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

Computational Details

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

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

- 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)

Review on literature on spatial big data

Heaton, M.J., Datta, A., Finley, A.O., Furrer, R., Guinness, J., Guhaniyogi, R., Gerber, F., Gramacy, R.B., Hammerling, D., Katzfuss, M. and Lindgren, F., 2018. *A case study competition among methods for analyzing large spatial data.* Journal of Agricultural, Biological and Environmental Statistics, pp.1-28.

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 θ;
  - $\{s_1^*, s_2^*, \ldots, s_r^*\}$ 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_θ 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_θ.
- 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 θ) for z.
- When $n > r$, the joint distribution of $\tilde{w}$ is singular (hence the name fixed-rank).

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_τ and V_z are positive definite matrices of sizes $n \times n$ and $r \times r$, respectively, and B_θ is $n \times r$.
- The low rank specification is $B_\theta z$ and the prior on z.
- D_τ (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
  - $z(s) = w(s)$
  - $z = w^* = (w(s_1^*), w(s_2^*), \ldots, w(s_r^*))^\top$ 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:

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

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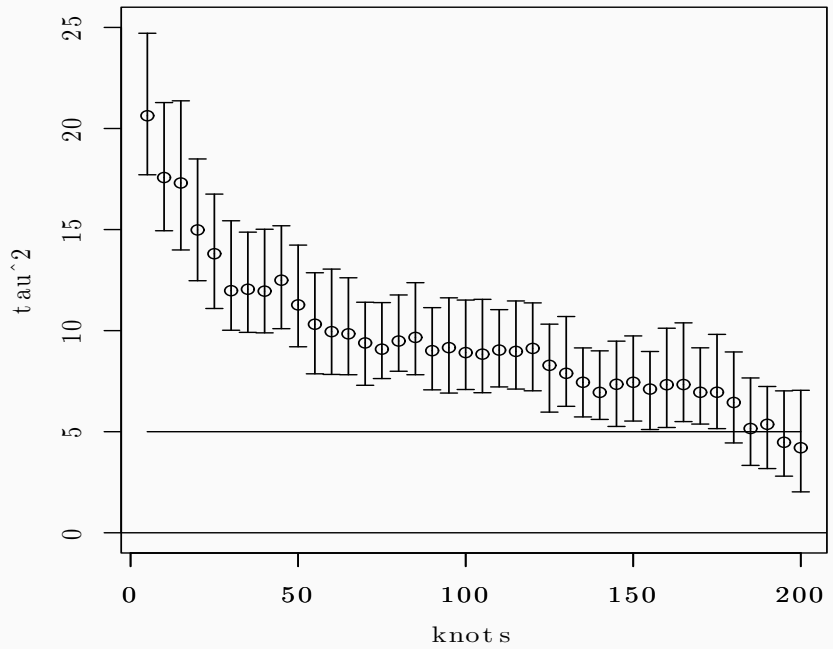
- The basis functions are *automatically* derived from the spatial covariance structure of the parent process $w(s)$:

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

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

- Note that $w(s) = \tilde{w}(s) + \eta(s)$. In low-rank processes, the residual process $\eta(s)$ is ignored.
- $\eta(s)$ 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: low-rank + sparse approximations

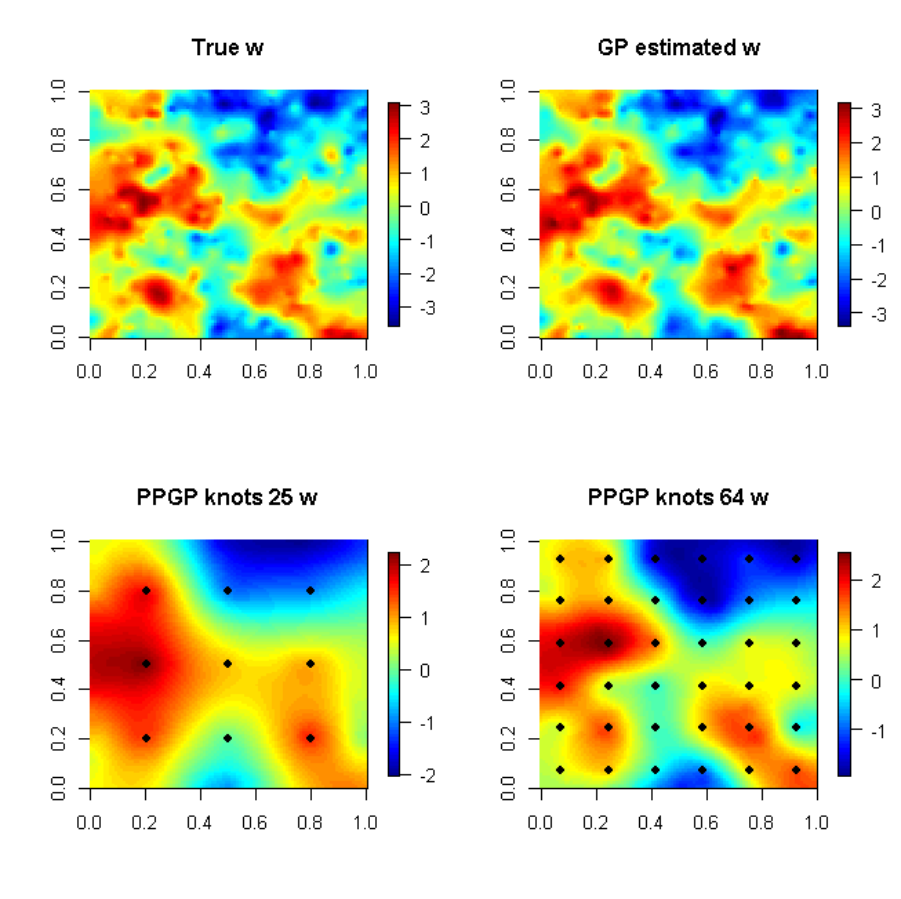
$$\tilde{w}_\epsilon(s) = \tilde{w}(s) + \tilde{\epsilon}(s) \, ,$$

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 becomes computationally expensive