Hierarchical spatial modelling for applied population and community ecology

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Modelling big spatial data

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Bayesian spatial linear model

$$y(\boldsymbol{s}_j) \sim \text{Normal}(\mu(\boldsymbol{s}_j), \tau^2)$$
$$\mu(\boldsymbol{s}_j) = \beta_0 + \beta_1 \cdot x_1(\boldsymbol{s}_j) + \text{w}(\boldsymbol{s}_j)$$
$$\mathbf{w} \sim \text{Multivariate Normal}(\mathbf{0}, \boldsymbol{C}(d, \sigma^2, \phi))$$

- Recall our use of Gaussian Processes (GPs) to model the spatial random effects

- Values of **w** are determined by the covariance matrix **C**.

- **C** is a J x J spatial covariance matrix (J is the number of spatial locations)

Covariance matrix with J = 5

$$
\begin{bmatrix}
k_{1,1} & k_{1,2} & k_{1,3} & k_{1,4} & k_{1,5} \\
k_{2,1} & k_{2,2} & k_{2,3} & k_{2,4} & k_{2,5} \\
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\end{bmatrix}
$$

Covariance between site 5 and site 3

Covariance matrix with J = 5

$$\begin{bmatrix} k_{1,1} & k_{1,2} & k_{1,3} & k_{1,4} & k_{1,5} \\ k_{2,1} & k_{2,2} & k_{2,3} & k_{2,4} & k_{2,5} \\ k_{3,1} & k_{3,2} & k_{3,3} & k_{3,4} & k_{3,5} \\ k_{4,1} & k_{4,2} & k_{4,3} & k_{4,4} & k_{4,5} \\ k_{5,1} & k_{5,2} & k_{5,3} & k_{5,4} & k_{5,5} \end{bmatrix}$$

What happens when J = 200? 1,000? 100,000?

Covariance between site 5 and site 3

Gaussian process

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- Flexible approach to account for spatial autocorrelation
- But... becomes extremely slow as the number of sites increases
- Not practical for data sets with hundreds of data points, let alone thousands.
- Computational bottleneck: dealing with a large, *dense* J x J matrix
- The "big n" problem

The "big n" problem underneath the hood

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- Estimating the parameters in our model requires calculating:

$$p(\mathbf{w}) \propto -\frac{1}{2}\log\left(\det(\boldsymbol{C})\right) - \frac{1}{2}\mathbf{w}^{\top}\boldsymbol{C}^{-1}\mathbf{w}$$

The "big n" problem underneath the hood

- Estimating the parameters in our model requires calculating:

$$p(\mathbf{w}) \propto -\frac{1}{2}\log(\det(\boldsymbol{C})) - \frac{1}{2}\mathbf{w}^{\top}\boldsymbol{C}^{-1}\mathbf{w}$$

- Storage requirements: $O(J^2)$ flops
- $\mathbf{C}$ is a dense matrix (i.e., there are no zeros)
- Computational complexity: $O(J^3)$ flops
- Computationally infeasible when J is even moderately large (e.g., 500)

