

# Nearest Neighbor Gaussian Processes for Large Spatial Data

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Consider again the spatially-varying intercept model for generic location  $\mathbf{s}$

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

where

$y(\mathbf{s})$  is the outcome,

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

$\boldsymbol{\beta}$  is a vector of  $p$  regression parameters,

$w(\mathbf{s})$  is a spatial random effect,

$\epsilon(\mathbf{s})$  is the independent noise process with variance  $\tau^2$ .

## Likelihood from (full rank) GP models

- Assuming  $w(\mathbf{s}) \sim GP(0, K_\theta(\cdot, \cdot))$  implies that for a set of  $n$  locations<sup>1</sup>

$$\mathbf{w} = (w(\mathbf{s}_1), w(\mathbf{s}_2), \dots, w(\mathbf{s}_n))^\top \sim MVN(\mathbf{0}, \mathbf{K}_\theta)$$

- 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  $\theta$  and many Markov chain Monte Carlo (MCMC) iterations

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

## Computation issues

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

Computationally infeasible for large datasets

## 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:** (Nychka et al., 2015; Johannesson et al., 2007; Katzfuss, 2017; Guhaniyogi and Sanso, 2020)
- **Sparsity:** (Solve  $\mathbf{Ax} = \mathbf{b}$  by (i) sparse  $\mathbf{A}$ , or (ii) sparse  $\mathbf{A}^{-1}$ )
  1. Covariance tapering (Furrer et al., 2006; Du et al., 2009; Kaufman et al., 2008; Stein, 2013; Shaby and Ruppert, 2012)
  2. GMRFs to GPs: INLA (Rue et al., 2009; Lindgren et al., 2011)
  3. LAGP Gramacy et al., 2014; Gramacy and Apley, 2015)
  4. **Nearest-neighbor Gaussian Process (NNGP)** models (Datta et al., 2016a,c,b; Finley et al., 2019a) builds on Vecchia (1988).

## Reduced (Low) rank models

- $\mathbf{K}_\theta \approx \mathbf{J}_\theta \mathbf{K}_\theta^* \mathbf{J}_\theta^\top + \mathbf{D}_\theta$
- $\mathbf{J}_\theta$  is  $n \times r$  matrix of spatial basis functions,  $r \ll n$
- $\mathbf{K}_\theta^*$  is  $r \times r$  spatial covariance matrix
- $\mathbf{D}_\theta$  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,  $\mathcal{S}^* = \{\mathbf{s}_1^*, \mathbf{s}_2^*, \dots, \mathbf{s}_r^*\}$ .
- $\mathbf{J}_\theta$  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

$$(\mathbf{J}_\theta \mathbf{K}_\theta^* \mathbf{J}_\theta^\top + \mathbf{D})^{-1} = \mathbf{D}^{-1} - \mathbf{D}^{-1} \mathbf{J}_\theta (\mathbf{K}_\theta^{*-1} + \mathbf{J}_\theta^\top \mathbf{D}^{-1} \mathbf{J}_\theta)^{-1} \mathbf{J}_\theta^\top \mathbf{D}^{-1}.$$

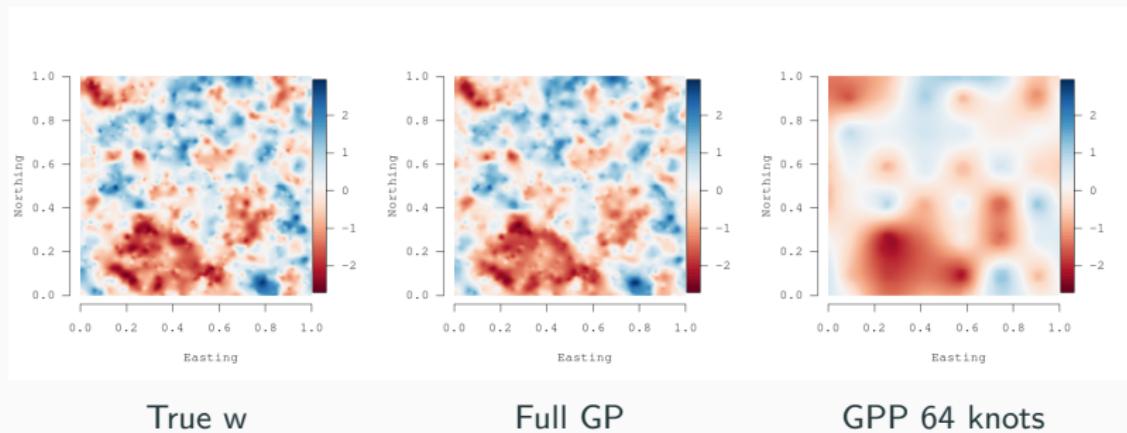
This is the famous Sherman-Woodbury-Morrison formula.

