# Scalable methods for large spatial data: Low rank predictive processes

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# Multivariate Gaussian likelihoods for geostatistical models

- $\mathscr{S} = \{s_1, s_2, \ldots, s_n\}$ are locations where data is observed
- $y(s_i)$ is outcome at the $i$-th location,
  $y = (y(s_1), y(s_2), \ldots, y(s_n))^\top$
- Model: $y \sim N(X\beta, C_\theta)$
- Estimating process parameters from the likelihood:

$$-\frac{1}{2}\log\det(C_\theta) - \frac{1}{2}(y - X\beta)^\top C_\theta^{-1}(y - X\beta)$$

- $C_\theta$ is usually dense with no exploitable structure
- Bayesian inference: Priors on $\{\beta, \theta\}$
- Need to calculate $\det(C_\theta)$ and quadratic forms of $C_\theta^{-1}$

# Predictions

- Conditional predictive density

$$p(y(s_0) \,|\, y, \theta, \beta) = N\left(y(s_0) \,\middle|\, \mu(s_0), \sigma^2(s_0)\right) \ .$$

- Kriging

$$\mu(s_0) = \mathrm{E}[y(s_0) \,|\, y, \theta] = x^\top(s_0)\beta + c_\theta^\top(s_0) C_\theta^{-1}(y - X\beta) \ ,$$
$$\sigma^2(s_0) = \mathrm{var}[y(s_0) \,|\, y, \theta] = C_\theta(s_0, s_0) - c_\theta^\top(s_0) C_\theta^{-1} c_\theta(s_0) \ .$$

- Again need to evaluate quadratic forms of $C_\theta^{-1}$

# Computational Details

- Cholesky decomposition: Any symmetric matrix $A$ can be factorized as $A = LDL^\top$ where $L$ is lower triangular and $D$ id diagonal
- Both $\det(C_\theta)$ and quadratic forms of $C_\theta^{-1}$ are best obtained via Cholesky decomposition of $C_\theta$

| | |
|---|---|
| Cholesky: | $\texttt{chol}(C_\theta) = LDL^\top$ ; |
| Determinant: | $\det(C_\theta) = \prod_{i=1}^n d_{ii}$ ; |
| Quadratic forms $a' C_\theta^{-1} b$ | $v = \texttt{trsolve}(L, a)$ ;<br>$C_\theta^{-1} a = u = \texttt{trsolve}(L^\top, D^{-1} v)$ ;<br>$a' C_\theta^{-1} b = u^\top b$ ; |

- Primary bottleneck is chol$(\cdot)$ requiring $O(n^2)$ storage and $O(n^3)$ memory
- Not feasible for large $n$

# Burgeoning literature on spatial big data

- Low-rank models (Wahba, 1990; Higdon, 2002; Kamman & Wand, 2003; Paciorek, 2007; Rasmussen & Williams, 2006; Stein 2007, 2008; Cressie & Johannesson, 2008; Banerjee et al., 2008; 2010; Gramacy & Lee 2008; Sang et al., 2011, 2012; Lemos et al., 2011; Guhaniyogi et al., 2011, 2013; Salazar et al., 2013; Katzfuss, 2016)
- Spectral approximations and composite likelihoods: (Fuentes 2007; Paciorek, 2007; Eidsvik et al. 2016)
- Multi-resolution approaches (Nychka, 2002; Johannesson et al., 2007; Matsuo et al., 2010; Tzeng & Huang, 2015; Katzfuss, 2016)
- Sparsity: (Solve $Ax = b$ by (i) sparse $A$, or (ii) sparse $A^{-1}$)
  1. Covariance tapering (Furrer et al. 2006; Du et al. 2009; Kaufman et al., 2009; Shaby and Ruppert, 2013)
  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 models (Vecchia 1988; Stein et al. 2004; Stroud et al 2014; Datta et al., 2016)

# Bayesian low rank models

- A *low rank* or *reduced rank* process approximates a *parent* process over a smaller set of points (*knots*).

- Start with a *parent process* $w(s)$ and construct $\tilde{w}(s)$

$$w(s) \approx \tilde{w}(s) = \sum_{j=1}^{r} b_\theta(s, s_j^*) z(s_j^*) = b_\theta^\top(s) z,$$

  where

  - $z(s)$ is *any* well-defined process (could be same as $w(s)$);
  - $b_\theta(s, s')$ is a family of basis functions indexed by parameters $\theta$;
  - $\{s_1^*, s_2^*, \ldots, s_r^*\}$ are the knots;
  - $b_\theta(s)$ and $z$ are $r \times 1$ vectors with components $b_\theta(s, s_j^*)$ and $z(s_j^*)$, respectively.