Simulation comparison

- *J = 1600,* fit a single-species spatial occupancy model

(A) True w

(B) Full GP (424 min)
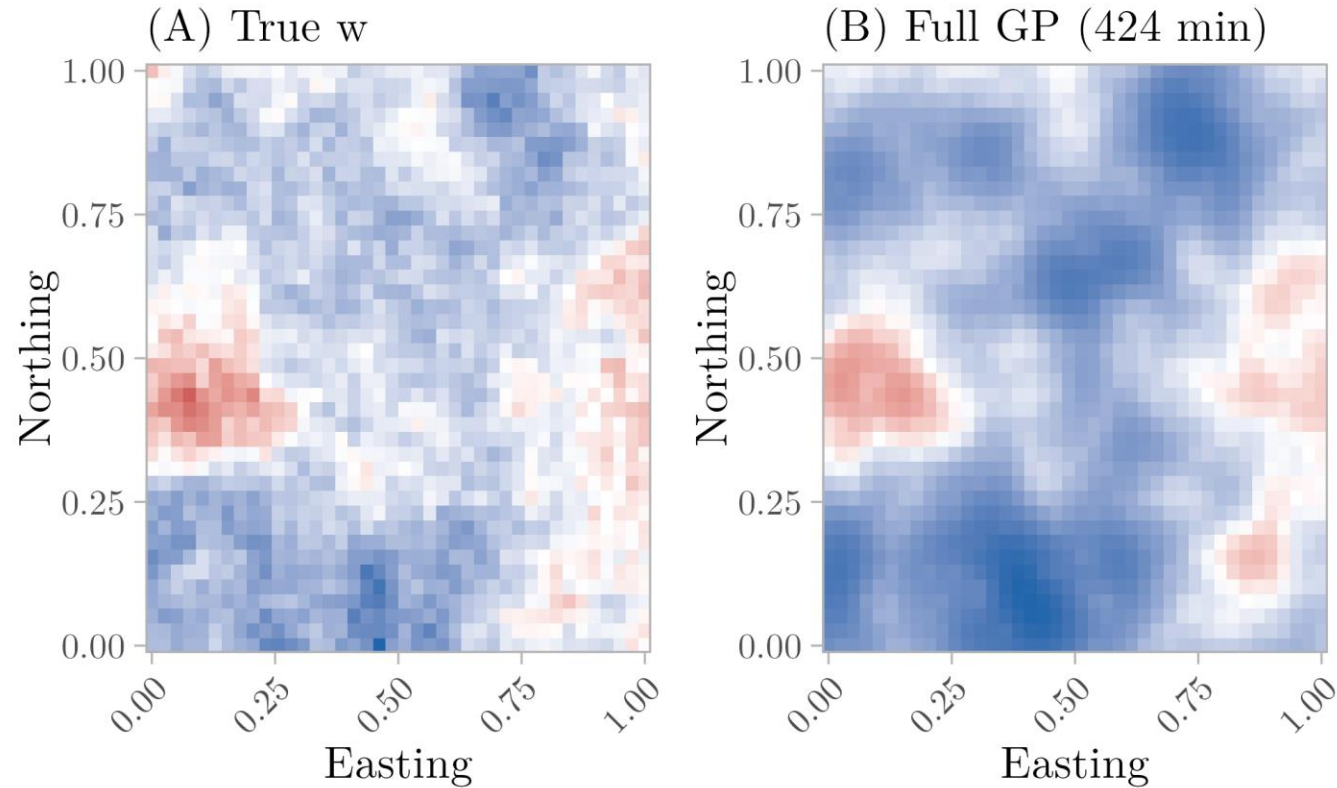
Solutions to the "big n" problem

A Case Study Competition Among Methods for Analyzing Large Spatial Data

Matthew J. HEATON, Abhirup DATTA, Andrew O. FINLEY,
Reinhard FURRER, Joseph GUINNESS, Rajarshi GUHANIYOGI,
Florian GERBER, Robert B. GRAMACY, Dorit HAMMERLING,
Matthias KATZFUSS, Finn LINDGREN, Douglas W. NYCHKA, Furong SUN,
and Andrew ZAMMIT-MANGION

Solutions to the "big n" problem

Low-rank methods: reduces the dimensionality of the covariance matrix (e.g., analogous to how a PCA takes a set of variables and reduces it to a smaller set)

