Scalable Gaussian Processes on Physically Constrained Domains

Spatial Modelling with Intrinsic Geometry

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Constrained Domains

- Groundwater

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Constrained Domains

- Groundwater
- Neighborhood/wildlife disconnected by barriers

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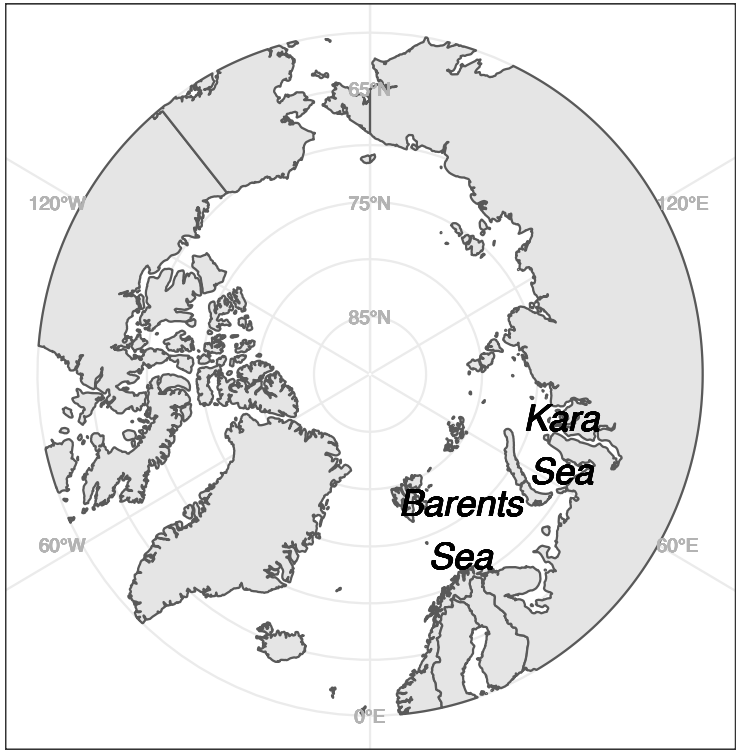
Constrained Domains



- Groundwater
- Neighborhood/wildlife disconnected by barriers
- Coastlines

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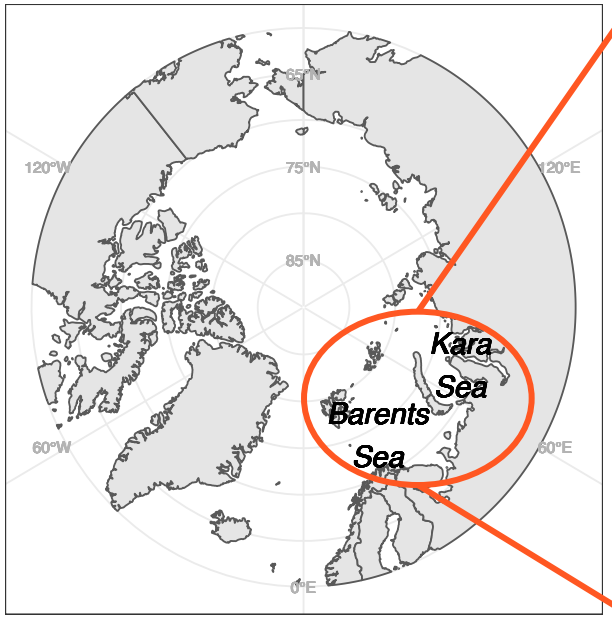
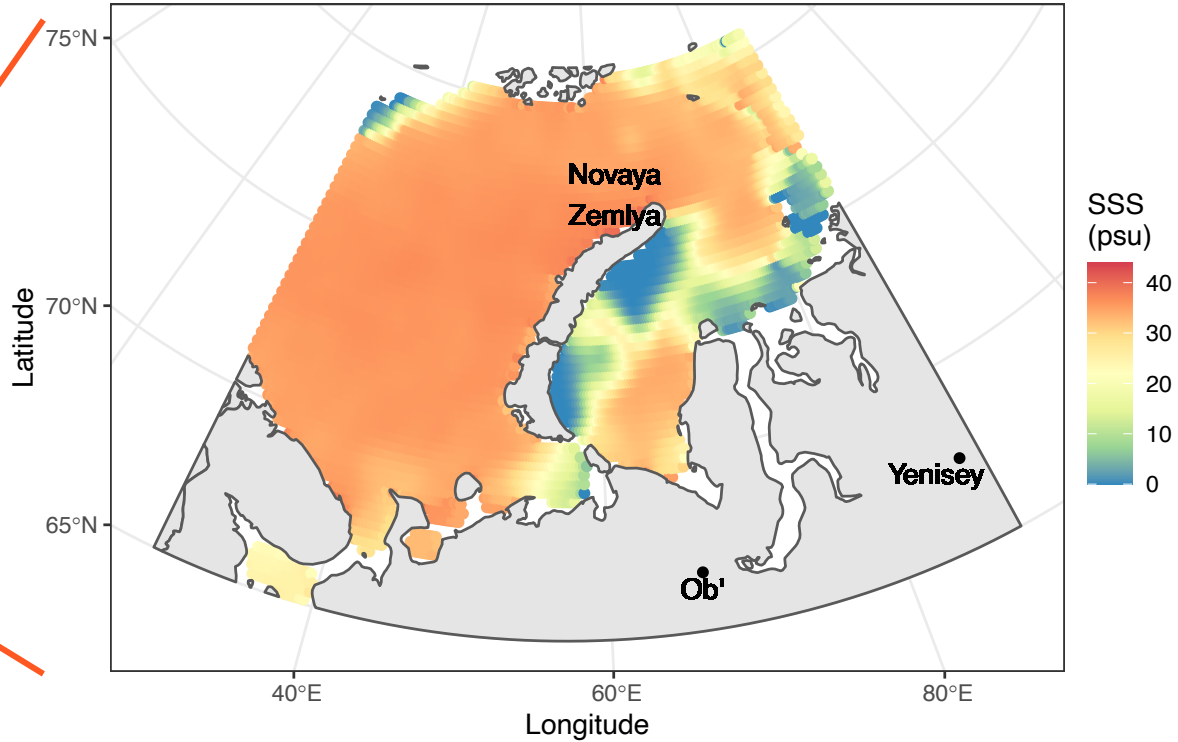
Constrained Domains



Sea Surface Salinity (SSS) over July 20 – July 31, 2017



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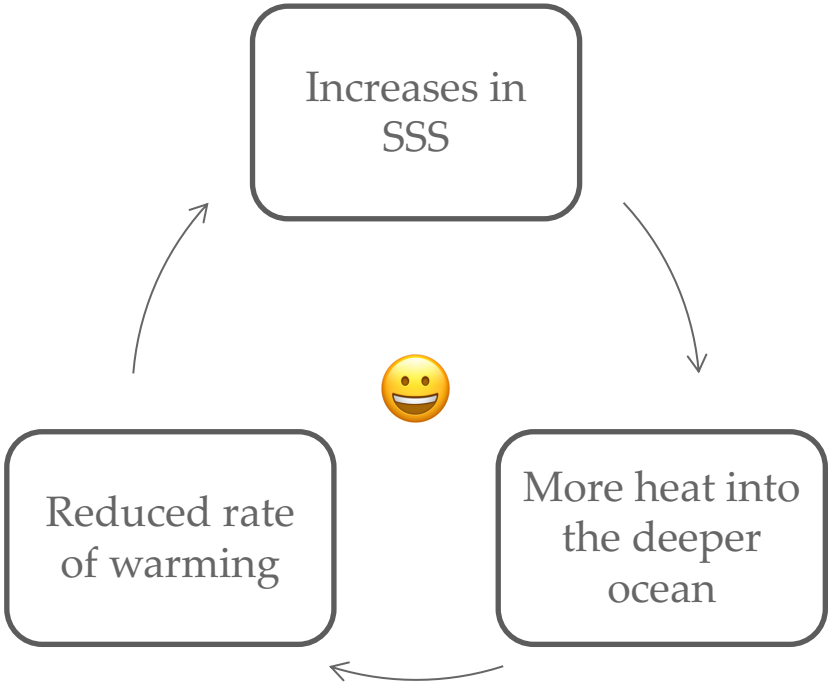
Background

- SSS helps understand changes in the Arctic.



