# Scalable methods for large spatial data: Nearest Neighbor Gaussian processes

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#### Review of Low rank Gaussian Predictive Process

#### **Pros**

- Choose knots  $S^* = \{s_1^*, s_2^*, \dots, s_r^*\}$
- $\tilde{w}(s) = E(w(s) | w(S^*)) + \eta(s)$
- $var(\tilde{w}) = A_{n \times r} Var(\tilde{w}(S^*))_{r \times r} A' + D_{n \times n}$
- Matrix identities ensure we only need to invert the  $r \times r$  matrix
- Computationally tractable FLOPs count O(nr<sup>2</sup>)
- Full Gaussian process (with a low-rank plus diagonal covariance function)
- Allows for coherent spatial interpolation at arbitrary resolution
- Can be used as prior for spatial random effects in any hierarchical setup for spatial data

#### Review of Low rank Gaussian Predictive Process

#### Cons

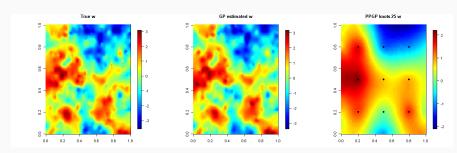


Figure: Comparing full GP vs low-rank GP

- Low rank models like the Predictive Process (PP) often tends 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 determinants
- Closely approximate full GP inference
- Proper Gaussian process model like the Predictive Process

• Write a joint density  $p(w) = p(w_1, w_2, ..., w_n)$  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  $w \sim N(0, C)$  this  $\Rightarrow$ 

$$w_1 = 0 + \eta_1;$$
  
 $w_2 = a_{21}w_1 + \eta_2;$   
... ... ...  
 $w_n = a_{n1}w_1 + a_{n2}w_2 + \cdots + a_{n,n-1}w_{n-1} + \eta_n;$ 

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• For Gaussian distribution  $w \sim N(0, C)$  this  $\Rightarrow$ 

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

$$\implies w = Aw + \eta; \quad \eta \sim N(0, D), \text{ where } D = diag(d_1, d_2, \dots, d_n).$$

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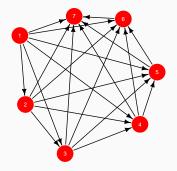
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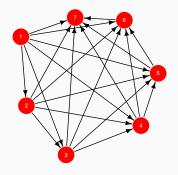
• Cholesky factorization:  $C = (I - A)^{-1}D(I - A)^{-\top}$  or  $C^{-1} = (I - A)'D^{-1}(I - A)$ 

- $w_{< i} = (w_1, w_2, \dots, w_{i-1})'$
- $c_i = Cov(w_i, w_{< i}), C_i = Var(w_{< i})$
- $i^{th}$  row of A and  $d_i = Var(\eta_i)$  are obtained from  $p(w_i \mid w_{< i})$  as follows:
  - Solve for  $a_{ij}$ 's from  $\sum_{i=1}^{i-1} a_{ij} w_i = E(w_i | w_{< i}) = c'_i C_i^{-1} w_{< i}$
  - $d_i = Var(w_i \mid w_{< i}) = \sigma^2 c'_i C_i^{-1} c_i$
- For large i, inverting  $C_i$  becomes slow
- The Cholesky factor approach for the full GP covariance matrix C does not offer any computational benefits

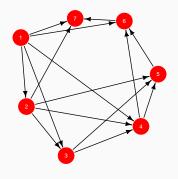
## Cholesky Factors and Directed Acyclic Graphs (DAGs)



- Number of non-zero entries (sparsity) of A equals number of arrows in the graph
- In particular: Sparsity of the i<sup>th</sup> row of A is same as the number of arrows towards i in the DAG

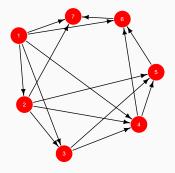


$$p(y_1)p(y_2 | y_1)p(y_3 | y_1, y_2)p(y_4 | y_1, y_2, y_3) \times p(y_5 | y_1, y_2, y_3, y_4)p(y_6 | y_1, y_2, \dots, y_5)p(y_7 | y_1, y_2, \dots, y_6).$$