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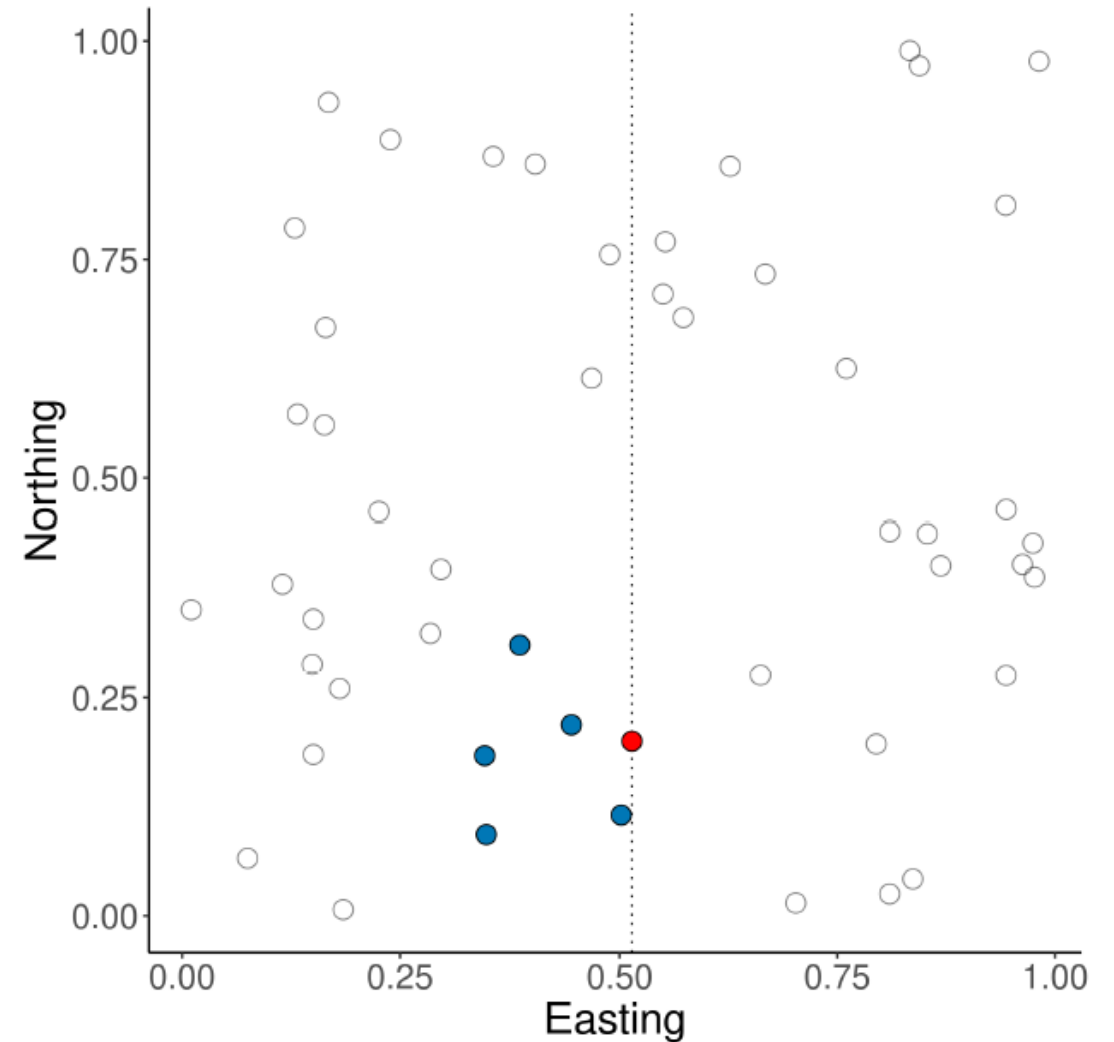
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- Conceptually:
    1. Order the spatial locations (e.g., along the x-axis)
    2. Determine the m nearest neighbors (subject to ordering) based on Euclidean (linear) distance
    3. The spatial random effect at each site only depends on values of its m nearest neighbors and is conditionally independent of all other values
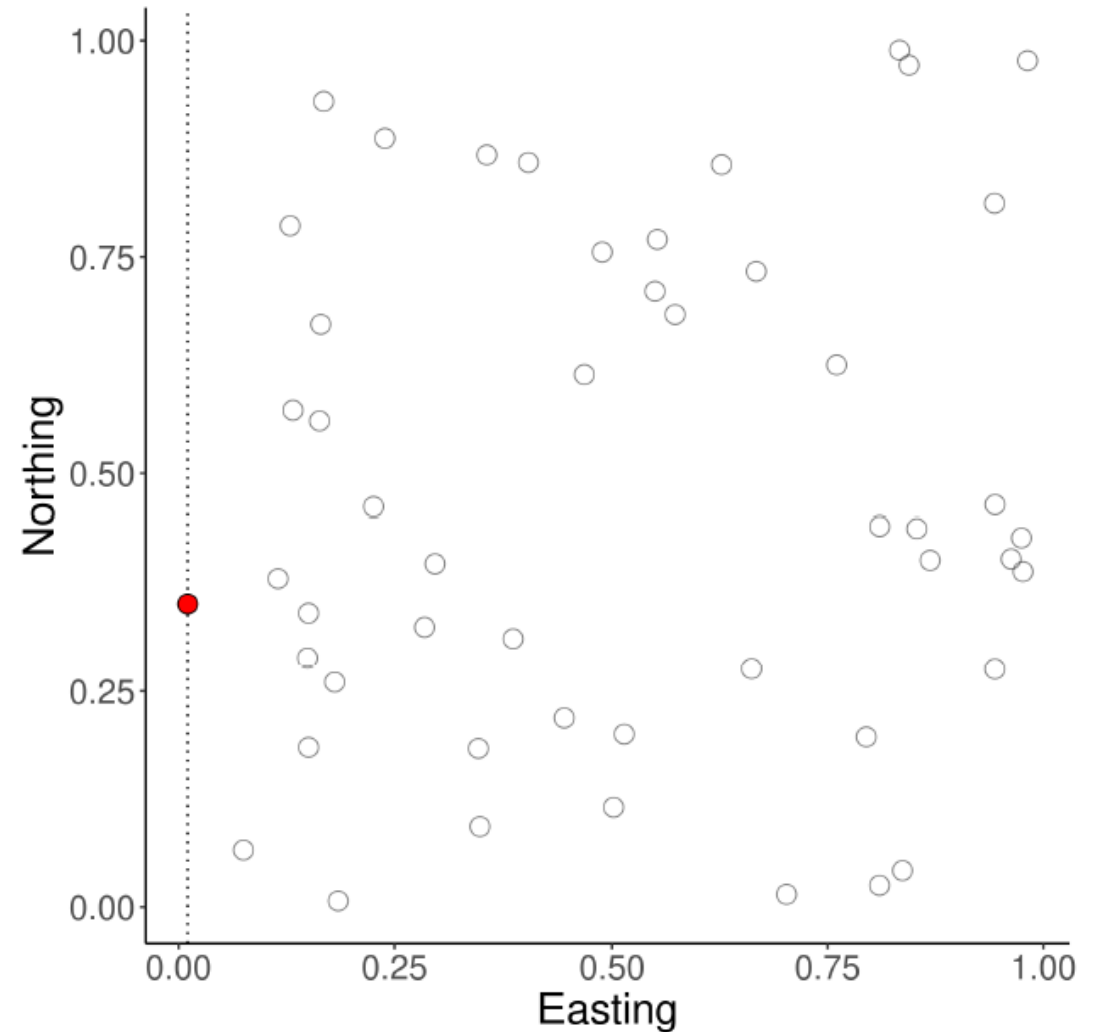
Choosing the neighbors

