each iteration for the NNGP model will be very fast, many more MCMC iterations may be required

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## Collapsed NNGP

## Collapsed NNGP

- Same model:

$$y(\mathbf{s}) = \mathbf{x}(\mathbf{s})^\top \boldsymbol{\beta} + w(\mathbf{s}) + \epsilon(\mathbf{s})$$

$$w(\mathbf{s}) \sim NNGP(0, K(\cdot, \cdot | \theta))$$

$$\epsilon(\mathbf{s}) \stackrel{iid}{\sim} N(0, \tau^2)$$

- Latent model:  $\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta} + \mathbf{w}, \tau^2 \mathbf{I})$ ;  $\mathbf{w} \sim N(\mathbf{0}, \tilde{\mathbf{K}}_\theta)$
- Collapsed model: Marginalizing out  $\mathbf{w}$ ,  $\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta}, \tau^2 \mathbf{I} + \tilde{\mathbf{K}}_\theta)$

$$\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta}, \tau^2 \mathbf{I} + \tilde{\mathbf{K}}_\theta)$$

- Only involves few parameters  $\boldsymbol{\beta}$ ,  $\tau^2$  and  $\theta = (\sigma^2, \phi)$
- Drastically reduces the MCMC dimensionality
- Gibbs sampler updates are based on sparse linear systems using  $\tilde{\mathbf{K}}_\theta^{-1}$  (e.g., use CHOLMOD)
- Improved MCMC convergence
- Can recover posterior distribution of  $\mathbf{w} | \mathbf{y}$
- Complexity of the algorithm depends on the design of the data locations and is not guaranteed to be  $O(n)$

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## Response NNGP

## Conjugate NNGP

- $w(\mathbf{s}) \sim GP(0, K(\cdot, \cdot | \theta)) \Rightarrow y(\mathbf{s}) \sim GP(\mathbf{x}(\mathbf{s})^\top \boldsymbol{\beta}, \Sigma(\cdot, \cdot | \tau^2, \theta))$
- $\Sigma(\mathbf{s}_i, \mathbf{s}_j) = K(\mathbf{s}_i, \mathbf{s}_j | \theta) + \tau^2 \delta(\mathbf{s}_i = \mathbf{s}_j)$  ( $\delta$  is Kronecker delta)
- We can directly derive the NNGP covariance function corresponding to  $\Sigma(\cdot, \cdot)$
- $\tilde{\Sigma}$  is the NNGP covariance matrix for the  $n$  locations
- Response model:  $\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta}, \tilde{\Sigma})$
- Storage and computations are guaranteed to be  $O(n)$
- Low dimensional MCMC  $\Rightarrow$  Improved convergence
- Cannot coherently recover  $\mathbf{w} | \mathbf{y}$

- Full GP model:  $\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta}, \Sigma)$  where  $\Sigma = \sigma^2 \mathbf{M}$

- $\mathbf{M} = \mathbf{R}(\phi) + \alpha \mathbf{I}$

- $\alpha = \tau^2 / \sigma^2$  is the ratio of the noise to signal variance

- $\tilde{\Sigma} = \sigma^2 \tilde{\mathbf{M}}$  where  $\tilde{\mathbf{M}}$  is the NNGP approximation for  $\mathbf{M}$

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- Full GP model:  $\mathbf{y} \sim N(\mathbf{X}\beta, \Sigma)$  where  $\Sigma = \sigma^2\mathbf{M}$
- $\mathbf{M} = \mathbf{R}(\phi) + \alpha\mathbf{I}$
- $\alpha = \tau^2/\sigma^2$  is the ratio of the noise to signal variance
- $\tilde{\Sigma} = \sigma^2\tilde{\mathbf{M}}$  where  $\tilde{\mathbf{M}}$  is the NNGP approximation for  $\mathbf{M}$
- If  $\phi$  and  $\alpha$  are known,  $\mathbf{M}$ , and hence  $\tilde{\mathbf{M}}$ , are known matrices
- The model becomes a standard Bayesian linear model
- Assume a *Normal Inverse Gamma* prior for  $(\beta, \sigma^2)^\top$
- $(\beta, \sigma^2)^\top \sim NIG(\mu_\beta, \mathbf{V}_\beta, a_\sigma, b_\sigma)$ , i.e.,  $\beta | \sigma^2 \sim N(\mu_\beta, \sigma^2\mathbf{V}_\beta)$  and  $\sigma^2 \sim IG(a_\sigma, b_\sigma)$
- Exact posterior distributions of  $\beta$  and  $\sigma^2$  are available