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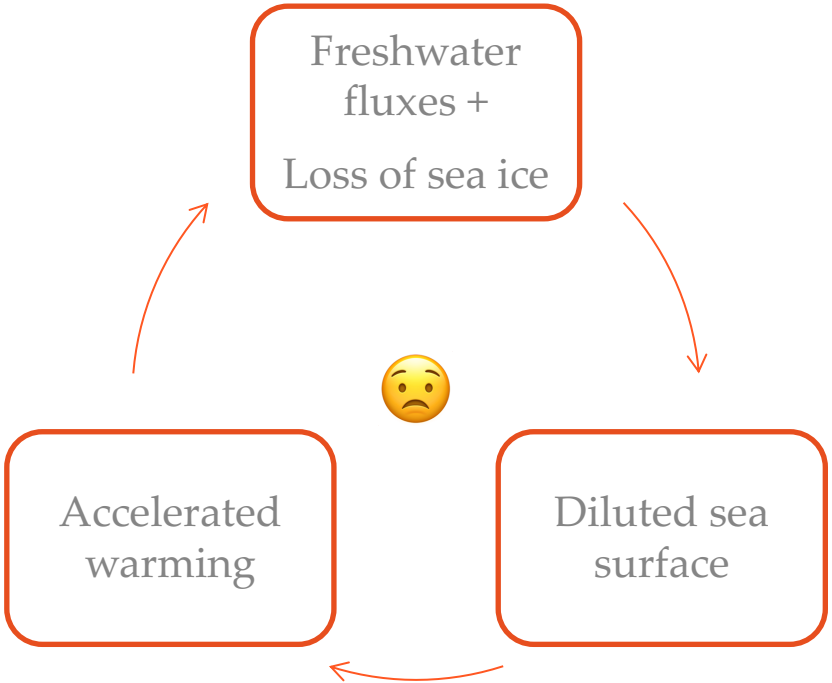
Background

- SSS helps understand changes in the Arctic.
- Kara Sea is one of the regions with a vulnerable feedback loop.
- Accurate prediction of SSS given unique domains is important to take actions before such regions fall into a vicious cycle of warming.



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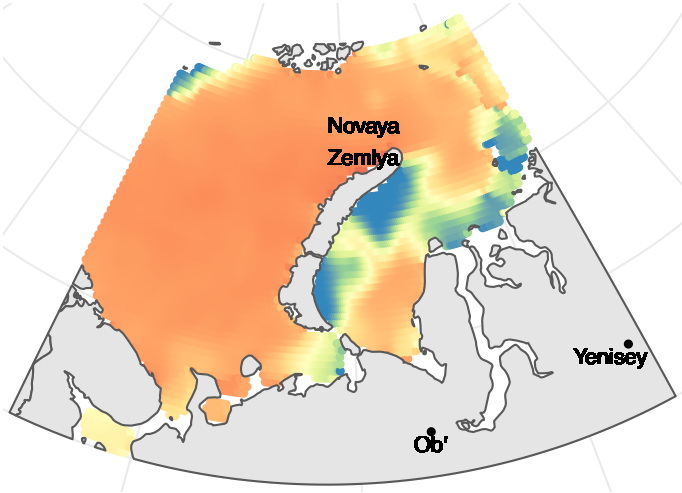
Background

Traditional spatial GP models

- Ignore the unique geometry of the domain.
  - Inappropriate smoothing over physical barriers
  - Likely produce sub-optimal results



- Have high computational cost $\mathcal{O}(n^3)$.
  - Prohibitive already if $n > 50{,}000$.
  - Recent & active development of scalable GP models whose computational cost grows linearly with n
    e.g., Vecchia (1988); Nearest Neighbor GP (NNGP) – Datta et al. (2016)

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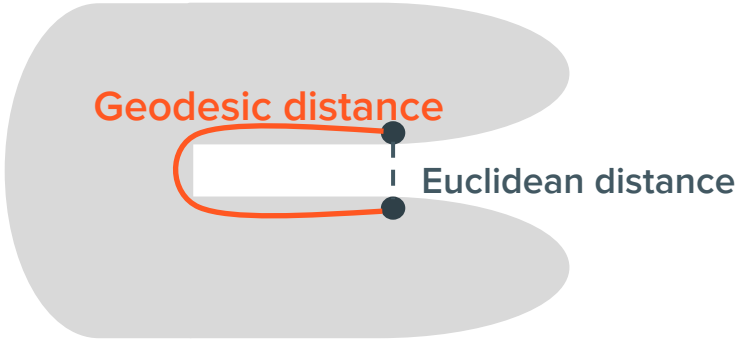
Literature

- Spline regression with partial differential equation (PDE) regularizations: Ramsay (2002); Wood et al. (2008); Sangalli et al. (2013)
- Based on stochastic PDEs (SPDEs): Bakka et al. (2019)
- Heat kernel-based GP approximations: Niu et al. (2019); Dunson et al. (2021)
- Geodesic distance in a covariance function of a scalable GP: Dai et al. (2021)



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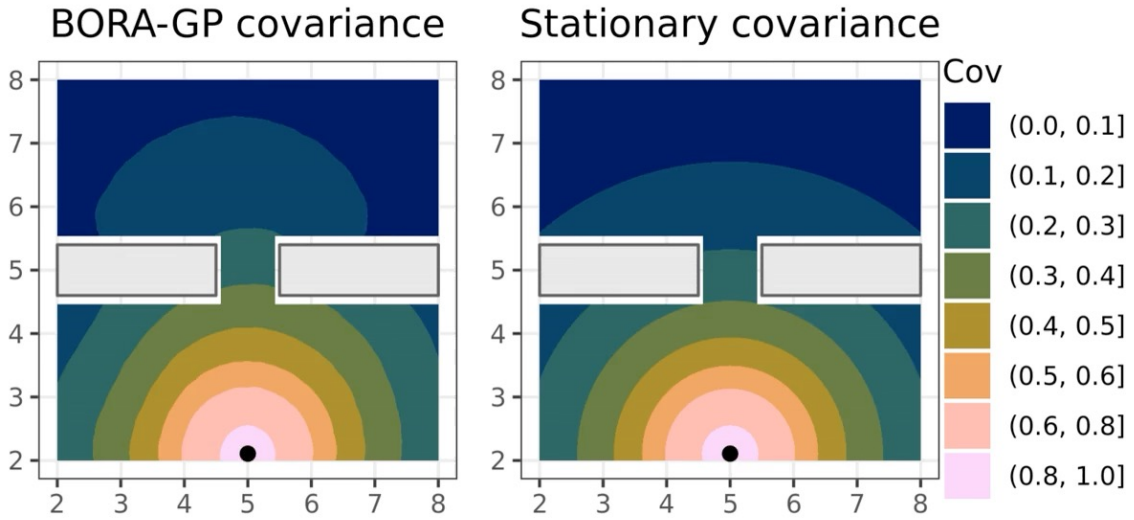
Goals