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

## 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  $\phi$
- Candidate models: Full GP and Gaussian Predictive Process (GPP) with 64 knots

# Oversmoothing due to reduced-rank models



**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.

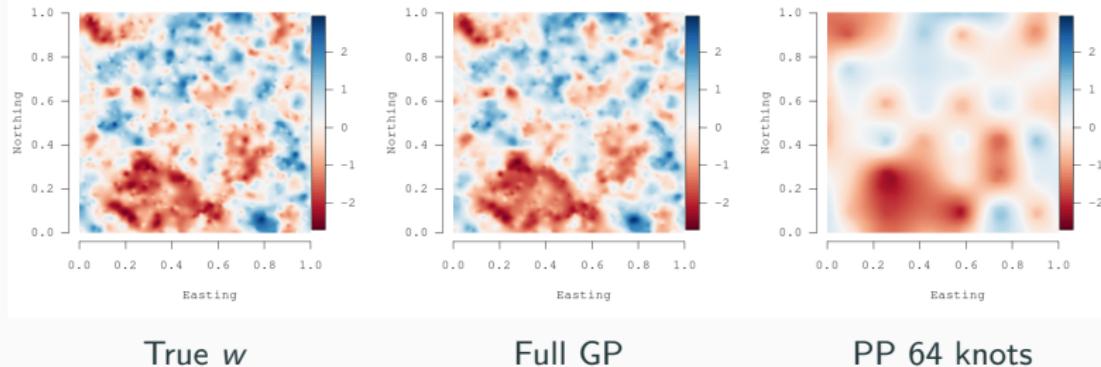
# Low rank Gaussian Predictive Process

## 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

# Sparse matrices

- 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

## 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  $\Rightarrow$

$$w_1 = 0 + \eta_1;$$

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

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

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

## Cholesky factors

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

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

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

## Cholesky factors

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

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

- Cholesky factorization:

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

## Cholesky factors

- 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  $\text{chol}(\mathbf{K}_\theta) = \mathbf{L} \mathbf{D} \mathbf{L}^\top$ , 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

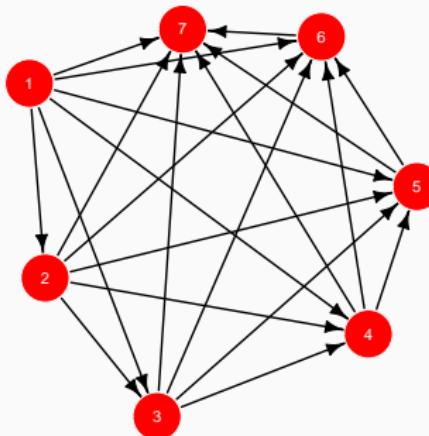
$$\sum_{j < i} a_{ij} w_j = E[w_i | w_{\{j < i\}}] \quad i = 2, \dots, n$$

- 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.

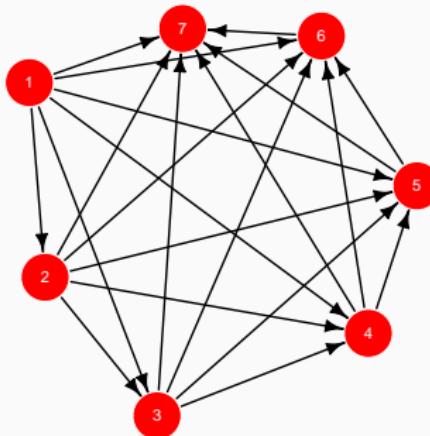
```
for(i in 1:(n-1)) {  
  A[i+1,1:i] = solve(K[1:i,1:i], K[1:i,i+1])  
  D[i+1,i+1] = K[i+1,i+1] - dot(K[i+1,1:i], A[i+1,1:i])  
}
```