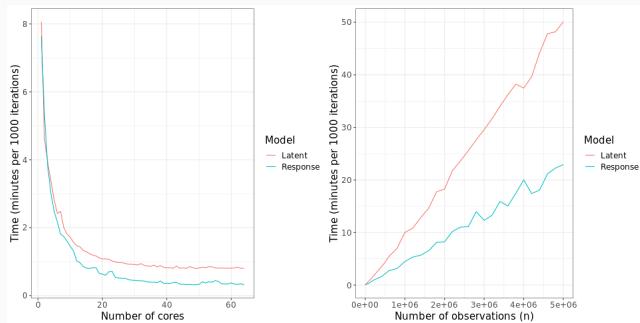
Can handle  $n$  in the 100s of millions!

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## Comparison of NNGP models

## Summary of Nearest Neighbor Gaussian Processes



**Figure:** (a) Runtime for 1000 MCMC iterations for  $n = 100000$  and different number of cores. (b) Runtime for 1000 MCMC iterations using 40 cores and  $n$  from 1000 to 5 million. Model type (latent and response) refers to different NNGP parameterizations, see Finley et al. 2022.

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- **Sparsity** inducing Gaussian process
- Constructed from sparse Cholesky factors based on  $m$  nearest neighbors
- **Scalability** in storage, inverse, and determinant of NNGP covariance matrix are all  $O(n)$
- **Proper Gaussian process**, allows for inference using hierarchical spatial models and predictions at arbitrary spatial resolution
- Closely approximates full GP inference, does not oversmooth like low rank models
- Extension to **multivariate NNGP**
- Collapsed and response NNGP models with improved MCMC convergence
- R packages `spNNGP` (Finley et al. 2022) and `spOccupancy` (Doser et al., 2022) on CRAN

## Some notes on efficient computing and high performance computing environments

## Code implementation

Andrew Finley<sup>1</sup> & Jeffrey Doser<sup>2</sup>

May 15, 2023

<sup>1</sup>Department of Forestry, Michigan State University.

<sup>2</sup>Department of Integrative Biology, Michigan State University.

Very useful libraries for efficient matrix computation:

1. Fortran BLAS (Basic Linear Algebra Subprograms, see Blackford et al. 2001). Started in late 70s at NASA JPL by Charles L. Lawson. See <http://www.netlib.orgblas>.
2. Fortran LAPACK (Linear Algebra Package, see Anderson et al. 1999). Started in mid 80s at Argonne and Oak Ridge National Laboratories. See <http://www.netlib.orglapack>.

Modern math software has a heavy reliance on these libraries, e.g., Matlab and *R*. Routines are also accessible via C, C++, Python, etc.

Many improvements on the standard BLAS and LAPACK functions, see, e.g.,

- Intel Math Kernel Library (MKL)
- AMD Core Math Library (ACML)
- Automatically Tuned Linear Algebra Software (ATLAS)
- Matrix Algebra on GPU and Multicore Architecture (MAGMA)
- OpenBLAS <http://www.openblas.net>
- vecLib (for Mac users only)

1

2

Key BLAS and LAPACK functions used in our setting.

| Function | Description                                                                                                                                                                  |
|----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| dpotrf   | LAPACK routine to compute the Cholesky factorization of a real symmetric positive definite matrix.                                                                           |
| dtrsv    | Level 2 BLAS routine to solve the systems of equations $\mathbf{Ax} = \mathbf{b}$ , where $\mathbf{x}$ and $\mathbf{b}$ are vectors and $\mathbf{A}$ is a triangular matrix. |
| dtrsm    | Level 3 BLAS routine to solve the matrix equations $\mathbf{AX} = \mathbf{B}$ , where $\mathbf{X}$ and $\mathbf{B}$ are matrices and $\mathbf{A}$ is a triangular matrix.    |
| dgemv    | Level 2 BLAS matrix-vector multiplication.                                                                                                                                   |
| dgemm    | Level 3 BLAS matrix-matrix multiplication.                                                                                                                                   |

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Consider different environments:

1. A **distributed system** consists of multiple autonomous computers (nodes) that communicate through a network. A computer program that runs in a distributed system is called a distributed program. Message Passing Interface (MPI) is a specification for an Application Programming Interface (API) that allows many computers to communicate.