- spOccupancy and spAbundance order sites along the horizontal axis (i.e., Easting)

- Example: NNGP with 5 neighbors

- Red point denotes the current site

- Blue points denote sites in the "neighbor set"

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How many neighbors?
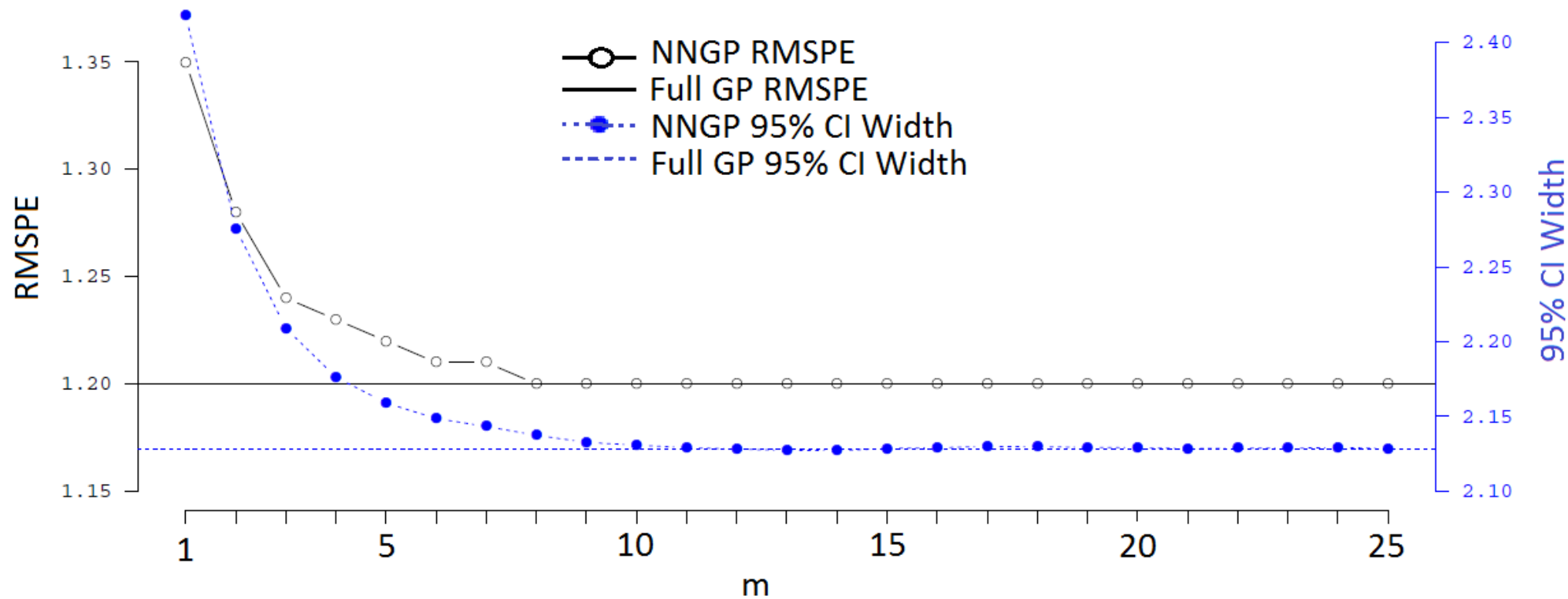
How many neighbors?
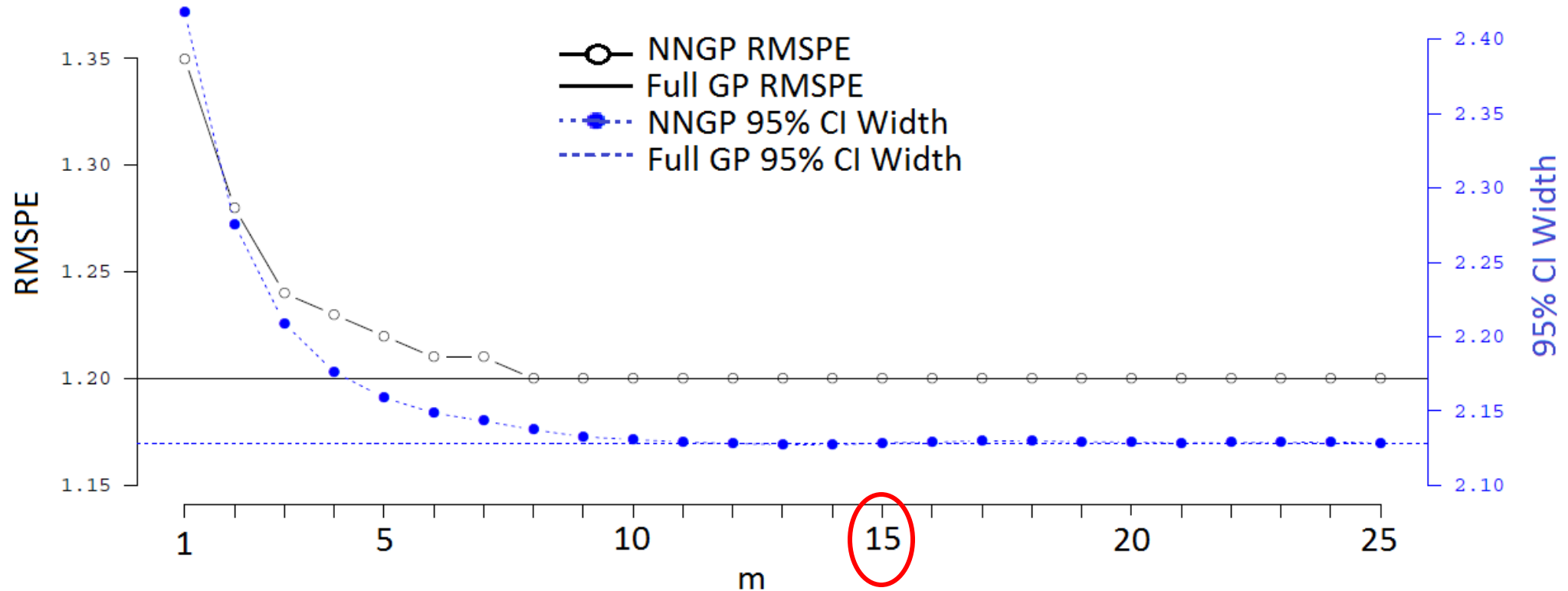
- m= 15 neighbors is often adequate (software default)
- Can compare smaller m using WAIC

Datta et al. (2016) JASA

NNGPs in more detail

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- Use a *sparse* matrix to approximate the dense Gaussian Process covariance matrix **C** (Datta et al. 2016)

- Based on rewriting the GP for **w** as a product of conditional densities.