# Bayesian low rank models (contd.)

- $\tilde{w} = (\tilde{w}(s_1), \tilde{w}(s_2), \ldots, \tilde{w}(s_n))^\top$ is represented as $\tilde{w} = B_\theta z$
- $B_\theta$ is $n \times r$ with $(i,j)$-th element $b_\theta(s_i, s_j^*)$
- Irrespective of how big $n$ is, we now have to work with the $r$ (instead of $n$) $z(s_j^*)$'s and the $n \times r$ matrix $B_\theta$.
- Since $r << n$, the consequential dimension reduction is evident.
- $\tilde{w}$ is a valid stochastic process in $r$-dimensions space with covariance:

$$\text{cov}(\tilde{w}(s), \tilde{w}(s')) = b_\theta^\top(s) V_z b_\theta(s') \ ,$$

  where $V_z$ is the variance-covariance matrix (also depends upon parameter $\theta$) for $z$.
- When $n > r$, the joint distribution of $\tilde{w}$ is singular.

# The Sherman-Woodbury-Morrison formulas

- Low-rank dimension reduction is similar to Bayesian linear regression
- Consider a simple hierarchical model (with $\beta = 0$):

$$N(z \mid 0, V_z) \times N(y \mid B_\theta z, D_\tau) \ ,$$

  where $y$ is $n \times 1$, $z$ is $r \times 1$, $D_\tau$ and $V_z$ are positive definite matrices of sizes $n \times n$ and $r \times r$, respectively, and $B_\theta$ is $n \times r$.
- The low rank specification is $B_\theta z$ and the prior on $z$.
- $D_\tau$ (usually diagonal) has the residual variance components.
- Computing var$(y)$ in two different ways yields

$$(D_\tau + B_\theta V_z B_\theta^\top)^{-1} = D_\tau^{-1} - D_\tau^{-1} B_\theta (V_z^{-1} + B_\theta^\top D_\tau^{-1} B_\theta)^{-1} B_\theta^\top D_\tau^{-1} \ .$$

- A companion formula for the determinant:

$$\det(D_\tau + B_\theta V_z B_\theta^\top) = \det(V_z) \det(D_\tau) \det(V_z^{-1} + B_\theta^\top D_\tau^{-1} B_\theta) \ .$$

# Predictive process models (Banerjee et al., *JRSS-B*, 2008)

- A particular low-rank model emerges by taking
  - $z(s) = w(s)$
  - $z = (w(s_1^*), w(s_2^*), \ldots, w(s_r^*))^\top$ as the realizations of the parent process $w(s)$ over the set of knots $\mathscr{S}^* = \{s_1^*, s_2^*, \ldots, s_r^*\}$,

  and then taking the conditional expectation:

$$\tilde{w}(s) = \mathrm{E}[w(s) \mid w^*] = b_\theta^\top(s) z \; .$$

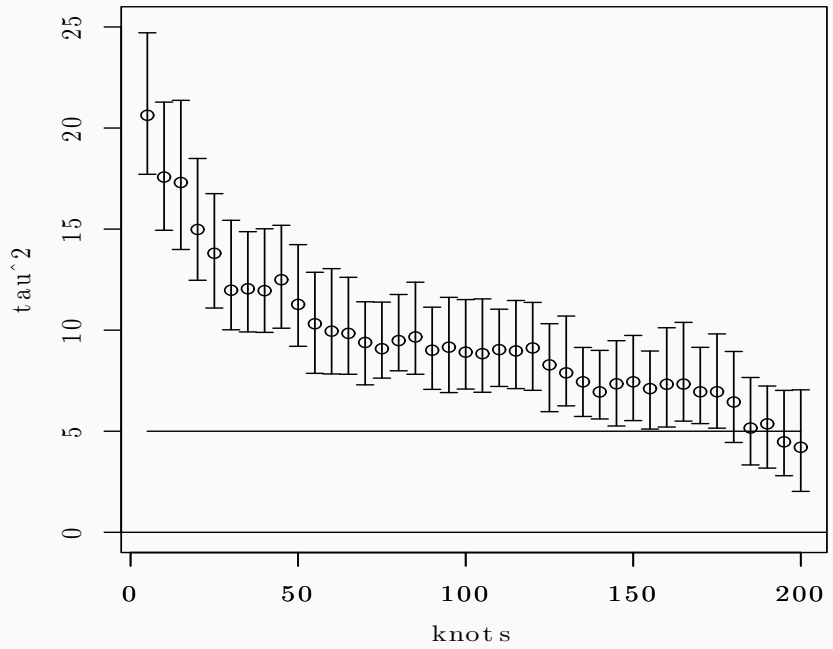
- The basis functions are *automatically* derived from the spatial covariance structure of the parent process $w(s)$:

$$b_\theta^\top(s) = \mathrm{cov}\{w(s), w^*\}\mathrm{var}^{-1}\{w^*\} = c_\theta(s, \mathscr{S}^*) C_\theta^{-1}(\mathscr{S}^*, \mathscr{S}^*) \; .$$

# Biases in low-rank models

- For the predictive process,

$$\begin{aligned} \text{var}\{w(s)\} &= \text{var}\{\text{E}[w(s) \mid w^*]\} + \text{E}\{\text{var}[w(s) \mid w^*]\} \\ &\geq \text{var}\{\text{E}[w(s) \mid w^*]\} = var(\tilde{w}(s)) \ . \end{aligned}$$