## Computing environments

Consider different environments:

1. A **distributed system** consists of multiple autonomous computers (nodes) that communicate through a network. A computer program that runs in a distributed system is called a distributed program. Message Passing Interface (MPI) is a specification for an Application Programming Interface (API) that allows many computers to communicate.
2. A **shared memory multiprocessing system** consists of a single computer with memory that may be simultaneously accessed by one or more programs running on multiple Central Processing Units (CPUs). OpenMP (Open Multi-Processing) is an API that supports shared memory multiprocessing programming.
3. A **heterogeneous system** uses more than one kind of processor, e.g., CPU & (Graphics Processing Unit) GPU or CPU & Intel's Xeon Phi Many Integrated Core (MIC).

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Which environments are right for large  $n$  settings?

- MCMC necessitates iterative evaluation of the likelihood which requires operations on large matrices.
- A specific hurdle is **factorization** to computing determinant and inverse of large dense covariance matrices.
- We try to model our way out and use computing tools to overcome the complexity (e.g., covariance tapering, Kaufman et al. 2008; low-rank methods, Cressie and Johannesson 2008; Banerjee et al. 2008, etc.).
- Due to **slow network communication** and transport of submatrices among nodes distributed systems are not ideal for these types of iterative large matrix operations.

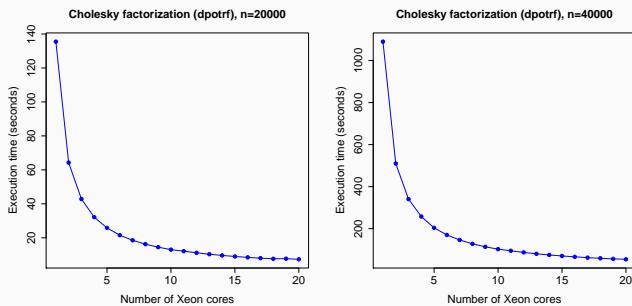
5

- My lab currently favors **shared memory multiprocessing** and **heterogeneous** systems.
- Newest unit is a Dell Poweredge with 384 GB of RAM, 2 threaded 10-core Xeon CPUs, and 2 Intel Xeon Phi Coprocessor with 61-cores (244 threads) running a Linux operating systems.
- Software includes OpenMP coupled with Intel MKL. MKL is a library of highly optimized, extensively threaded math routines designed for Xeon CPUs and Phi coprocessors (e.g., BLAS, LAPACK, ScaLAPACK, Sparse Solvers, Fast Fourier Transforms, and vector RNGs).



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So what kind of speed up to expect from threaded BLAS and LAPACK libraries.



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## R and threaded BLAS and LAPACK

The BLAS and LAPACK that “ships” with R is single-threaded, but these can be replaced with multi-threaded libraries.

### Windows

- Microsoft R Open: The Enhanced R Distribution  
<https://mran.microsoft.com/open> comes with MKL  
<https://software.intel.com/en-us/mkl>.
- Replace existing R's `libRblas.so` with OpenBLAS library `libopenblas.so`. OpenBLAS is available here  
<http://www.openblas.net>.

### Max OS X

- Mac vecLib obtained via XCode. Use install notes [here](#).

### Linux/Unix

- MKL, OpenBLAS, ACML (compile R against MKL or post compile symbolic link of `libRblas.so` to `libopenblas.so`).
- Some additional gains using Intel icc and ifort compilers.

## Modeling non-Gaussian spatial data

Jeffrey Doser<sup>1</sup> & Andrew Finley<sup>2</sup>

May 15, 2023

<sup>1</sup>Department of Integrative Biology, Michigan State University.

<sup>2</sup>Department of Forestry, Michigan State University.

- Often data sets preclude Gaussian modeling:  $y(\mathbf{s})$  may not even be continuous
- Examples:
  - Binary: presence or absence of a species at location  $\mathbf{s}$ .
  - Count: abundance of a species at location  $\mathbf{s}$ .
  - Categorical: counts of trees by size class at location  $\mathbf{s}$ .
- Replace Gaussian likelihood by exponential family member (Diggle, Tawn, and Moyeed (1998)).