- Aim to construct a new **scalable** **nonstationary** GP that incorporates **constrained domains**.
  - Physically sensible kriging
  - Physically sensible covariance behaviors



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Existing Scalable Methods

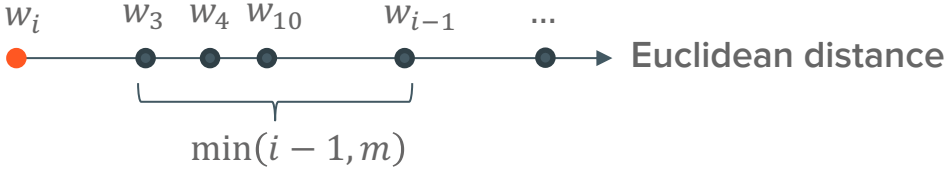
- Bayesian hierarchical spatial regression

$$y = X\beta + w + \epsilon,\ \epsilon \sim N(0, \tau^2 I_n),\quad w(s) \sim GP\big(0, C(\cdot,\cdot\,|\theta)\big)$$

  - Vecchia (1988) cheaply approximates the likelihood.

$$p(w_1, \cdots, w_n) = \prod_{i=1}^{n} p(w_i | w_1, \cdots, w_{i-1}) \approx \prod_{i=1}^{n} p(w_i | w_{im})$$

    - Nearest neighbors w_{im}:



    - $w_{im} = \{w_1, w_2, w_3, \cdots, w_{i-2}, w_{i-1}\}$ ➡ Sparse precision matrix ➡ Scalability

  - NNGP (Datta et al. 2016) extends it to a process based on directed acyclic graphs (DAG).

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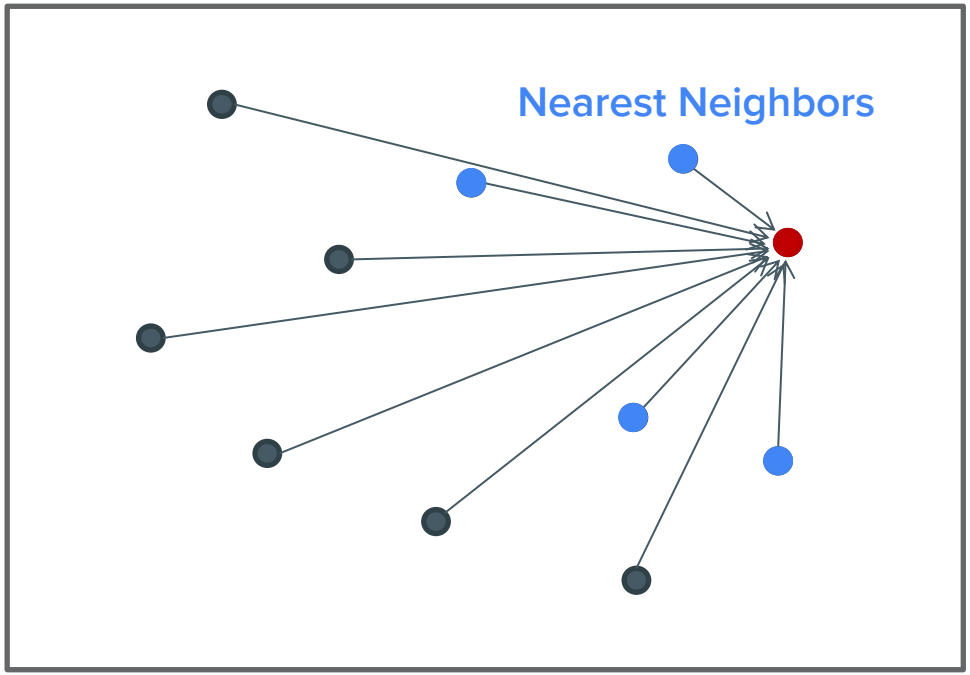
Existing Scalable Methods

- Visualization of sparsity using DAGs

$m = 4$



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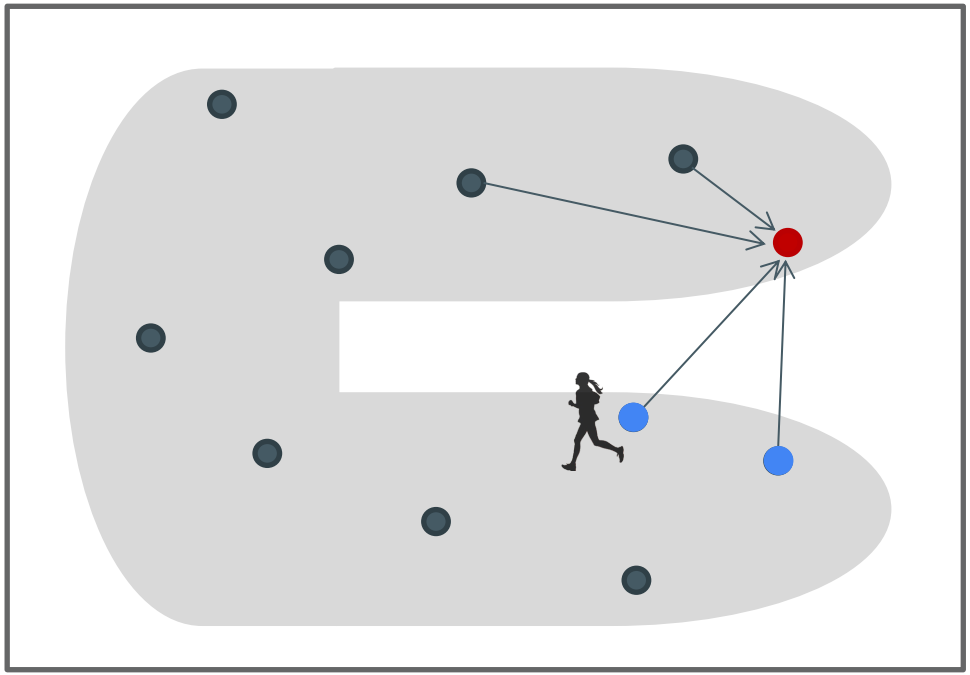
Existing Scalable Methods

- What if we know that our measurements lie in a constrained domain?

$m = 4$



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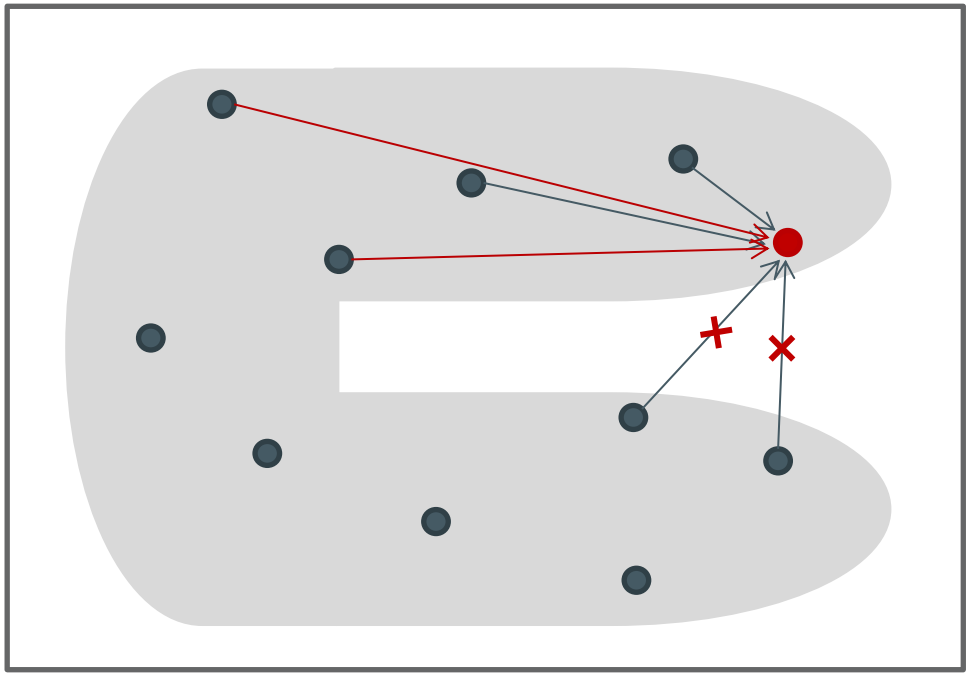
Our Proposal