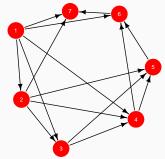


$$p(y_1)p(y_2 \mid y_1)p(y_3 \mid y_1, y_2)p(y_4 \mid y_1, y_2, y_3)$$

$$p(y_5 \mid y_4, y_2, y_3, y_4)p(y_6 \mid y_1, y_2, y_3, y_4, y_5)p(y_7 \mid y_1, y_2, y_3, y_4, y_6, y_6)$$



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



- 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:

$$E[w_i \mid w_{N(i)}] = \sum_{j \in N(i)} a_{ij} w_j = c_{i,N(i)} C_{N(i)}^{-1} w_{N(i)}$$

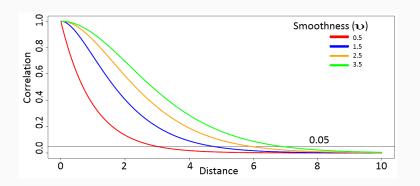
$$Var[w_i | w_{N(i)}] = d_i = \sigma_i^2 - c_{i,N(i)} C_{N(i)}^{-1} c_{N(i),i}$$

• The above matrix is only  $m \times m$ 

### Choosing neighbor sets

Matern Covariance Function:

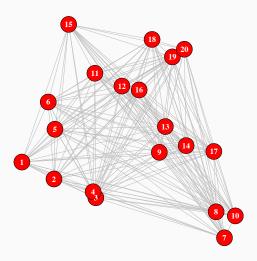
$$C(s_i, s_j) = \frac{1}{2^{\nu-1}\Gamma(\nu)}(||s_i - s_j||\phi)^{\nu} \mathscr{K}_{\nu}(||s_i - s_j||\phi); \ \phi > 0, \nu > 0,$$



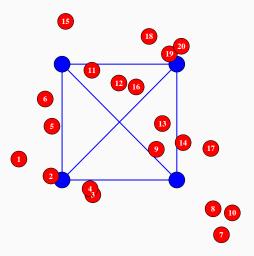
### Choosing neighbor sets

- Spatial covariance functions decay with distance
- Vecchia (1988):  $N(s_i) = m$ —nearest neighbors of  $s_i$  in  $s_1, s_2, \ldots, s_{i-1}$ 
  - 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 (2016) can also be used