## Non-Gaussian spatial data

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- **First stage:**  $y(\mathbf{s}_i)$  are conditionally independent given  $\beta$  and  $w(\mathbf{s}_i)$ . Here we use a canonical link function, say  $g(E[y(\mathbf{s}_i)]) = \eta(\mathbf{s}_i) = \mathbf{x}(\mathbf{s}_i)^\top \beta + w(\mathbf{s}_i)$ .

- **First stage:**  $y(\mathbf{s}_i)$  are conditionally independent given  $\beta$  and  $w(\mathbf{s}_i)$ . Here we use a canonical link function, say  $g(E[y(\mathbf{s}_i)]) = \eta(\mathbf{s}_i) = \mathbf{x}(\mathbf{s}_i)^\top \beta + w(\mathbf{s}_i)$ .
- **Second stage:** Model  $w(\mathbf{s}_i)$  as a Gaussian process:

$$\mathbf{w} \sim N(\mathbf{0}, \sigma^2 \mathbf{R}(\phi))$$

- **First stage:**  $y(\mathbf{s}_i)$  are conditionally independent given  $\beta$  and  $w(\mathbf{s}_i)$ . Here we use a canonical link function, say  $g(E[y(\mathbf{s}_i)]) = \eta(\mathbf{s}_i) = \mathbf{x}(\mathbf{s}_i)^\top \beta + w(\mathbf{s}_i)$ .

- **Second stage:** Model  $w(\mathbf{s}_i)$  as a Gaussian process:

$$\mathbf{w} \sim N(\mathbf{0}, \sigma^2 \mathbf{R}(\phi))$$

- Additional GLMM flexibility comes at a computational cost: lose conjugacy of  $\beta, \mathbf{w}$
- Requires more Metropolis steps. Particularly costly for  $\mathbf{w}$
- Practical consequence: slower, less efficient algorithms
- Prediction and interpolation proceed as with the Gaussian case

- **Third stage:** Priors and hyperpriors.

- Suppose  $y(\mathbf{s}_i) \sim \text{Binomial}(N(\mathbf{s}_i), \psi(\mathbf{s}_i))$ , where  $N(\mathbf{s}_i)$  is the number of trials and  $\psi(\mathbf{s}_i)$  is the probability of success.

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- Both yield closed form full conditional distributions for all parameters except  $\phi$ .

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- Define  $\kappa(\mathbf{s}_i) = y(\mathbf{s}_i) - N(\mathbf{s}_i)/2$
- Resulting Gibbs sampler is remarkably similar to that of a Gaussian model with response  $y(\mathbf{s}_i)^* = \kappa(\mathbf{s}_i)/\omega(\mathbf{s}_i)$  and heteroskedastic variances  $\tau^2(\mathbf{s}_i) = 1/\omega(\mathbf{s}_i)$ .

## Pólya-Gamma data augmentation

- Suppose  $y(\mathbf{s}_i) \sim Bernoulli(\psi(\mathbf{s}_i))$ .

$$\begin{aligned} \psi(\mathbf{s}_i)^{y(\mathbf{s}_i)}(1 - \psi(\mathbf{s}_i))^{1-y(\mathbf{s}_i)} &= \frac{\exp(\mathbf{x}(\mathbf{s}_i)^\top \beta + \mathbf{w}(\mathbf{s}_i))^{y(\mathbf{s}_i)}}{1 + \exp(\mathbf{x}(\mathbf{s}_i)^\top \beta + \mathbf{w}(\mathbf{s}_i))} \\ &= \exp(\kappa(\mathbf{s}_i)(\mathbf{x}(\mathbf{s}_i)^\top \beta + \mathbf{w}(\mathbf{s}_i))) \times \\ &\quad \int \exp\left(-\frac{\omega(\mathbf{s}_i)}{2}(\mathbf{x}(\mathbf{s}_i)^\top \beta + \mathbf{w}(\mathbf{s}_i))^2\right) \\ &\quad p(\omega(\mathbf{s}_i) | 1, 0) d\omega(\mathbf{s}_i), \end{aligned}$$

- $p(\omega(\mathbf{s}_i) | 1, 0)$  is the Pólya-Gamma PDF with parameters 1 and 0
- With Gaussian priors on  $\beta$  and IG prior on  $\sigma^2$ , full conditionals for  $\beta$ ,  $\sigma^2$ , and  $w$  are available in closed form.  $\phi$  updated with MH.
- See Polson, Scott, Windle (2013) JASA