- Leads to overestimation of the nugget

# Bias-adjusted or modified predictive processes

- In low-rank processes, $w(s) = \tilde{w}(s) + \eta(s)$. What is lost in $\eta(s)$?
- $\eta(s)$ is a Gaussian process with covariance structure

$$\begin{aligned}\text{Cov}\{\eta(s), \eta(s')\} &= K_{\eta,\theta}(s, s') \\ &= C_\theta(s, s') - c_\theta(s, \mathscr{S}^*) C_\theta^{-1}(\mathscr{S}^*, \mathscr{S}^*) c_\theta(\mathscr{S}^*, s') \, .\end{aligned}$$

- Remedy:

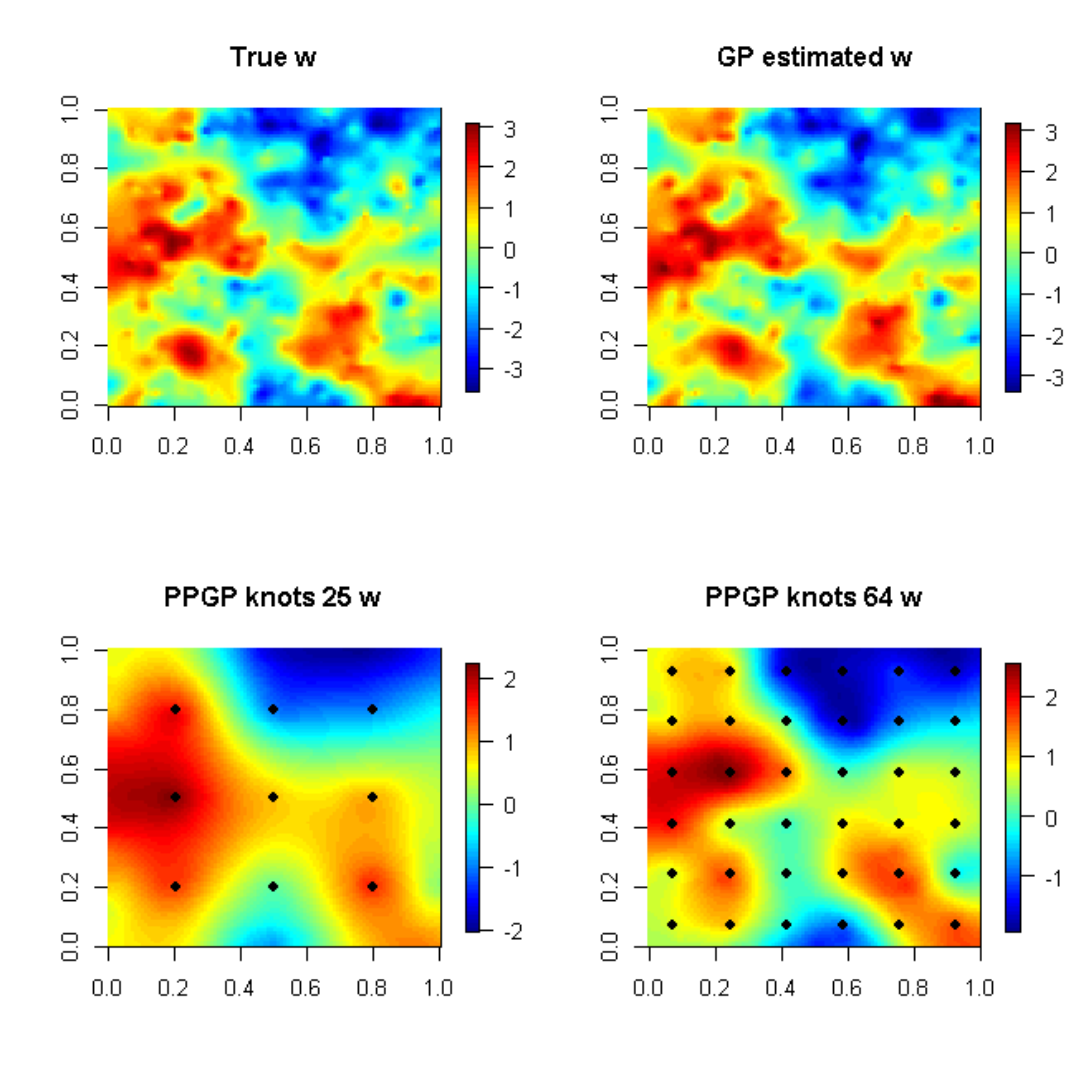
$$\tilde{w}_\epsilon(s) = \tilde{w}(s) + \tilde{\epsilon}(s) \, ,$$

where $\tilde{\epsilon}(s) \overset{ind}{\sim} N(0, \delta^2(s))$ and

$$\delta^2(s) = \text{var}\{\eta(s)\} = C_\theta(s, s) - c_\theta(s, \mathscr{S}^*) C_\theta^{-1}(\mathscr{S}^*, \mathscr{S}^*) c_\theta(\mathscr{S}^*, s) \, .$$

- Other improvements suggested by Sang et al. (2011, 2012) and Katzfuss (2017).

# Oversmoothing in low rank models




Low rank models oversmooths unless we use more knots which