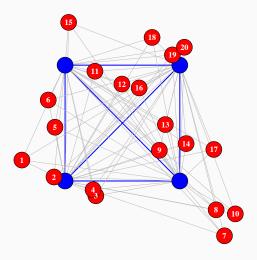


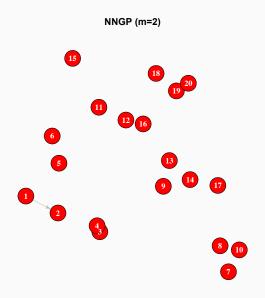


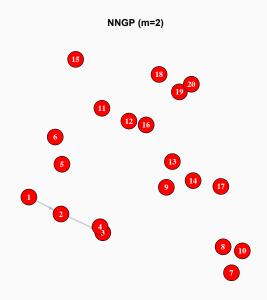
#### **Predictive Process**

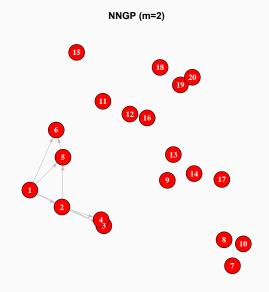


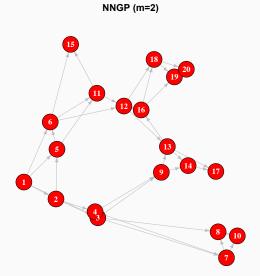
#### **Predictive Process**





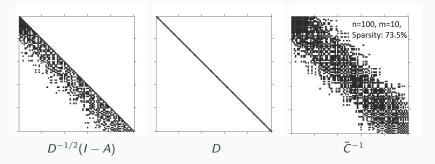






## Sparse precision matrices

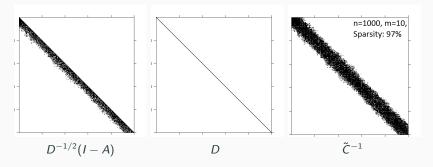
- The neighbor sets and the covariance function  $C(\cdot,\cdot)$  define a sparse Cholesky factor  $D^{-1/2}(I-A)$  of the spatial precision (inverse-covariance) matrix
- $N(w \mid 0, C) \approx N(w \mid 0, \tilde{C})$ ;  $\tilde{C}^{-1} = (I A)^{\top} D^{-1} (I A)$



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

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#### **Extension to a Process**

- We have defined  $w \sim N(0, \tilde{C})$  over the set of data locations  $S = \{s_1, s_2, \dots, s_n\}$
- For  $s \notin S$ , define N(s) as set of *m*-nearest neighbors of *s* in *S*
- Define  $w(s) = \sum_{i:s_i \in N(s)} a_i(s)w(s_i) + \eta(s)$  where  $\eta(s) \stackrel{ind}{\sim} N(0, d(s))$ 
  - a<sub>i</sub>(s) and d(s) are once again obtained by solving m × m system respectively as the m-nearest neighbor kriging mean weights and kriging variance
- Well-defined GP over entire domain
  - Nearest Neighbor GP (NNGP) Datta et al. (2016)<sup>1</sup>

//www.tandfonline.com/doi/abs/10.1080/01621459.2015.1044091

<sup>1</sup>https:

## Hierarchical spatial regression with NNGP

#### **Spatial linear model**

$$y(\mathbf{s}) = x(\mathbf{s})'\beta + w(\mathbf{s}) + \epsilon(\mathbf{s})$$

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

## Hierarchical spatial regression with NNGP

### Full Bayesian Model

$$N(y \mid X\beta + w, \tau^{2}I) \times N(w \mid 0, \tilde{C}(\sigma^{2}, \phi)) \times N(\beta \mid \mu_{\beta}, V_{\beta})$$
$$\times IG(\tau^{2} \mid a_{\tau}, b_{\tau}) \times IG(\sigma^{2} \mid a_{\sigma}, b_{\sigma}) \times Unif(\phi \mid a_{\phi}, b_{\phi})$$

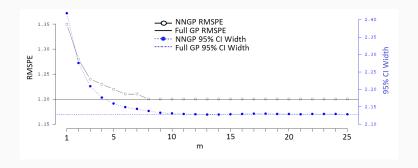
#### Gibbs sampler:

- Conjugate full conditionals for  $\beta$ ,  $\tau^2$ ,  $\sigma^2$  and  $w(s_i)$ 's
- ullet Metropolis step for updating  $\phi$
- Posterior predictive distribution at any location using composition sampling:

$$\int N(y(s) | x(s)'\beta + w(s), \tau^2 I) \times N(w(s) | a(s)'w_R, d(s)) \times$$

$$p(w, \beta, \tau^2, \sigma^2, \phi | y) d(w, \beta, \tau^2, \sigma^2, \phi)$$

## **Choosing** m



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

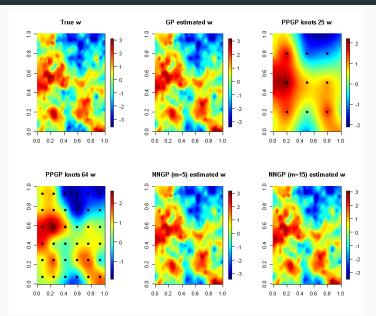
### Storage and computation

- 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

### spNNGP package in R

- Implements the MCMC for spatial regression model using NNGP
- Full posterior distributions of all parameters available (similar to spBayes)
- Suitable for parallel computing
- Implements NNGP variants like the response model and the MCMC-free conjugate model
- Very suitable for analyzing very large spatial datasets (upto millions of locations)

### **Predicted surfaces of** *w*



### Reducing parameter dimensionality

- The Gibbs sampler algorithm for the NNGP updates  $w(s_1), w(s_2), \dots, w(s_n)$  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
- Solution: Back to the marginalized model?