NNGPs in more detail

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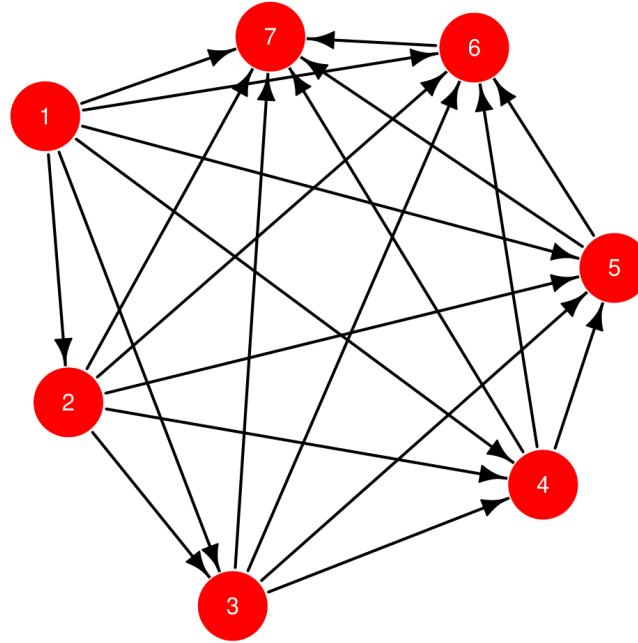- $\mathbf{w} \sim \text{Normal}(\mathbf{0}, C)$ is equivalent to

$$p(w_1)p(w_2 \mid w_1)p(w_3 \mid w_1, w_2) \cdots p(w_n \mid w_1, w_2, \ldots, w_{n-1})$$
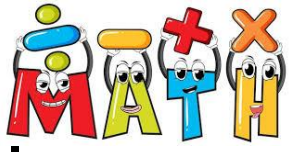
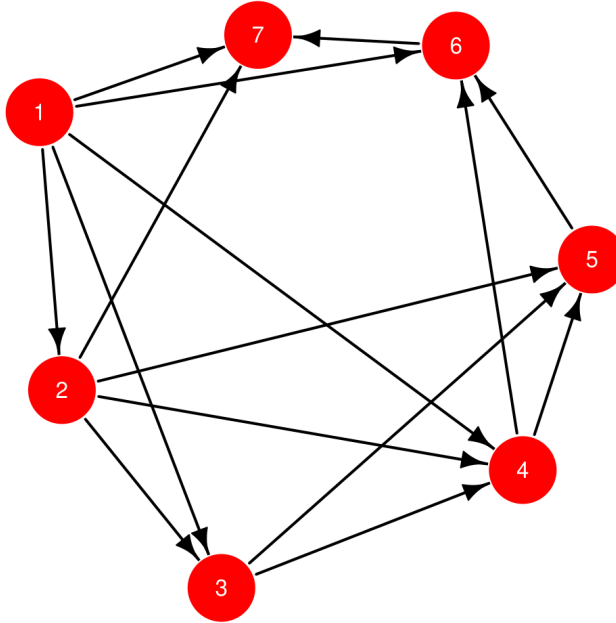# Introducing sparsity via graphical models