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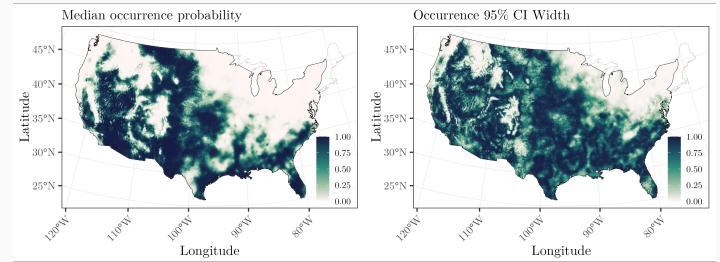
## Example: species distribution modeling

- Objective: predict the distribution of Loggerhead Shrike across the US

$$\begin{aligned} y(\mathbf{s}_i) &\sim Bernoulli(\psi(\mathbf{s}_i)) \\ \text{logit}(\psi(\mathbf{s}_i)) &= \mathbf{x}(\mathbf{s}_i)^\top \beta + \mathbf{w}(\mathbf{s}_i) \\ \mathbf{w} &\sim N(\mathbf{0}, \sigma^2 \mathbf{R}(\phi)) \\ \beta &\sim N(\mu_\beta, \Sigma_\beta) \\ \sigma^2 &\sim IG(a_\sigma, b_\sigma) \\ \phi &\sim Uniform(l, u) \\ \omega(\mathbf{s}_i) &\sim PG(1, 0) \end{aligned}$$

## Example: species distribution modeling

- Posterior predictive inference proceeds as with the Gaussian case



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## Some practical considerations

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- Priors for  $\sigma^2$  and  $\phi$  may need to be more informative, particularly for binary data.
- Be careful with non-identity link functions when thinking about priors.
- Pólya-Gamma data augmentation also applicable for Negative Binomial count data, but slow for large counts and can be unstable.

## Software

- **spBayes**
  - Univariate and multivariate, full GPs or predictive processes
  - Gaussian, Binomial (no Pólya-Gamma data augmentation), Poisson
- **spNNGP**
  - Univariate, NNGPs
  - Gaussian, Binomial
- **spOccupancy**
  - Univariate and multivariate, focus on modeling wildlife distributions, full GPs or NNGPs
  - Bernoulli
- **spAbundance**  
(<https://github.com/doserjef/spAbundance>)
  - Univariate and multivariate, focus on modeling wildlife/plant abundance, NNGPs
  - Gaussian, Poisson, Negative Binomial

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## Spatial Factor Models for Multivariate Spatial Data

Jeffrey Doser<sup>1</sup> & Andrew Finley<sup>2</sup>

May 15, 2023

<sup>1</sup>Department of Integrative Biology, Michigan State University.

<sup>2</sup>Department of Forestry, Michigan State University.

## Multivariate spatial data

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## Multivariate spatial generalized linear model

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  - Atmospheric modeling:** at a given site we observe surface temperature, precipitation and wind speed
- We anticipate dependence between measurements
  - at a particular location
  - across locations

- Spatial generalized linear model for  $h$ -variate spatial data for  $j = 1, 2, \dots, h$  and  $i = 1, \dots, n$ :

$$y_j(\mathbf{s}_i) \sim f(\mu_j(\mathbf{s}_i), \tau_j)$$

$$\mu_j(\mathbf{s}_i) = g^{-1}(\eta_j(\mathbf{s}_i)) = \mathbf{x}(\mathbf{s}_i)^\top \boldsymbol{\beta}_j + \mathbf{w}_j^*(\mathbf{s}_i)$$

- We can imagine modeling  
 $\mathbf{w}^*(\mathbf{s}_i) = (w_1^*(\mathbf{s}_i), w_2^*(\mathbf{s}_i), \dots, w_h^*(\mathbf{s}_i))'$  as an  $h$ -variate Gaussian process

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- Could model using Multivariate NNGP as discussed previously with SVCs, works well when  $h < 5$ .
- But what about when  $h$  is large (e.g., 10, 100)?