### Collapsed NNGP

• Same model:

$$y(s) = x(s)'\beta + w(s) + \epsilon(s)$$
  
 $w(s) \sim NNGP(0, C(\cdot, \cdot | \theta))$   
 $\epsilon(s) \stackrel{\text{iid}}{\sim} N(0, \tau^2)$ 

- Vector form  $y \sim N(X\beta + w, \tau^2 I)$ ;  $w \sim N(0, \tilde{C}(\theta))$
- Collapsed model: Marginalizing out w, we have  $y \sim N(X\beta, \tau^2 I + \tilde{C}(\theta))$

### Collapsed NNGP

#### Model

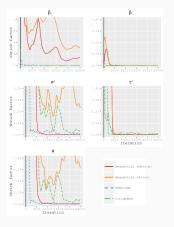
$$y \sim N(X\beta, \tau^2 I + \tilde{C}(\theta))$$

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

### Response NNGP

- $w(s) \sim GP(0, C(\cdot, \cdot | \theta)) \Rightarrow y(s) \sim GP(x(s)'\beta, \Sigma(\cdot, \cdot | \tau^2, \theta))$
- $\Sigma(s_i, s_j) = C(s_i, s_j | \theta) + \tau^2 \delta(s_i = s_j)$  ( $\delta$  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:  $y \sim N(X\beta, \tilde{\Sigma})$
- Storage and computations are guaranteed to be O(n)
- Low dimensional MCMC ⇒ Improved convergence
- Cannot coherently recover  $w \mid y$

## MCMC convergence



**Figure:** MCMC convergence diagnostics using Gelman-Rubin shrink factor for different NNGP models <sup>2</sup> for a simulated dataset

<sup>&</sup>lt;sup>2</sup>Finley et al. (2019): https://www.tandfonline.com/doi/abs/10.1080/10618600.2018.1537924?journalCode=ucgs20

- Original full GP model:  $y(s) \stackrel{ind}{\sim} N(x(s)'\beta + w(s), \tau^2)$
- $w(s) \sim \mathit{GP}$  with a stationary covariance function  $C(\cdot, \cdot \mid \sigma^2, \phi)$
- $Cov(w) = \sigma^2 R(\phi)$
- Full GP model:  $y \sim N(X\beta, \Sigma)$  where  $\Sigma = \sigma^2 M$
- $M = R(\phi) + \alpha I$
- $\alpha = \tau^2/\sigma^2$  is the ratio of the noise to signal variance
- Response NNGP model:  $y \sim N(X\beta, \tilde{\Sigma})$
- ullet  $ilde{\Sigma}=\sigma^2 ilde{M}$  where  $ilde{M}$  is the NNGP approximation for M

- $y \sim N(X\beta, \sigma^2 \tilde{M})$
- If  $\phi$  and  $\alpha$  are known, M, and hence  $\tilde{M}$ , are known matrices
- The model becomes a standard Bayesian linear model
- Assume a *Normal Inverse Gamma (NIG)* prior for  $(\beta, \sigma^2)'$
- $(\beta, \sigma^2)' \sim NIG(\mu_{\beta}, V_{\beta}, a_{\sigma}, b_{\sigma})$ , i.e.,  $\beta \mid \sigma^2 \sim N(\mu_{\beta}, \sigma^2 V_{\beta})$  and  $\sigma^2 \sim IG(a_{\sigma}, b_{\sigma})$

•  $y \sim N(X\beta, \sigma^2 \tilde{M})$ ,  $\tilde{M}$  is known

#### Joint likelihood:

$$N(y \mid X\beta, \sigma^2 \tilde{M}) \times N(\beta \mid \mu_{\beta}, \sigma^2 V_{\beta}) \times IG(\sigma^2 \mid a_{\sigma}, b_{\sigma})$$

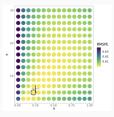
•  $y \sim N(X\beta, \sigma^2 \tilde{M})$ ,  $\tilde{M}$  is known

