Low-Rank and Predictive Process Models

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Multivariate Gaussian likelihoods for geostatistical models

- $\mathscr{L} = \{s_1, s_2, \ldots, s_n\}$ 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: $y \sim N(X\beta, K_\theta)$
- Estimating process parameters from the likelihood:
$$-\frac{1}{2}\log\det(K_\theta) - \frac{1}{2}(y - X\beta)^\top K_\theta^{-1}(y - X\beta)$$
- K_θ is usually dense with no exploitable structure
- Bayesian inference: Priors on $\{\beta, \theta\}$
- Challenges: Storage and $\texttt{chol}(K_\theta) = LDL^\top$.

Prediction and interpolation

- 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" (spatial prediction/interpolation)

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

- Bayesian "kriging" computes (simulates) posterior predictive density:

$$p(y(s_0)\,|\,y) = \int p(y(s_0)\,|\,y,\theta,\beta)p(\beta,\theta\,|\,y)\mathrm{d}\beta\mathrm{d}\theta$$

Computational Details

- Compute the mean and variance (for any given $\{\beta, \theta\}$ and s_0):

$$\begin{aligned} &\text{Solve for } u: && K_\theta u = k_\theta(s_0)\ ; \\ &\text{Predictive mean:} && x^\top(s_0)\beta + u^\top(y - X\beta)\ ; \\ &\text{Predictive variance:} && K_\theta(s_0, s_0) - u^\top k_\theta(s_0)\ . \end{aligned}$$

- Compute the mean and variance (for any given $\{\beta, \theta\}$ and s_0):

$$\begin{aligned} &\text{Cholesky:} && \texttt{chol}(K_\theta) = LDL^\top\ ; \\ &\text{Solve for } v: && v = \texttt{trsolve}(L, k_\theta(s_0))\ ; \\ &\text{Solve for } u: && u = \texttt{trsolve}(L^\top, D^{-1}v)\ ; \\ &\text{Predictive mean:} && x^\top(s_0)\beta + u^\top(y - X\beta)\ ; \\ &\text{Predictive variance:} && K_\theta(s_0, s_0) - u^\top k_\theta(s_0)\ . \end{aligned}$$

- Primary bottleneck is chol$(\cdot)$

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 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.

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:

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

Practical implementation for Bayesian low rank models

- In practical implementation, better to avoid SWM formulas.

$$\underbrace{\begin{bmatrix} D_\tau^{-1/2} y \\ 0 \end{bmatrix}}_{y_*} = \underbrace{\begin{bmatrix} D_\tau^{-1/2} B_\theta \\ V_z^{-1/2} \end{bmatrix}}_{B_*} z + \underbrace{\begin{bmatrix} e_1 \\ e_2 \end{bmatrix}}_{e_*}.$$

- $e_* \sim N(0, I_{n+r})$.
- $V_z^{1/2}$ and $D_\tau^{1/2}$ are matrix square roots of of V_z and D_τ, respectively.
- If D_τ is diagonal (as is common), then $D_\tau^{1/2}$ is simply the square root of the diagonal elements of D_τ.
- $V_z^{1/2} = \texttt{chol}(V_z)$ is the triangular (upper or lower) Cholesky factor of the $r \times r$ matrix V_z.
- Use `backsolve` to efficiently obtain $V_z^{-1/2} z$

Practical implementation for Bayesian low rank models (contd.)

- The marginal density of $p(y_* \mid \theta, \tau)$ after integrating out z now corresponds to the normal linear model

$$y_* = B_* \hat{z} + e_* \ ,$$

where $\hat{z}$ is the ordinary least-square estimate of z.

- Use `lm` function to compute $\hat{z}$ applying the QR decomposition to B_*.
- Thus, we estimate the Bayesian linear model

$$p(\theta, \tau) \times N(y_* \mid B_* \hat{z}, I_{n+r})$$

- MCMC will generate posterior samples for $\{\theta, \tau\}$.
- *Recover* the posterior samples for z from those of $\{\theta, \tau\}$:

$$p(z \mid y) = \int N(z \mid \hat{z}, M) \times p(\theta, \tau \mid y) \mathrm{d}\theta \mathrm{d}\tau$$

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

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 $\mathscr{L}^* = \{s_1^*, s_2^*, \ldots, s_r^*\}$,

  and then taking the conditional expectation:

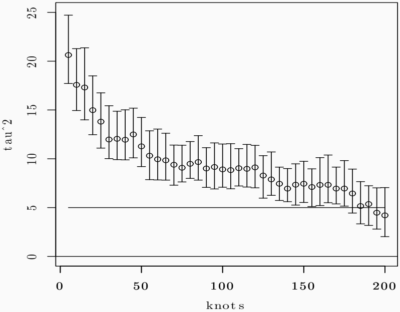
$$\tilde{w}(s) = \mathrm{E}[w(s) \mid w^*] = b_\theta^\top(s) z \; .$$

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

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

Biases in low-rank models

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



- For the predictive process,

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

Bias-adjusted or modified predictive processes

- $\eta(s)$ is a Gaussian process with covariance structure

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

- Remedy:

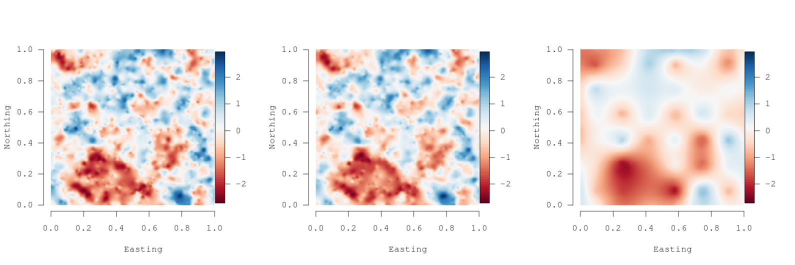
$$\tilde{w}_\epsilon(s) = \tilde{w}(s) + \tilde{\epsilon}(s) \ ,$$

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

$$\delta^2(s) = \mathrm{var}\{\eta(s)\} = K_\theta(s, s) - K_\theta(s, \mathscr{L}^*)K_\theta^{-1}(\mathscr{L}^*, \mathscr{L}^*)K_\theta(\mathscr{L}^*, s) \ .$$

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

Oversmoothing in low rank models



True w Full GP PPGP 64 knots

Figure: Comparing full GP vs low-rank GP with 2500 locations. Figure (1c) exhibits oversmoothing by a low-rank process (predictive process with 64 knots)