Introducing sparsity via graphical models

$$p(w_1)p(w_2 \mid w_1)p(w_3 \mid w_1, w_2)p(w_4 \mid w_1, w_2, w_3)$$
$$\times p(w_5 \mid w_1, w_2, w_3, w_4)p(w_6 \mid w_1, w_2, \ldots, w_5)$$
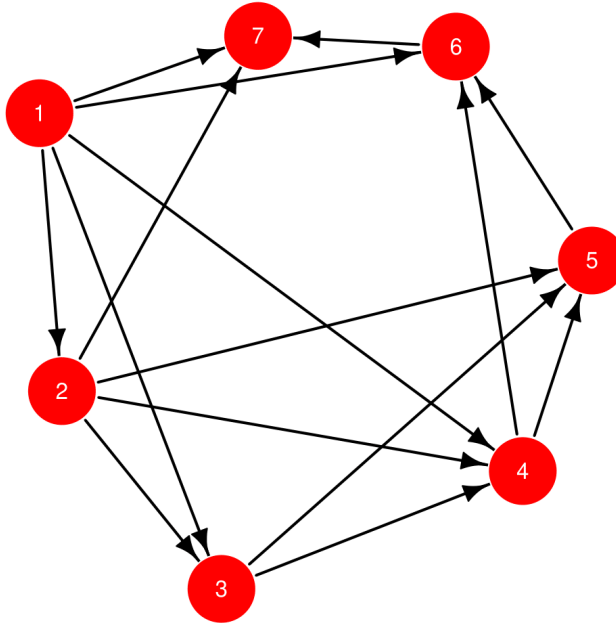$$\times p(w_7 \mid w_1, w_2, \ldots, w_6).$$

Introducing sparsity via graphical models

$$p(w_1)p(w_2 \mid w_1)p(w_3 \mid w_1, w_2)p(w_4 \mid w_1, w_2, w_3)$$
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$$\times p(w_7 \mid w_1, w_2, w_3, w_4, w_5, w_6)$$

Introducing sparsity via graphical models
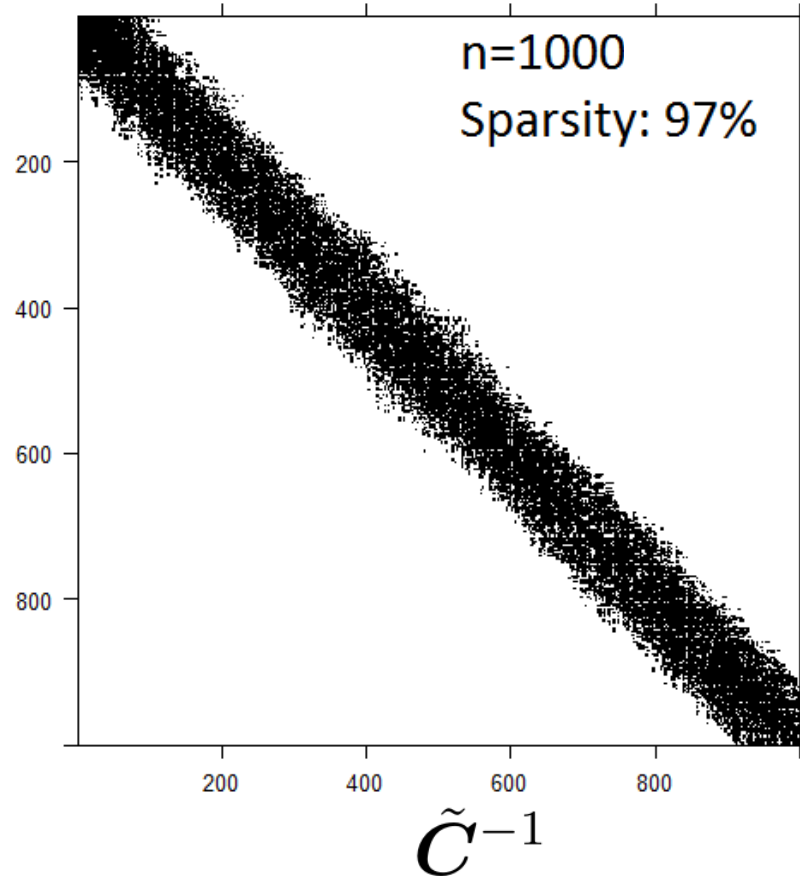
Size of neighbor set is ≤ m

$$p(w_1)p(w_2 \mid w_1)p(w_3 \mid w_1, w_2)p(w_4 \mid w_1, w_2, w_3)$$

$$\times \, p(w_5 \mid \cancel{w_1}, w_2, w_3, w_4)p(w_6 \mid w_1, \cancel{w_2}, \cancel{w_3}, w_4, w_5)$$

$$\times \, p(w_7 \mid w_1, w_2, \cancel{w_3}, \cancel{w_4}, \cancel{w_5}, w_6)$$