# Cholesky Factors and Directed Acyclic Graphs (DAGs)



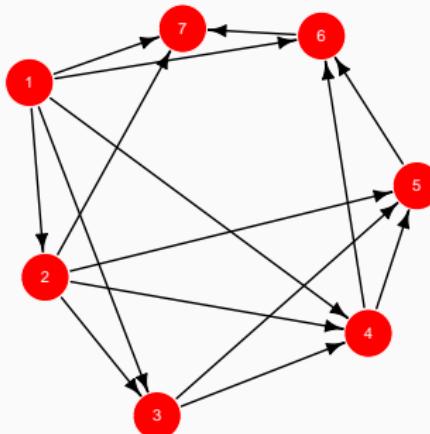
- Number of non-zero entries (**sparsity**) of  $\mathbf{A}$  equals number of arrows in the graph
- In particular: Sparsity of the  $i^{th}$  row of  $\mathbf{A}$  is same as the number of arrows towards  $i$  in the DAG

# Introducing sparsity via graphical models



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

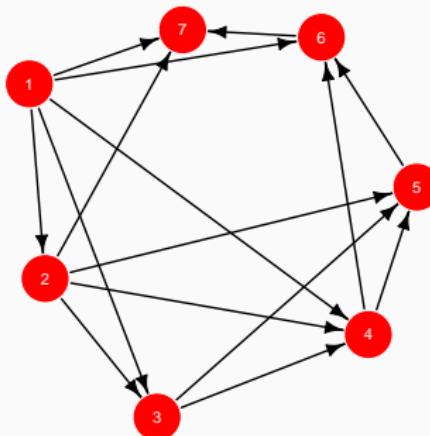
# Introducing sparsity via graphical models



$$p(y_1)p(y_2 | y_1)p(y_3 | y_1, y_2)p(y_4 | y_1, y_2, y_3)$$

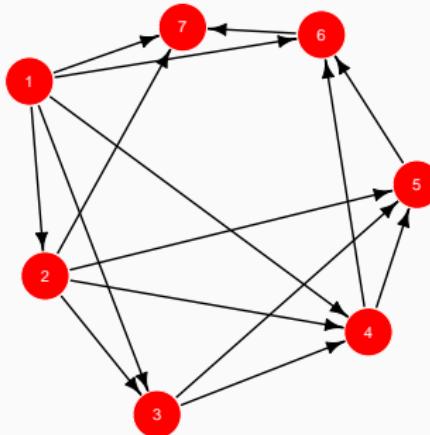
$$p(y_5 | \cancel{y_1}, y_2, y_3, y_4)p(y_6 | y_1, \cancel{y_2}, \cancel{y_3}, y_4, y_5)p(y_7 | y_1, y_2, \cancel{y_3}, \cancel{y_4}, \cancel{y_5}, y_6)$$

# Introducing sparsity via graphical models



- 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  $p(w_i | \{w_k : k < i\})$

# Introducing sparsity via graphical models



- $N(i)$  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  $m \times m$

- Non-zero elements of sparse **A** and **D** are computed:

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

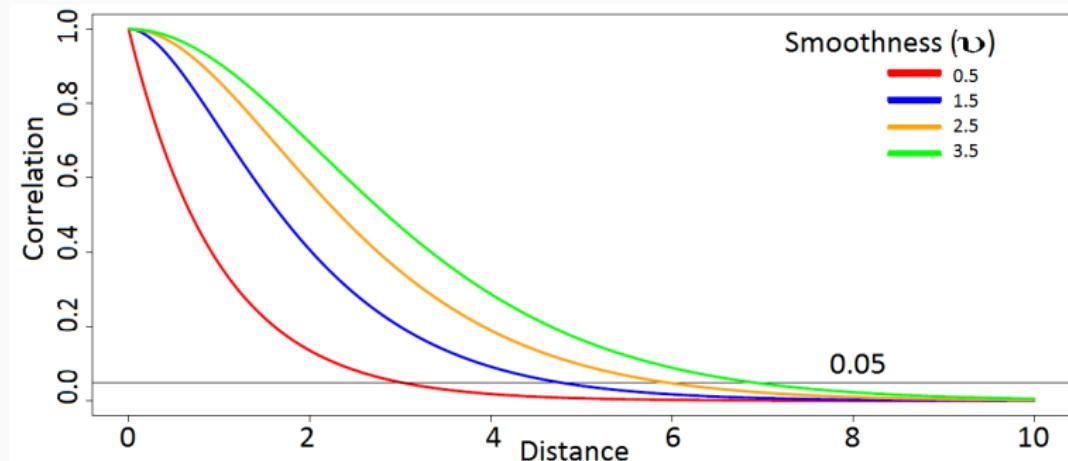
```
for(i in 1:(n-1)) {  
    Pa = N[i+1] # neighbors of i+1  
    A[i+1,Pa] = solve(K[Pa,Pa], K[i+1,Pa])  
    D[i+1,i+1] = K[i+1,i+1] - dot(K[i+1,Pa],A[i+1,Pa])  
}
```