- **B**arrier **O**verlap-**R**emoval **A**cyclic directed graph **G**aussian **P**rocess (BORA-GP*)

$m = 4$



*Credit: Michele Peruzzi

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Our Proposal

1. Specify a multivariate normal distribution over a fixed finite set $R = \{r_1, \cdots, r_k\} \subset \mathcal{D}$

$$w_R = \big(w(r_1), \cdots, w(r_k)\big)^T \sim N\big(0, \tilde{C}_R\big) = \prod_{i=1}^{k} N(w(r_i); M_{r_i} w_{[r_i]}, V_{r_i})$$

- $M_{r_i} = C_{r_i,[r_i]} C_{[r_i]}^{-1}$, $V_{r_i} = C_{r_i} - C_{r_i,[r_i]} C_{[r_i]}^{-1} C_{[r_i],r_i}$
- C: base covariance function
- $[r_i]$: set of spatial locations in R whose straight line to r_i does not overlap barriers (physically sensible neighbors of r_i of size $\min(i-1, m)$)

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Our Proposal

2. Extend it to the whole domain $\mathcal{D}$

$$\forall u \in \mathcal{D} \setminus R,\ w(u)|w_R \sim N(M_u w_{[u]}, V_u)$$

- $[u] \subset R$ physically sensible neighbors of size m

➡ 1 & 2 define a valid scalable process

$$w(s) \sim \text{BORA–GP}(0, \tilde{C}(\cdot,\cdot\,|\theta))$$

- $\tilde{C}$ is nonstationary: covariance between any two locations depends on R through their neighbor sets.

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Neighbor Search Algorithm

Algorithm 1: Neighbor search for reference locations

Input: The number of neighbors m, the reference locations $\mathcal{R} = \{\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k\}$, and barriers $\mathcal{B}$

Output: Neighbor set $[\boldsymbol{r}_i] \subset \mathcal{R}$ of size $\min(m, i-1)$, $\forall \boldsymbol{r}_i \in \mathcal{R}$

Note: The reference locations are arranged in some ordering.

/* First-order neighbors */

for $i = 1, \ldots, m+1$ **do**
  $[\boldsymbol{r}_i] = \{\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{i-1}\}^*$
for $i = m+2, \ldots, k$ **do**
  Sort† $\{\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{i-1}\}$ by Euclidean distance to $\boldsymbol{r}_i$, enumerated by $\{\boldsymbol{r}_{\pi_1}, \ldots, \boldsymbol{r}_{\pi_{i-1}}\}$
  for $j = 1, \ldots, i-1$ **do**
    if $\overrightarrow{\boldsymbol{r}_{\pi_j}\boldsymbol{r}_i}$ does not intersect with $\mathcal{B}$ **then**
      $\boldsymbol{r}_{\pi_j} \in [\boldsymbol{r}_i]$
    if $\#([\boldsymbol{r}_i])^\ddagger = m$ **then**
      break

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Neighbor Search Algorithm

```
   /* Second-order neighbors                                          */
10 for i such that 0 < #([r_i]) = m_1 < m  do
11     Sort [r_i]_2 := [[r_i]]^§ \[r_i] by sum of Euclidean distances¶
12     if #([r_i]_2) ≥ m − m_1 then
13         Include the first m − m_1 elements of [r_i]_2 in [r_i]
14     else
15         Include all elements of [r_i]_2 in [r_i] and repeat from step 10 as necessary.
```

Neighbor Search Algorithm

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Neighbor Search Algorithm

1 **for** i such that $[\boldsymbol{r}_i] = \emptyset$ **do**
2 Sort m nearest grid points by Euclidean distance to $\boldsymbol{r}_i$, enumerated by $\{\boldsymbol{l}_{i1}, \ldots, \boldsymbol{l}_{im}\}$
3 **for** $t = 1, \ldots, m$ **do**
4 **if** $\overrightarrow{\boldsymbol{l}_{it}\boldsymbol{r}_i}$ does not intersect with $\mathcal{B}$ **then**
5 **for** $j = 1, \ldots, i-1$ **do**
6 **if** $\overrightarrow{\boldsymbol{r}_{\pi_j}\boldsymbol{l}_{it}}$ does not intersect with $\mathcal{B}$ **then**
7 $\boldsymbol{r}_{\pi_j} \in [\boldsymbol{r}_i]$
8 **if** $\#([\boldsymbol{r}_i]) > 0$ **then**
9 **break**

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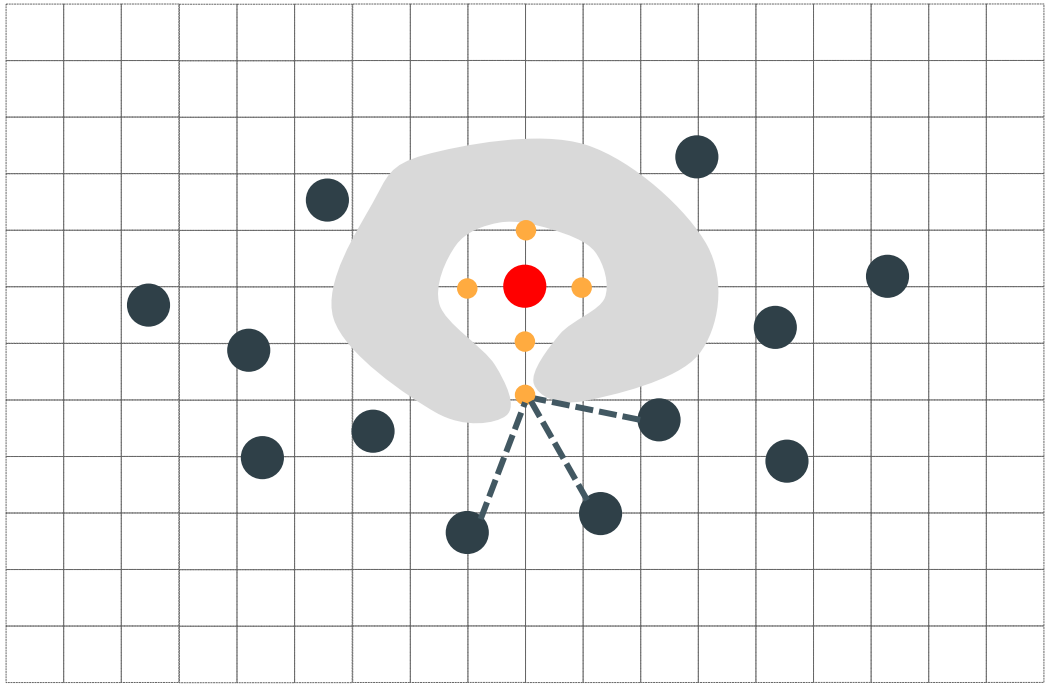
Neighbor Search Algorithm