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## Spatial Factor Model

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- We represent the  $h \times 1$  vector  $\mathbf{w}^*(\mathbf{s}_i)$  as a linear combination of latent spatial factors and factor loadings:

$$\mathbf{w}^*(\mathbf{s}_i) = \boldsymbol{\Lambda} \mathbf{w}(\mathbf{s}_i)$$

- $\boldsymbol{\Lambda}$  is an  $h \times q$  loadings matrix and  $\mathbf{w}(\mathbf{s}_i)$  is a  $q \times 1$  vector of realizations from  $q$  independent spatial GPs

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- $\boldsymbol{\Lambda}$  is an  $h \times q$  loadings matrix and  $\mathbf{w}(\mathbf{s}_i)$  is a  $q \times 1$  vector of realizations from  $q$  independent spatial GPs
- In traditional factor analysis,  $\mathbf{w}(\mathbf{s}_i)$  are realizations from independent standard normal random variables.

- Choosing  $q \ll h$  leads to substantial computational reductions.
- Simple to code: just sample from  $q$  independent GPs as with basic univariate models.
- Yields a non-separable multivariate cross-covariance function between location  $\mathbf{s}_i$  and  $\mathbf{s}_{i'}$ :  

$$\text{cov}(\mathbf{w}^*(\mathbf{s}_i), \mathbf{w}^*(\mathbf{s}_{i'})) = \sum_{k=1}^q \rho_k(\mathbf{s}_i, \mathbf{s}_{i'}, \phi_k) \boldsymbol{\lambda}_k \boldsymbol{\lambda}_k^\top$$
- Can simply replace the  $q$  full GPs with their corresponding NNGPs to yield a spatial factor NNGP model
- Identifiability constraints on  $\boldsymbol{\Lambda}$ : fix upper triangle to 0 and diagonal to 1. See Ren and Banerjee (2013) *Biometrics*

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## Priors

## Gibbs sampler

- Standard normal priors for the lower triangle of  $\boldsymbol{\Lambda}$
  - We like to model response-specific regression coefficients  $\beta_j$  hierarchically. For each  $r = 1, \dots, p$  covariate, we model  $\beta_{j,r}$  following
- $$\beta_{j,r} \sim N(\mu_{\beta_r}, \tau_{\beta_r}^2)$$
- Gaussian hyperpriors for  $\mu_{\beta_r}$  and IG or half-Cauchy priors for  $\tau_{\beta_r}^2$
  - Independent uniform priors for spatial decay parameters  $\phi$

- Full conditionals are in closed form for all parameters except  $\phi$  for Gaussian and Binomial responses.
- Update  $\phi$  with an Adaptive Metropolis-within-Gibbs algorithm (Roberts and Rosenthal 2009)
- See Taylor-Rodriguez et al. 2019 for Gaussian sampler, spOccupancy website for Pólya-Gamma sampler

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## Why we like spatial factor models

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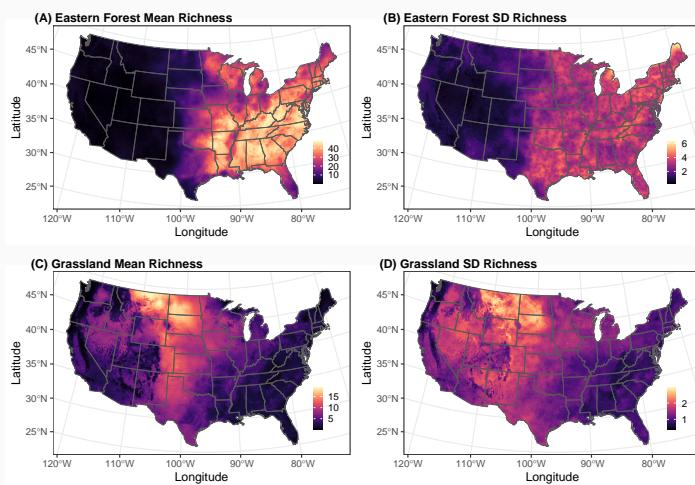
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- Relatively fast and efficient (well, at least for Gaussian and Binomial).
- Factors and factor loadings can be used for model-based ordination.
- Straightforward extensions to spatially-varying coefficient models.