- 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.

# Choosing neighbor sets

Matern Covariance Function:

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



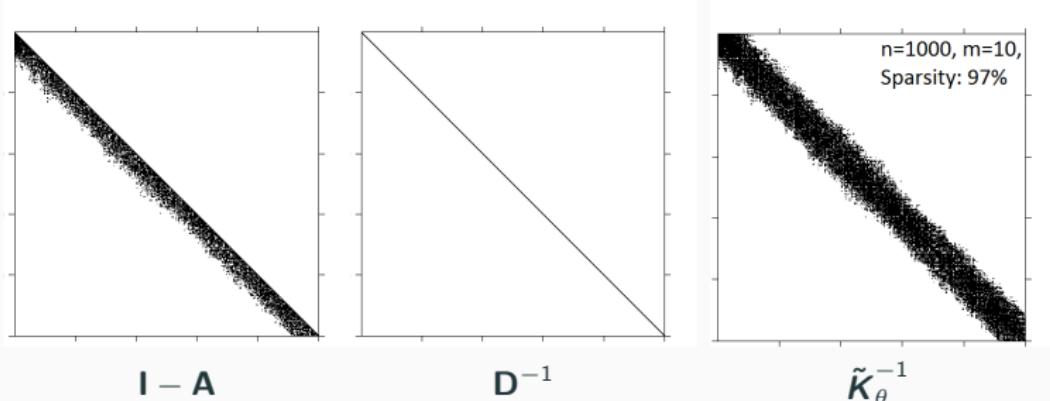
## Choosing neighbor sets

- Spatial covariance functions decay with distance
- Vecchia (1988):  $N(\mathbf{s}_i) = m$ —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)

## Nearest neighbors

# 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  $\eta(\mathbf{s}) \stackrel{ind}{\sim} N(0, d(\mathbf{s}))$ 
  - $a_i(\mathbf{s})$  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)

# 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  $GP(0, (\cdot, \cdot, | \sigma^2, \phi))$
- $\epsilon(\mathbf{s}) \stackrel{\text{iid}}{\sim} N(0, \tau^2)$  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  $w(\mathbf{s})$