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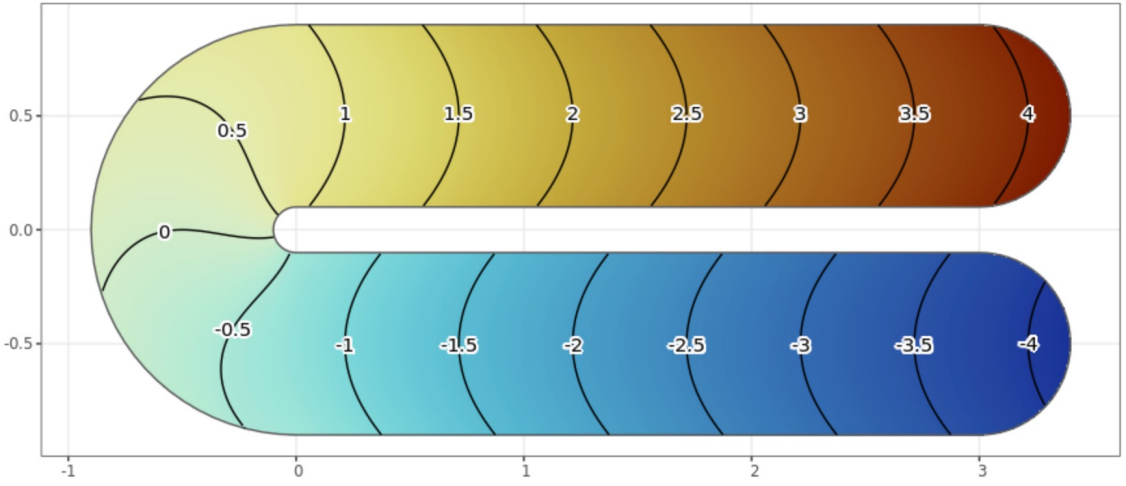
BORA-GP vs. NNGP

- BORA-GP proposes a new set of neighbors *conforming to barriers* in the NNGP framework.
- BORA-GP reduces to NNGP if no barriers.
- BORA-GP can enjoy nice properties of NNGP
  - ✓ Scalability
  - ✓ Nonstationarity
  - ✓ Standalone process
  - ✓ Versatility with any covariance functions
  - ✓ Straightforward extensions to multivariate, non-Gaussian data, etc.
- End-goal for BORA-GP vs. side product for NNGP

Modified Horseshoe

- $y(s) = w(s) + \epsilon(s),\ \epsilon(s) \sim N(0, \tau^2),\ \tau = 0.1$
- $w(s)$ generated as suggested in Wood et al. (2008)
- Compare BORA-GP with NNGP and Barrier SGF (Bakka et al. 2019)
- 30 replicates for each combination of n = 300, 600, 1000 and m = 10, 15, 20



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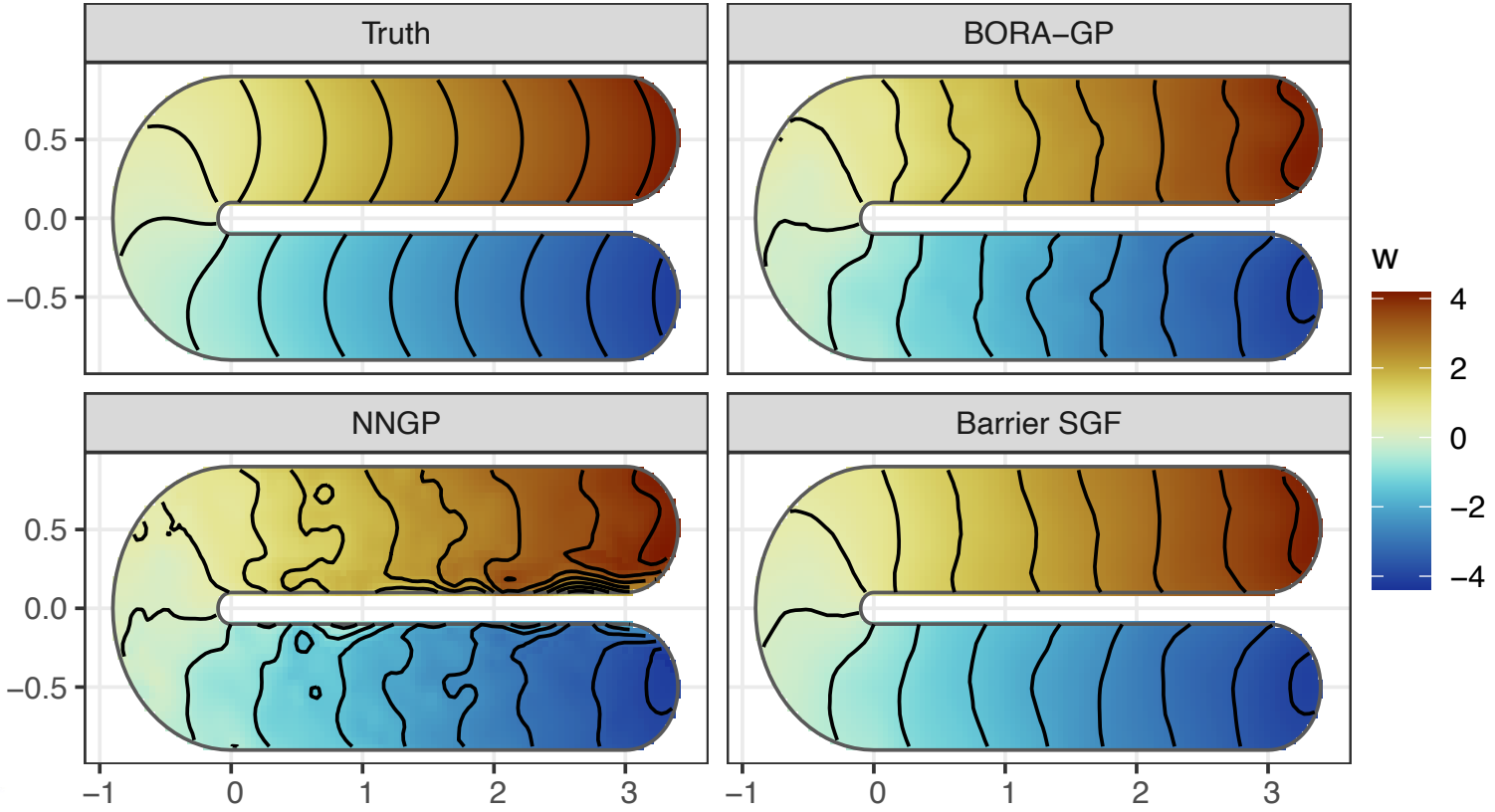
Modified Horseshoe