#### Joint likelihood:

$$N(y \mid X\beta, \sigma^2 \tilde{M}) \times N(\beta \mid \mu_{\beta}, \sigma^2 V_{\beta}) \times IG(\sigma^2 \mid a_{\sigma}, b_{\sigma})$$

- Conjugate posterior distribution  $(\beta, \sigma^2) | y \sim NIG(\mu_\beta^*, V_\beta^*, a_\sigma^*, b_\sigma^*)$
- $\mu_{\beta}^*$ ,  $V_{\beta}^*$ ,  $a_{\sigma}^*$  and  $b_{\sigma}^*$  can be calculated in O(n) time
- Exact posterior distributions, means, and variances of  $\beta$  and  $\sigma^2$  are available in closed form
- $y(s) | y \sim t_{2a^*_{\sigma}}(m(s), \frac{b^*_{\sigma}}{a^*_{\sigma}}v(s))$ , i.e., follows a *t*-distribution
- ullet Exact posterior predictive distributions of  $y(s) \mid y$  for any s
- No MCMC required for parameter estimation or prediction

# Choosing $\alpha$ and $\phi$



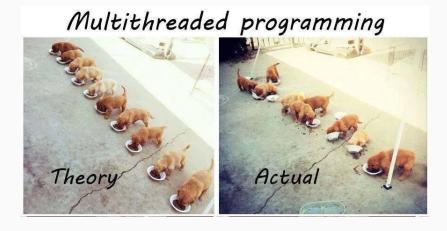
**Figure:** Simulation experiment in Finley et al,  $2020^3$ : True value (+) of  $(\alpha, \phi)$  and estimated value (  $\circ$ ) using 5-fold cross validation

- $\phi$  and  $\alpha$  are chosen using K-fold cross validation over a grid of possible values
- Unlike MCMC, cross-validation can be completely parallelized
- $\bullet$  Resolution of the grid for  $\phi$  and  $\alpha$  can be decided based on computing resources available
- In practice, a reasonably coarse grid often suffices https://arxiv.org/pdf/2001.09111.pdf

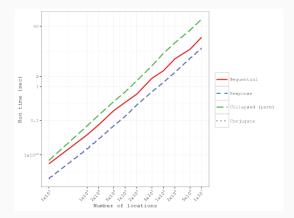
#### **Scalability**

- Computation and storage requirements are O(n)
- One evaluation time similar to the response NNGP model
- Unlike response NNGP, does not involve any serial MCMC iterations
- For K fold cross validation and G combinations of  $\phi$  and  $\alpha$ , total number of evaluations is KG
- Embarassingly parallel: Each of the KG evaluations can proceed in parallel

# Statutory figure on embarrassingly parallel computing



# Comparison of run times



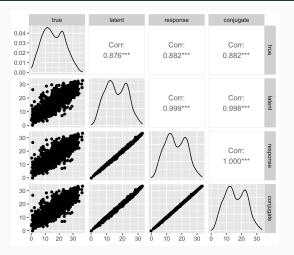
**Figure:** Run times of different NNGP models with increasing sample size for a simulated dataset<sup>4</sup>

<sup>&</sup>lt;sup>4</sup>Finley et al. (2019): https://www.tandfonline.com/doi/abs/10.1080/10618600.2018.1537924?journalCode=ucgs20

# Comparison of Bayesian NNGP models

	Sequential	Collapsed	Response	Conjugate
O(n) time	Yes	No	Yes	Yes
Recovery of w   y	Yes	Yes	No	No
MCMC dimensionality	High	Low	Low	MCMC-free
Fully Bayesian inference	Yes	Yes	Yes	No
Embarassingly parallel	No	No	No	Yes

### Comparing predictions of different NNGP models



**Figure:** Comparing hold-out predictions from of forest canopy height different NNGP models using the Bonanza Creek Experimental Forest dataset of spNNGP package