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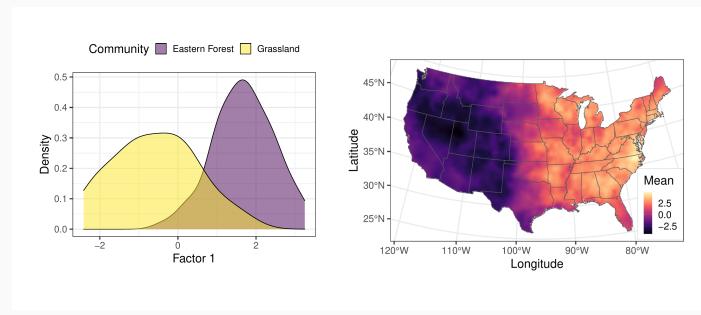
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## Example: bird communities across the continental US



## Example: bird communities across the continental US

Visualization of the first spatial factor and corresponding factor loadings



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## Some downsides to spatial factor models

## Software

- Convergence assessment is not always straightforward
- Sensitivity to initial values
- Order of the first  $q$  responses has important implications for convergence and mixing.
- Assume a multivariate stochastic process can be represented as a linear combination of independent univariate processes

- `spOccupancy`: spatial NNGP and non-spatial factor models for binary data
- `spAbundance`: Gaussian, Poisson, and NB spatial NNGP and non-spatial factor models.
- `boral`: many distributions for non-spatial and spatial factor models (Hui 2015 *MEE*; spatial use full GPs fit in JAGS)
- `Hmsc`: spatial models using NNGPs (Tikhonov et al. 2019; *MEE*)
- `spBFA`: a variety of spatial models with some nifty priors (Berchuck et al. 2022 *Bayesian Analysis*)

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## Exercise

Modeling the distribution of 10 tree species across Vermont

## Application of Spatially-Varying Coefficient Models

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May 15, 2023

<sup>1</sup>Department of Integrative Biology, Michigan State University.

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## Spatially-Varying Coefficient Models

## SVC GLMMs

- Extension of spatial regression approaches that allow regression coefficients to vary across space, and not just the intercept
- SVC models are random slopes models, with spatial structure given to the random slopes

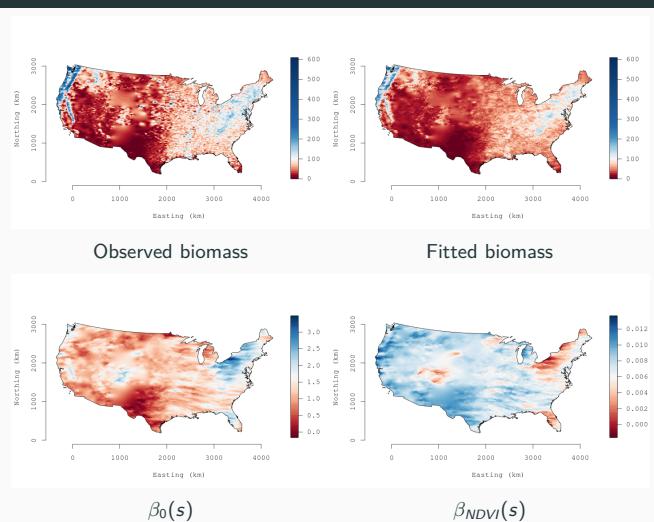
$$\begin{aligned}y(\mathbf{s}_i) &\sim f(\mu(\mathbf{s}_i), \tau) \\ \mu(\mathbf{s}_i) &= g^{-1}(\eta(\mathbf{s}_i)) = \mathbf{x}(\mathbf{s}_i)^\top \tilde{\beta}(\mathbf{s}_i) \\ \tilde{\beta}_r(\mathbf{s}_i) &= \beta_r + w_r(\mathbf{s}_i) \text{ for each } r = 1, \dots, p\end{aligned}$$

- We can model  $w(\mathbf{s}_i)$  using a GP, predictive process, or **NNGP**
- We can envision modeling  $w(\mathbf{s}_i)$  in two ways:
  1. Multivariate NNGP (see previous forest biomass example)
  2. **Independent NNGPs**
- Here we focus on the latter
- Pros and cons to both approaches, similar to correlations between random slopes and intercepts in mixed models

## Potential benefits of SVC models

- Improved predictive performance
- Tremendous flexibility to accommodate spatial variability in effects
- Hypothesis testing and generation
- Accommodate highly non-linear relationships
- Model spatial variability in trends over time