Sparsity via NNGP

$$\text{Normal}(\mathbf{w} \mid \mathbf{0}, C) \approx \text{Normal}(\mathbf{w} \mid \mathbf{0}, \tilde{C})$$

n=1000
Sparsity: 97%

$\tilde{C}^{-1}$

NNGP-derived
covariance matrix

Bayesian spatial NNGP linear model

$$y(\boldsymbol{s}_j) \sim \text{Normal}(\mu(\boldsymbol{s}_j), \tau^2)$$

$$\mu(\boldsymbol{s}_j) = \beta_0 + \beta_1 \cdot x_1(\boldsymbol{s}_j) + \text{w}(\boldsymbol{s}_j)$$

$$\mathbf{w} \sim \text{Multivariate Normal}(\mathbf{0}, \tilde{\boldsymbol{C}}(d, \sigma^2, \phi))$$

- All we do is replace the covariance matrix from the GP with the NNGP-derived covariance matrix. Otherwise, it's exactly the same!
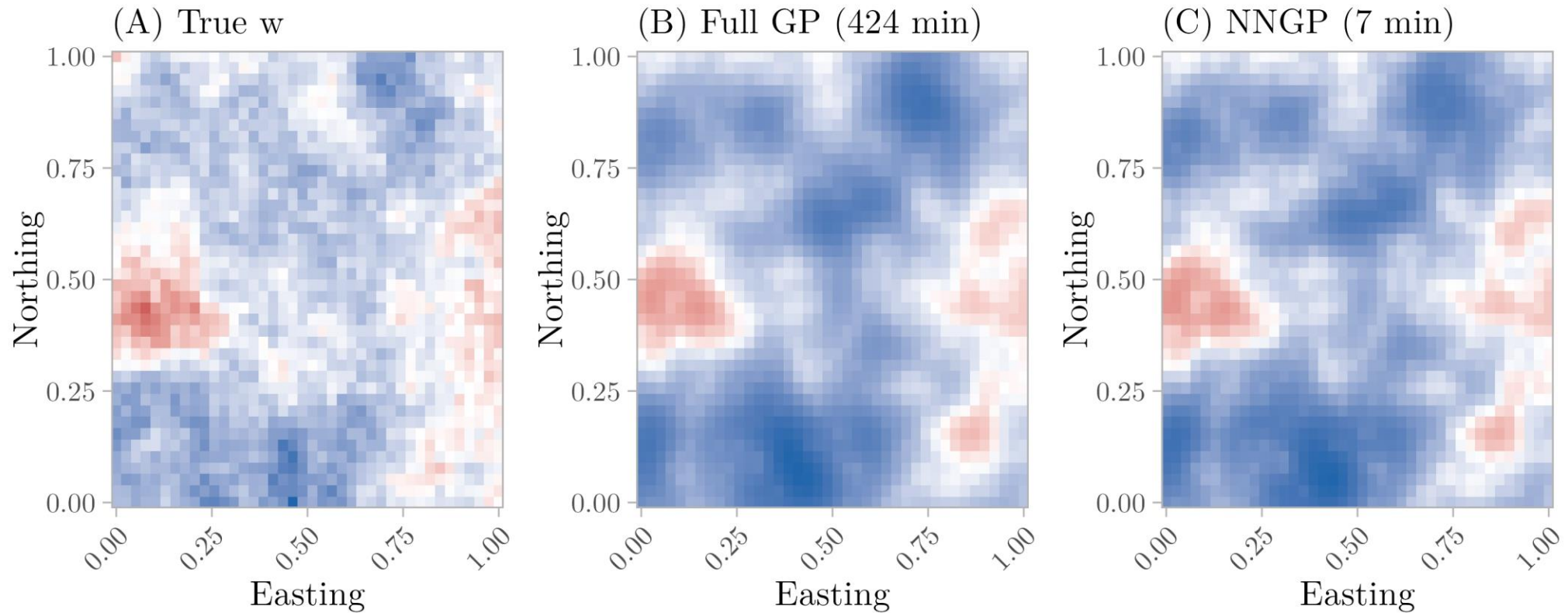
Storage and computation

- Storage
  - Never need to store J x J distance matrix
  - Stores smaller m x m matrices (m is the number of neighbors)
  - Total storage requirements: $O(Jm^2)$
- Computation:
  - Only involves inverting small m x m matrices
  - $O(Jm^3)$ flops
- Since m << J, NNGP offers great scalability for big spatial data

Simulation comparison

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(A) True w   (B) Full GP (424 min)   (C) NNGP (7 min)

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