# Hierarchical spatial regression with NNGP

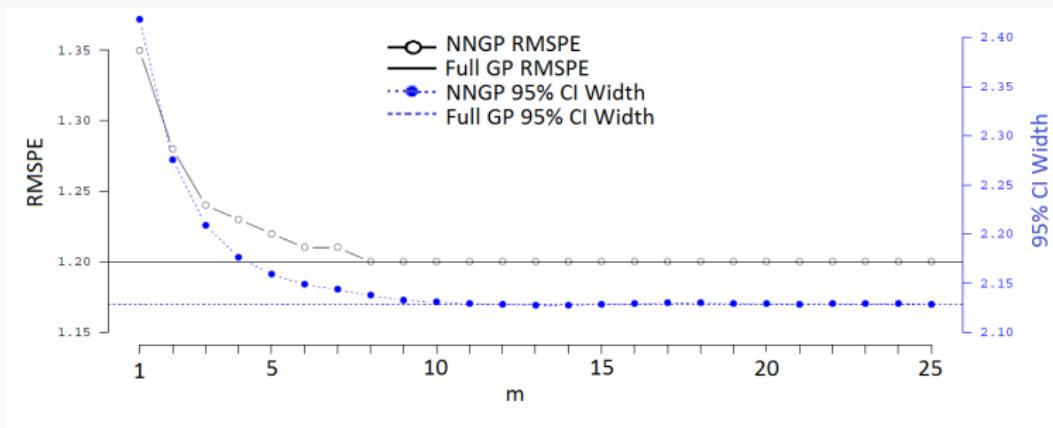
## Full Bayesian Model

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

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

## Choosing $m$



- 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

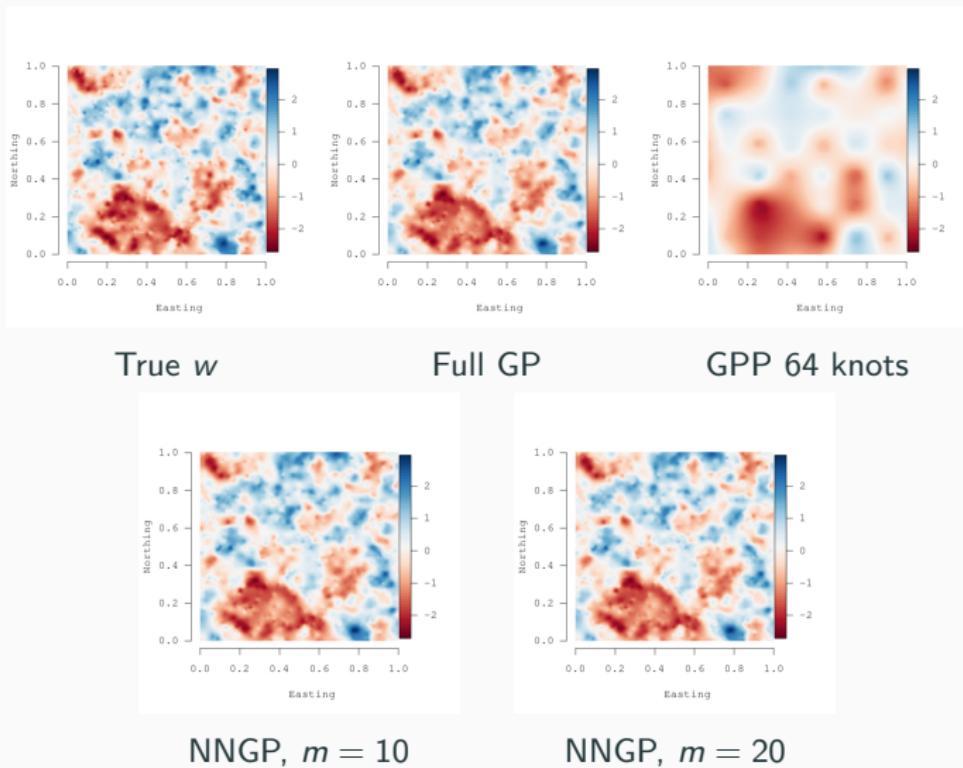
# Storage and computation

- 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

## 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  $\phi$
- Candidate models: Full GP, Gaussian Predictive Process (GPP) with 64 knots and NNGP

# Fitted Surfaces



**Figure:** Univariate synthetic data analysis

# Parameter estimates

	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)	1.03 (0.69, 1.34)
$\beta_1$	5	5.01 (4.99, 5.03)	5.01 (4.99, 5.03)	5.03 (4.99, 5.06)	5.01 (4.99, 5.03)
$\sigma^2$	1	0.96 (0.78, 1.23)	0.94 (0.77, 1.20)	1.29 (0.96, 2.00)	0.94 (0.76, 1.23)
$\tau^2$	0.1	0.10 (0.08, 0.13)	0.10 (0.08, 0.13)	0.08 (0.04, 0.13)	0.10 (0.08, 0.12)
$\phi$	12	12.93 (9.70, 16.77)	13.36 (9.99, 17.15)	<b>5.61 (3.48, 8.09)</b>	13.52 (9.92, 17.50)

## Model evaluation

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

- 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

## Multivariate spatial linear model

- Spatial linear model for  $q$ -variate spatial data:  
 $y_i(\mathbf{s}) = \mathbf{x}_i^\top(\mathbf{s})\boldsymbol{\beta}_i + w_i(s) + \epsilon_i(s)$  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