## Improved predictive performance

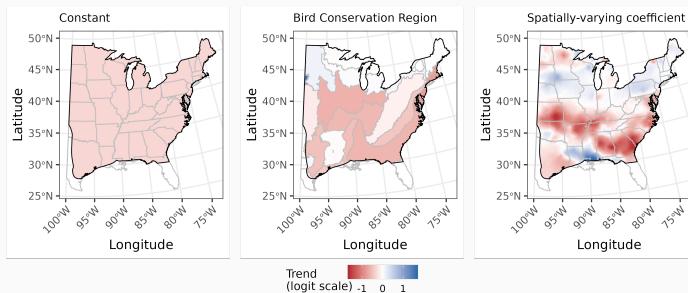


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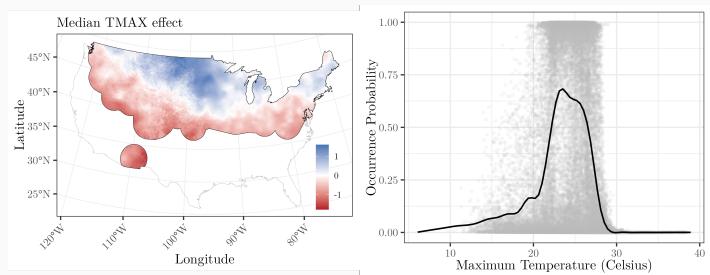
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## More flexibility to accommodate spatial variability in effects

Gray Catbird occurrence trend across the eastern US from 2000-2019



## Example: Effect of max temperature on Bobolink occurrence



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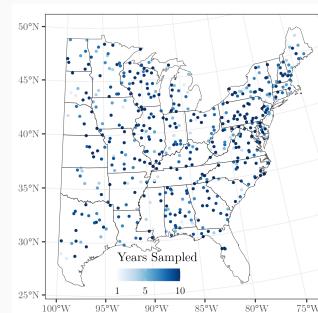
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## Software

- `spBayes`: univariate Gaussian SVC with full GPs
- `spOccupancy`: univariate Binomial SVC with NNGPs (multivariate on its way)
- `varycoef`: maximum likelihood Gaussian SVCs (Dambon et al. 2021 *Spatial Stats.*)
- `sdmTMB`: penalized likelihood and Bayesian SVC GLMMs (Anderson et al. 2022 *bioRxiv*)

## Exercise: 10-year occurrence trend of Wood Thrush

- Data come from USGS North American Breeding Bird Survey
- We desire to account for observational biases in detection of the birds (i.e., false negatives).
- Add on an additional observational layer to our hierarchical model



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## Exercise: Process model

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- Let  $z_t(\mathbf{s}_i)$  denote the true presence (1) or absence (0) of the species at site  $i = 1, \dots, 500$  during year  $t = 1, \dots, 10$ .
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- If the bird was detected at a site and year, we know  $z_t(\mathbf{s}_i) = 1$ . If not, it might be there and we just missed it during the surveys.

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## Exercise: Process model

## Exercise: Observation model

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- If the bird was detected at a site and year, we know  $z_t(\mathbf{s}_i) = 1$ . If not, it might be there and we just missed it during the surveys.
- We model  $z_t(\mathbf{s}_i)$  just as before with a Bernoulli GLM, with a SVC for trend

$$z_t(\mathbf{s}_i) \sim \text{Bernoulli}(\psi_t(\mathbf{s}_i))$$

$$\text{logit}(\psi_t(\mathbf{s}_i)) = \tilde{\beta}_0(\mathbf{s}_i) + \tilde{\beta}_1(\mathbf{s}_i) \cdot \text{YEAR}_t$$

- $\tilde{\beta}_0(\mathbf{s}_i)$  and  $\tilde{\beta}_1(\mathbf{s}_i)$  are modeled as independent SVCS with NNGPs

- Let  $y_{t,k}(\mathbf{s}_i)$  denote the observed detection (1) or nondetection (0) of the bird at site  $i$  during year  $t$  and survey  $k = 1, \dots, 5$ .
- We model  $y_{t,k}(\mathbf{s}_i)$  conditional on the true presence/absence of the species  $z_t(\mathbf{s}_i)$

$$y_{t,k}(\mathbf{s}_i) \mid z_t(\mathbf{s}_i) \sim \text{Bernoulli}(p_{i,t,k} \cdot z_t(\mathbf{s}_i))$$

$$\text{logit}(p_{i,t,k}) = \alpha_0 + \alpha_1 \cdot \text{DAY}_{i,t,k} + \alpha_2 \cdot \text{DAY}_{i,t,k}^2$$

- A key assumption for identifiability is that  $z_t(\mathbf{s}_i)$  does not change across the 5 replicate surveys at site  $i$  during year  $t$ .

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