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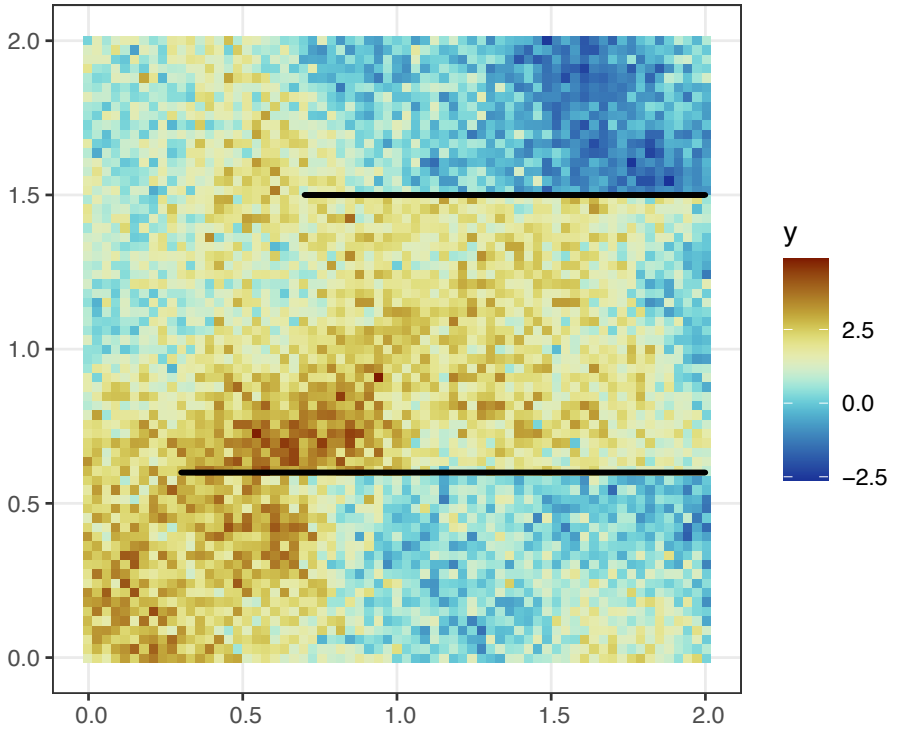
Domain with Faults

- $y(s) = \beta_0 + x(s)\beta_1 + w(s) + \epsilon(s)$, $\epsilon(s) \sim N(0, 0.1^2)$
- $\beta_0 = 1,\ \beta_1 = 0.5,\ x(s) \sim N(0,1)$
- $w(s)$ generated by BORA-GP
  - $m = 15$
  - Matérn base covariance function with $\sigma^2 = 1,\ \nu = 1.5,\ \phi = 4$
- 4,489 locations in a domain with two faults
- One example out of 30 replicates



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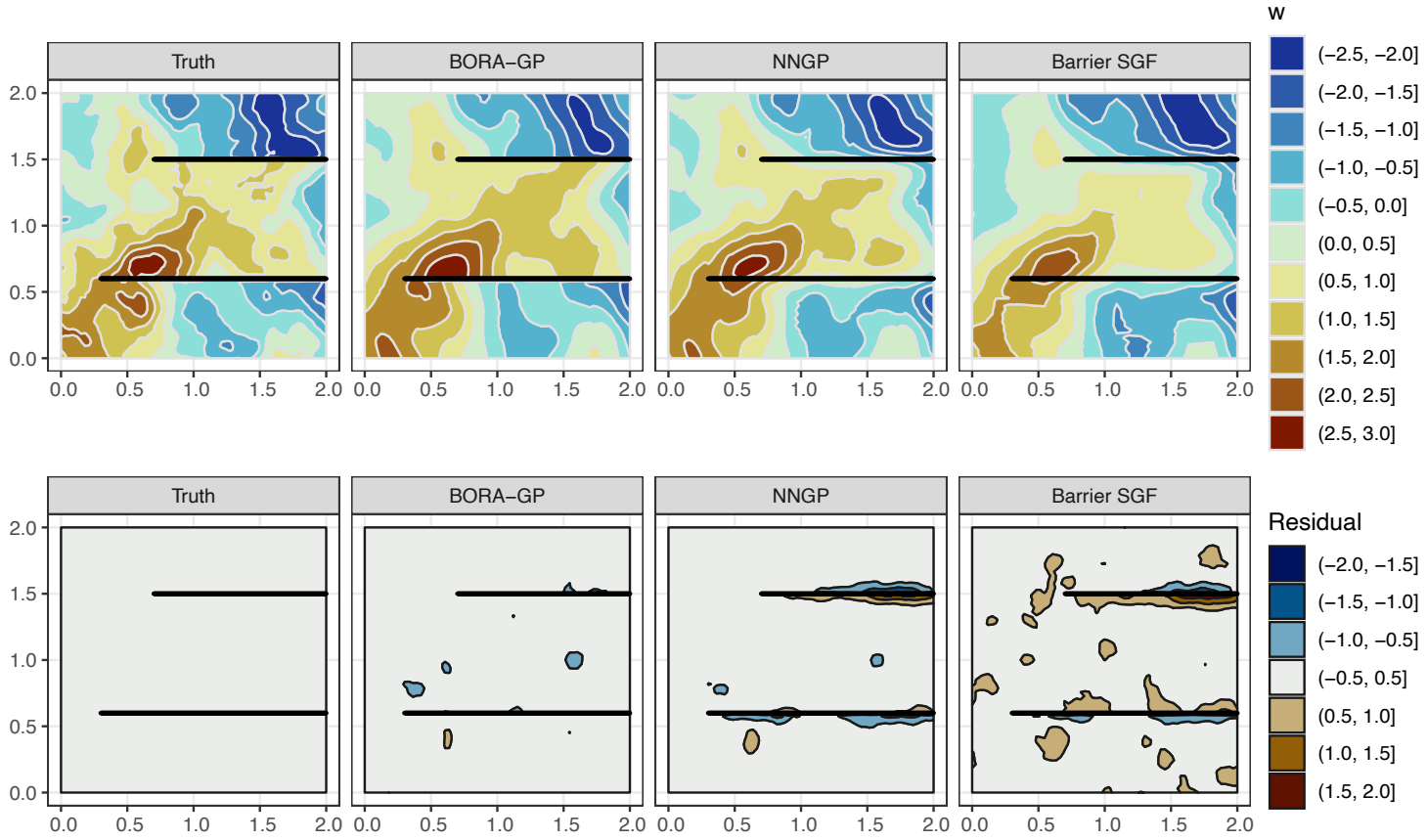
Domain with Faults