## Multivariate GPs

- $\text{Cov}(w(\mathbf{s}_i), w(\mathbf{s}_j)) = K(s_i, s_j \mid \theta)$  – a  $q \times q$  cross-covariance matrix
- Choices for the function  $K(\cdot, \cdot \mid \theta)$ 
  - Multivariate Matérn
  - Linear model of co-regionalization
- For data observed at  $n$  locations, all choices lead to a dense  $nq \times nq$  matrix  $\mathbf{K}_\theta = \text{Cov}(w(\mathbf{s}_1), w(\mathbf{s}_2), \dots, w(\mathbf{s}_n))$
- Not scalable when  $nq$  is large

## Multivariate NNGPs

- Cholesky factor approach similar to the univariate case

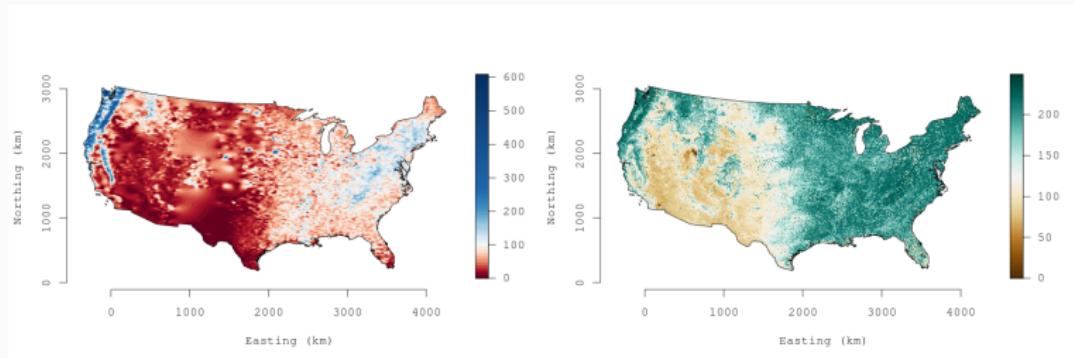
$$\begin{bmatrix} \mathbf{w}(\mathbf{s}_1) \\ \mathbf{w}(\mathbf{s}_2) \\ \mathbf{w}(\mathbf{s}_3) \\ \vdots \\ \mathbf{w}(\mathbf{s}_n) \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 & 0 \\ \mathbf{A}_{21} & 0 & 0 & \dots & 0 & 0 \\ \mathbf{A}_{31} & \mathbf{A}_{32} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{A}_{n1} & \mathbf{A}_{n2} & \mathbf{A}_{n3} & \dots & \mathbf{A}_{n,n-1} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{w}(\mathbf{s}_1) \\ \mathbf{w}(\mathbf{s}_2) \\ \mathbf{w}(\mathbf{s}_3) \\ \vdots \\ \mathbf{w}(\mathbf{s}_n) \end{bmatrix} + \begin{bmatrix} \boldsymbol{\eta}(\mathbf{s}_1) \\ \boldsymbol{\eta}(\mathbf{s}_2) \\ \boldsymbol{\eta}(\mathbf{s}_3) \\ \vdots \\ \boldsymbol{\eta}(\mathbf{s}_n) \end{bmatrix}$$

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

Only differences:

- $\mathbf{w}(\mathbf{s}_i)$  and  $\boldsymbol{\eta}(\mathbf{s}_i)$ '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.,  $q > 5$ ).