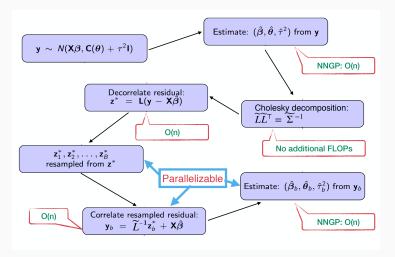
# The BRISC package<sup>6</sup>

- Uses maximum-likelihood based estimation from the response NNGP model
- BRISC\_estimation for parameter estimation
- BRISC\_prediction for spatial predictions using NNGP
- BRISC\_bootstrap NNGP-based Bootstrap for Rapid Inference on Spatial Covariances (Saha and Datta, 2018)<sup>5</sup> to obtain parameter confidence intervals
- New feature: BRISC\_simulation for fast approximate simulation of large scale Gaussian Process realizations

<sup>&</sup>lt;sup>5</sup>https://onlinelibrary.wiley.com/doi/abs/10.1002/sta4.184

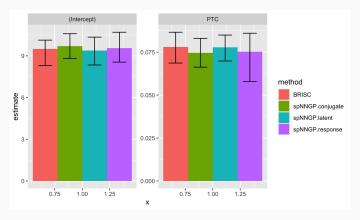
<sup>6</sup>https://cran.r-project.org/web/packages/BRISC/BRISC.pdf

#### **BRISC:** Fast NNGP-based spatial bootstrap



**Figure:** BRISC algorithm for bootstrapping of all parameters in the spatial linear model. This is implemented in the BRISC\_bootstrap function of the BRISC package.

### Comparing inference from different NNGP models

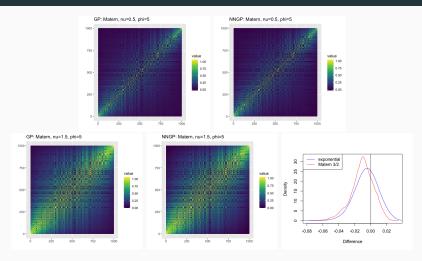


**Figure:** Comparing estimates of the intercept and the slope on Percent tree cover (PTC) for forest canopy height (FCH) in the Bonanza Creek Experimental Forest dataset using different NNGP models

# Fast simulation of large Gaussian Process datasets

- Input: n locations  $s_1, \ldots, s_n$  and a GP covariance matrix  $\Sigma$  on these locations
- Generating  $y_{sim} \sim N(0, \Sigma)$  requires to store  $\Sigma$  and calculate its Cholesky factor  $(O(n^2)$  storage and  $O(n^3)$  FLOPs)
- $\bullet$  The NNGP covariance matrix  $\widetilde{\Sigma} \approx \Sigma$
- ullet BRISC\_simulation generates  $y_{sim} \sim \mathcal{N}(0,\widetilde{\Sigma})$ 
  - Generate z ∼ N(0, I)
  - Generate sparse Cholesky factor  $L = D^{-1/2}(I A)$  of  $\widetilde{\Sigma}^{-1}$
  - Solve sparse triangular system:  $Ly_{sim} = z$  to obtain  $y_{sim} \sim N(0, \widetilde{\Sigma})$
  - O(n) storage and FLOPs
- Fast approximate large-scale simulation of GP realizations

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**Figure:** Simulation of Gaussian random fields using full GP and NNGP. The last figure plots the density of the difference between the sample covariance matrices generated from full GP and NNGP.

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Covariance function	Sample size	NNGP	full GP
exponential	1000	3	12
	2500	6	83
	5000	11	464
	10000	31	NA
	100000	831	NA
Matérn <sub>3/2</sub>	1000	4	11
	2500	8	81
	5000	18	459
	10000	48	NA
	100000	698	NA

**Table:** Computation times (in seconds) for simulating 10000 random draws from a full GP and NNGP.

<sup>&</sup>lt;sup>7</sup>https://arxiv.org/pdf/2102.13299.pdf

## Summary of Nearest Neighbor Gaussian Processes

- Sparsity inducing Gaussian process constructed from sparse Cholesky factors based on m nearest neighbors
- Scalability: 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
- Collapsed and response NNGP models with improved MCMC convergence
- spNNGP package in R for analyzing large spatial data using NNGP models
- Applications in spatial bootstrap, simulation of large Gaussian fields using the BRISC package