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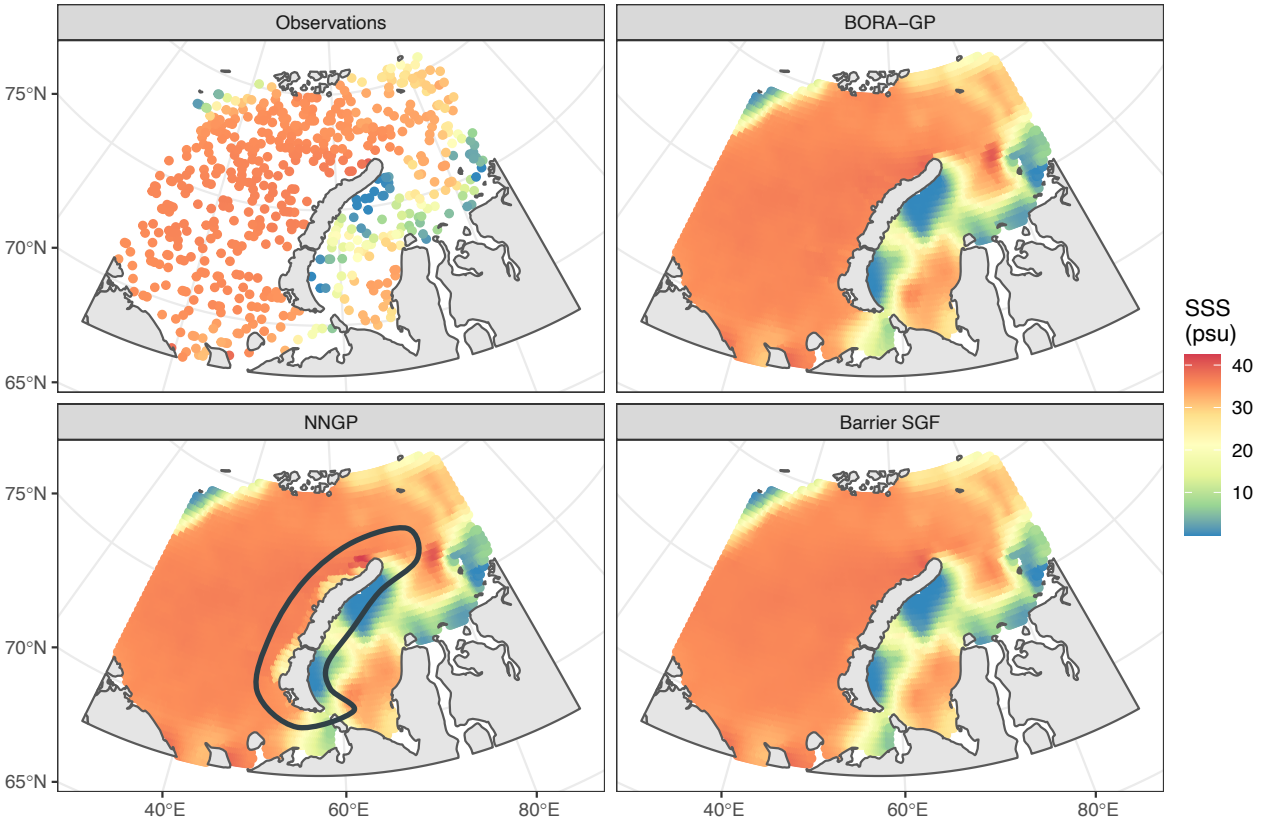
Analysis

- Bayesian spatial regression

$$y(s) = \beta_0 + w(s) + \epsilon(s),\ \ \epsilon(s) \sim N(0, \tau^2),$$
$$w(s) \sim \text{BORA-GP}(0, \tilde{C}(\cdot,\cdot\,|\theta))$$

- $y(s)$: sqrt of SSS in late July of 2017
- Data from Soil Moisture Active Passive (SMAP) V5.0 at a 60km spatial resolution
- Number of obs n = 589 out of 8,418 measurements
- 10,315 new spatial locations to predict (7,829 labeled + 2,486 unlabeled)
- Matérn covariance function with $\nu = 1$ as a base C
- For BORA-GP & NNGP, m = 15

Analysis



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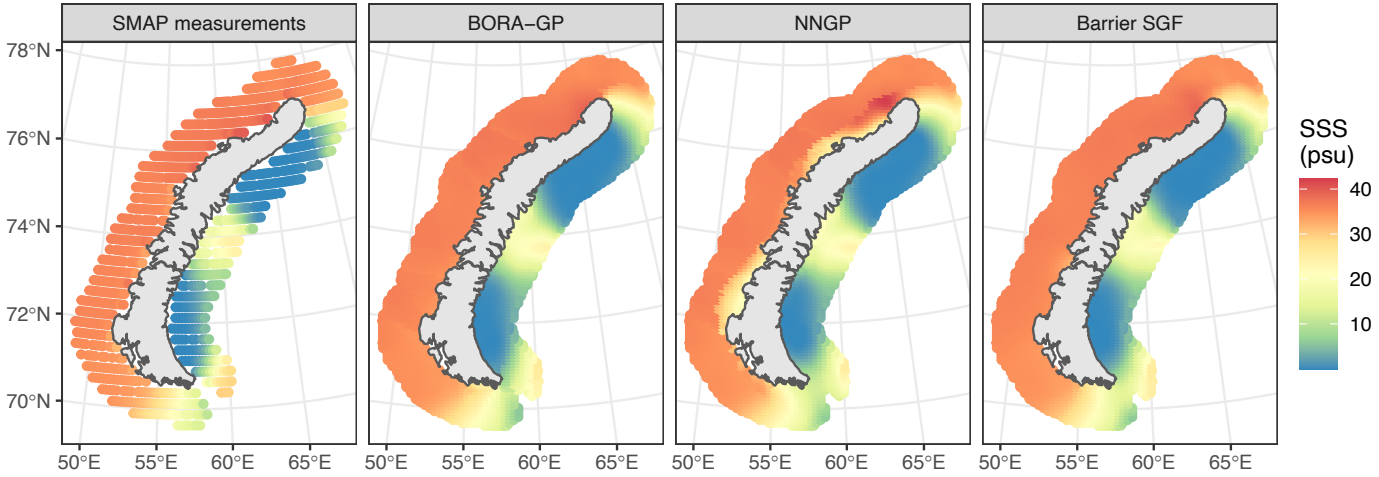
Analysis



	BORA-GP	NNGP	Barrier SGF
RMSPE	**0.325**	0.412	0.332
MAPE	**0.147**	0.218	0.159
95% CI coverage	**0.950**	0.911	0.875
Mean 95% CI width	1.140	1.196	**0.876**

>48%

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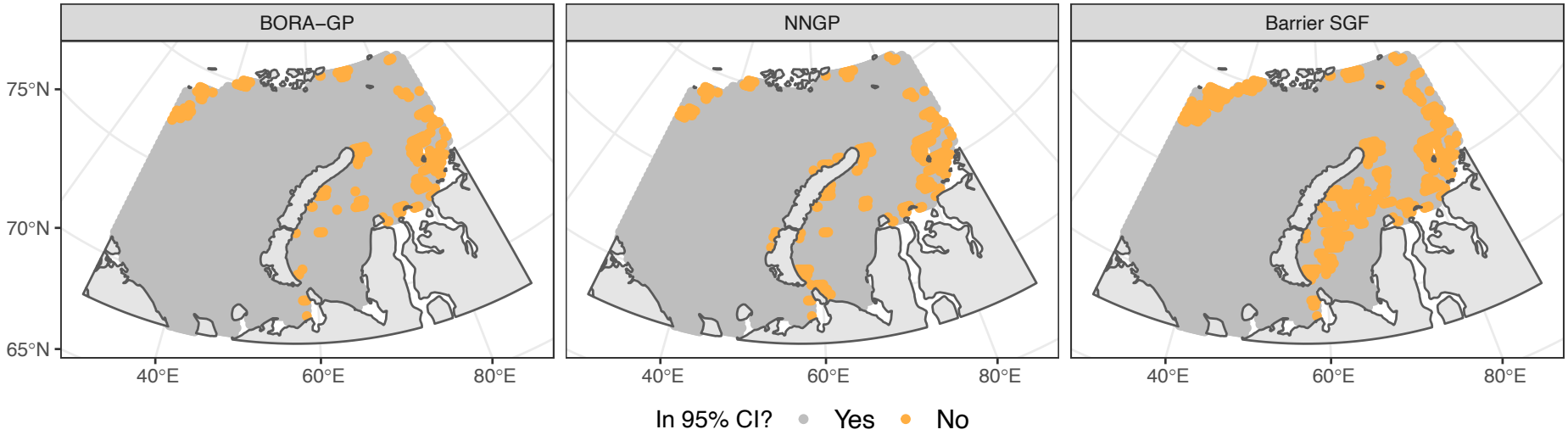
Analysis



- Low salinity is a key to understand various ocean processes!
  - Strong stratification: less circulation of nutrients → limited productivity of phytoplankton
  - Acidification: negative impacts on marine species, marine food-webs, reefs in coastal protection against storms