# U.S. Forest biomass data



Observed biomass

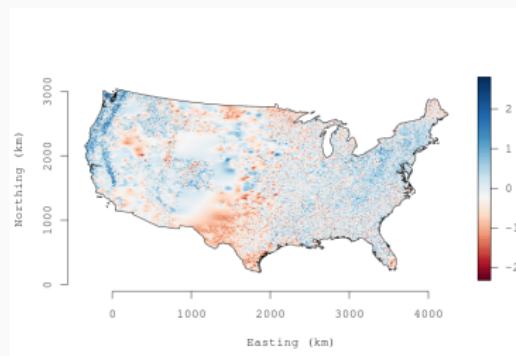
NDVI

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

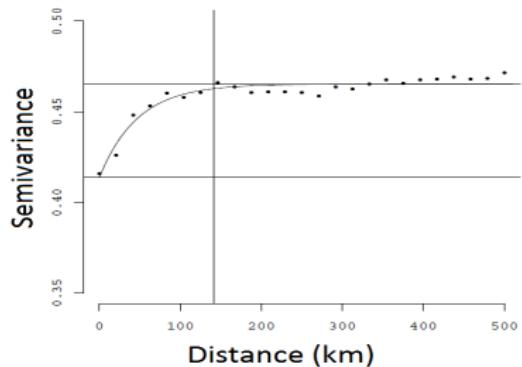
# U.S. Forest biomass data

## Non Spatial Model

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



Residuals



Variogram of residuals

**Strong spatial pattern among residuals**

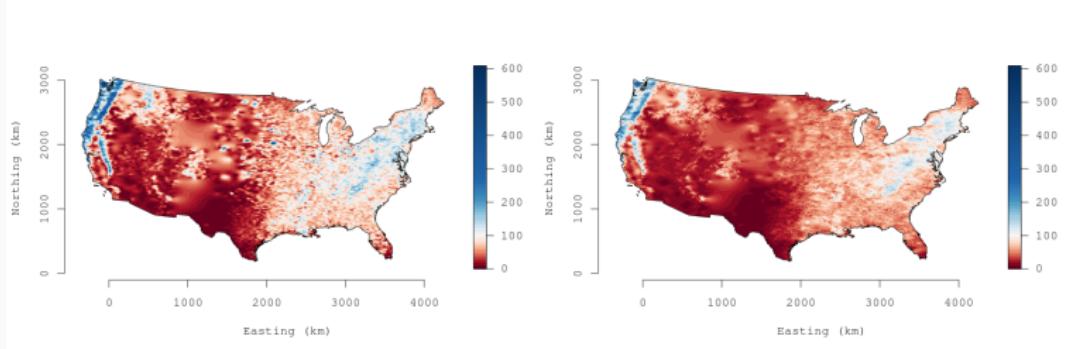
## Forest biomass dataset

- $n \approx 10^5$  (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

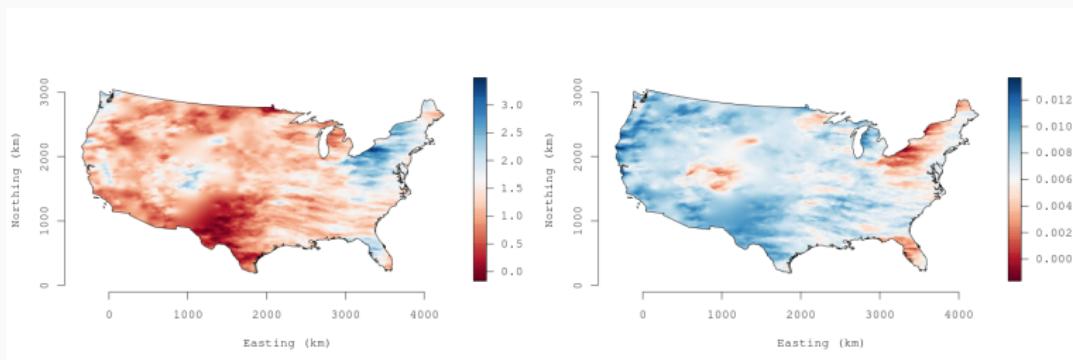
- $\text{Biomass}(s) = \beta_0(s) + \beta_1(s)\text{NDVI}(s) + \epsilon(s)$
- $\mathbf{w}(s) = (\beta_0(s), \beta_1(s))^\top \sim \text{Bivariate NNGP}(0, \tilde{K}(\cdot, \cdot | \theta)), m = 5$
- Time  $\approx 6\text{ seconds}$  per iteration
- Full inferential output: 41 hours (25000 MCMC iterations)

# Forest biomass data



Observed biomass

Fitted biomass



$$\beta_0(s)$$

$$\beta_{NDVI}(s)$$

## Reducing parameter dimensionality

- 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

# Collapsed NNGP

- Same model:

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

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

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

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

## Collapsed NNGP

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

- Only involves few parameters  $\boldsymbol{\beta}$ ,  $\tau^2$  and  $\boldsymbol{\theta} = (\sigma^2, \phi)$
- 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  $\mathbf{w} \mid \mathbf{y}$
- Complexity of the algorithm depends on the design of the data locations and is **not guaranteed to be  $O(n)$**

## Response NNGP

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

## Conjugate NNGP

- Full GP model:  $\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta}, \boldsymbol{\Sigma})$  where  $\boldsymbol{\Sigma} = \sigma^2 \mathbf{M}$
- $\mathbf{M} = \mathbf{R}(\phi) + \alpha \mathbf{I}$
- $\alpha = \tau^2 / \sigma^2$  is the ratio of the noise to signal variance
- Response NNGP model:  $\mathbf{y} \sim N(\mathbf{X}\boldsymbol{\beta}, \tilde{\boldsymbol{\Sigma}})$
- $\tilde{\boldsymbol{\Sigma}} = \sigma^2 \tilde{\mathbf{M}}$  where  $\tilde{\mathbf{M}}$  is the NNGP approximation for  $\mathbf{M}$

## Conjugate NNGP

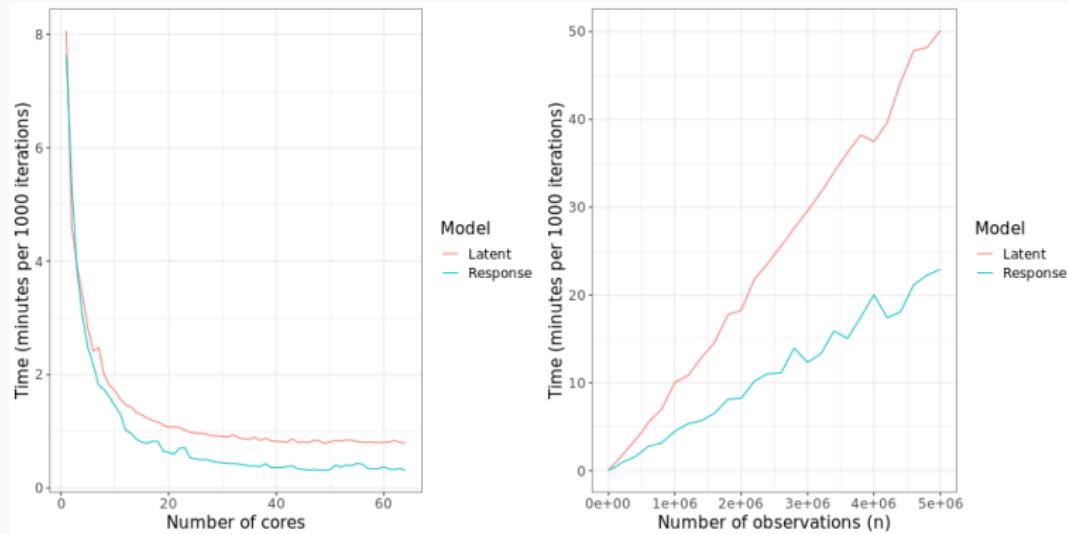
- Full GP model:  $\mathbf{y} \sim N(\mathbf{X}\beta, \Sigma)$  where  $\Sigma = \sigma^2 \mathbf{M}$
- $\mathbf{M} = \mathbf{R}(\phi) + \alpha \mathbf{I}$
- $\alpha = \tau^2 / \sigma^2$  is the ratio of the **noise to signal variance**
- Response NNGP model:  $\mathbf{y} \sim N(\mathbf{X}\beta, \tilde{\Sigma})$
- $\tilde{\Sigma} = \sigma^2 \tilde{\mathbf{M}}$  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 (NIG)** 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!

# Comparison of NNGP models

	Latent	Collapsed	Response	Conjugate
$O(n)$ time	Yes	No	Yes	Yes
Recovery of $\mathbf{w}   \mathbf{y}$	Yes	Yes	No	Yes
Parameter dimensionality	High	Low	Low	Low
Inference on $\theta$	Yes	Yes	Yes	Partially

# Comparison of NNGP models



**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.

## Summary of Nearest Neighbor Gaussian Processes

- 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