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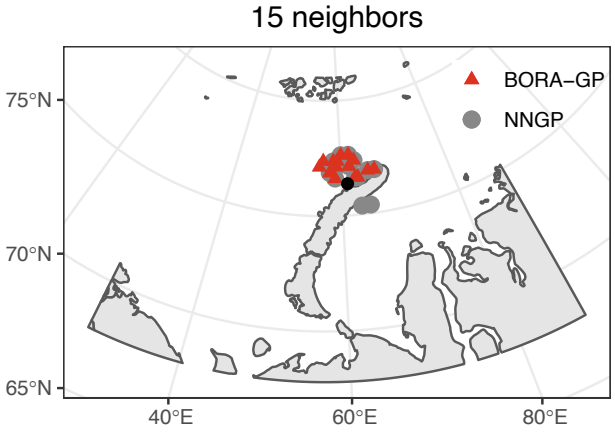
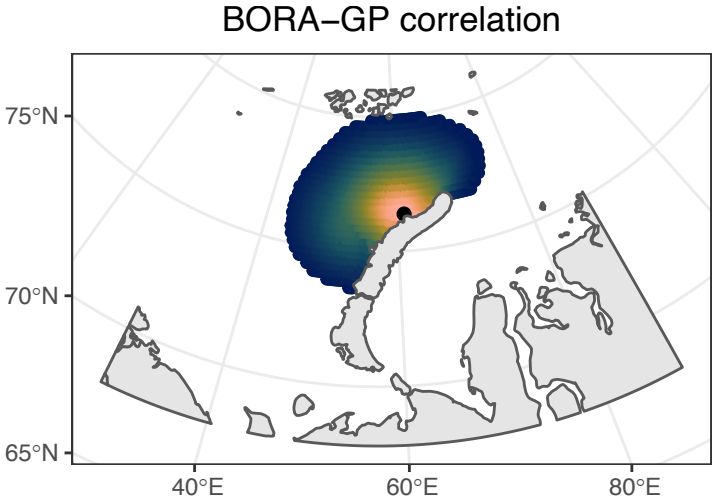
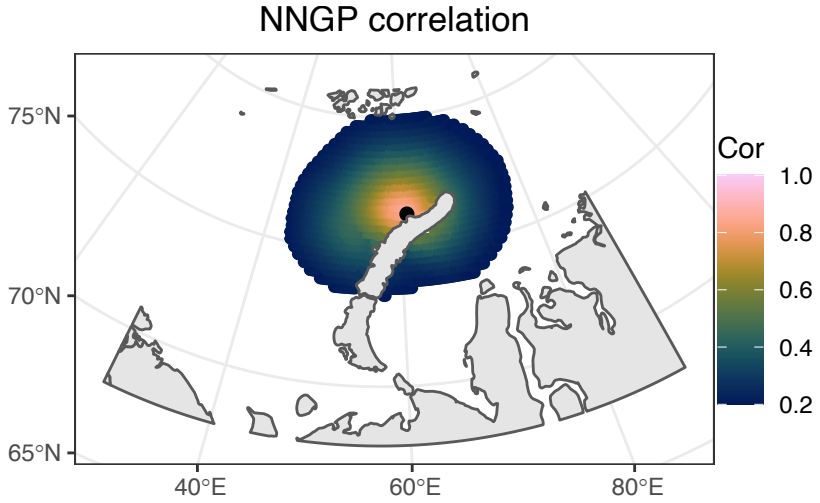
Analysis







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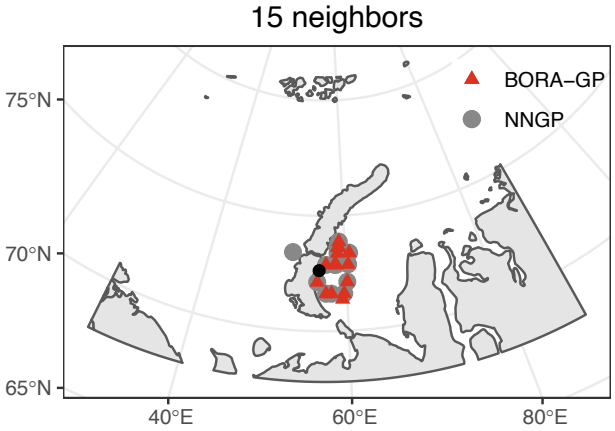
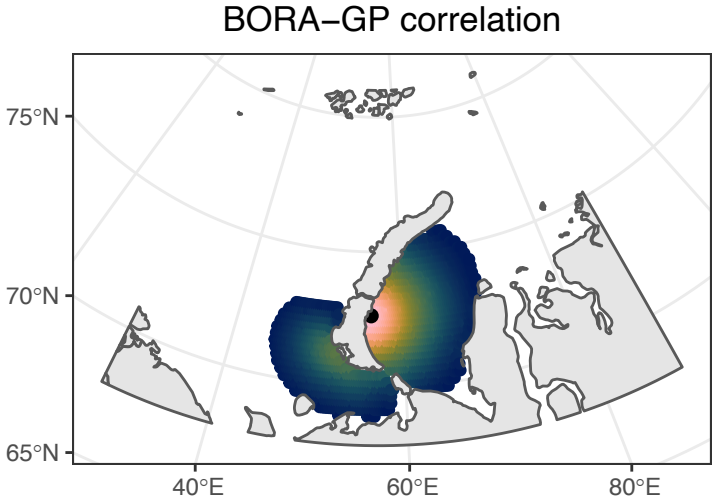
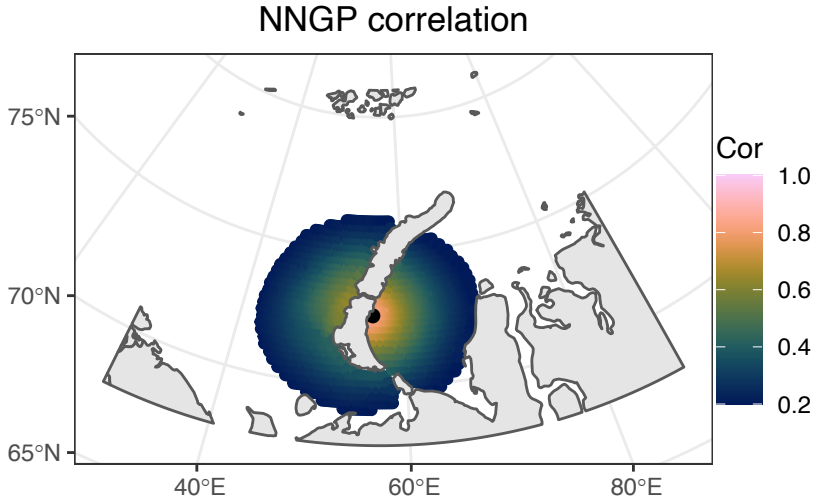
Analysis







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Conclusions & Discussions

- BORA-GP considers geometric features of domains and produces
  - physically sensible neighbors,
  - plausible nonstationary covariance behaviors,
  - physically sensible prediction.
- Users familiar with NNGP can use BORA-GP seamlessly.
- Assume hard barriers (Horseshoe, sliding doors, line barriers, complex coastlines and islands, etc.)
- Extend it to a soft barrier
  - For any location s, each reference location r receives a weight that decreases as either Euclidean distance between s and r increases or a directed edge from r to s overlaps barriers.
  - Locations crossing barriers can still receive a small but positive probability.

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Thank you!

Paper and an R package coming soon

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