On Gaussian Process Models for High-Dimensional Geostatistical Datasets

Sudipto Banerjee
Joint work with Abhirup Datta, Andrew O. Finley and Alan E. Gelfand

University of California, Los Angeles, USA

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Space debris
Motivating Example

U.S. Forest biomass data

Figure: Observed biomass (left) and NDVI (right)

- Forest biomass data collected between 1999 and 2006 at 114,371 plots
- Normalized Difference Vegetation Index (NDVI) calculated in July 2006
- NDVI is a measure of greenness and is used as a covariate in Forest Biomass Regression Models
Non Spatial Model

Model

\[ \text{Biomass} = \beta_0 + \beta_1 \text{NDVI} + \text{error}, \quad \hat{\beta}_0 = 1.043, \hat{\beta}_1 = 0.0093 \]

Figure: Heat map (left) and variogram (right) of residuals reflecting spatial correlation
Spatially-varying regression models

- \[ Y(s) = \beta_0(s) + \beta_1(s)X(s) + e(s) \]

- Produce maps for intercept and slope:
  \[ \{ \beta_0(s) : s \in D \subset \mathbb{R}^d \} \text{ and } \{ \beta_1(s) : s \in D \subset \mathbb{R}^d \} \]

- This would be rich: understand spatially-varying impact of predictors on outcome.

- Model-based predictions: \( Y(s_0) \mid \{ y(s_1), y(s_2), \ldots, y(s_n) \} \).
Gaussian (spatial) process

- \( \{w(s) : s \in D \subset \mathbb{R}^d\} \sim GP(0, K_\theta(s, t)) \) implies
  
  \[
  w = (w(s_1), w(s_2), \ldots, w(s_n))^\top \sim N(0, K_\theta)
  \]

  for every finite set of points \( s_1, s_2, \ldots, s_n \).

- \( K_\theta = \{K_\theta(s_i, s_j)\} \) is a spatial variance-covariance matrix

- Stationary: \( K_\theta(s, t) = K_\theta(t - s) \). Isotropy: \( K_\theta(s, t) = K_\theta(||t - s||) \).

- Bochner: Covariance function \( \Leftrightarrow \) characteristic function.
Matérn covariance:

\[ K_\theta(s, t) = \frac{\sigma^2}{2^{\phi_2} - 1 \Gamma(\phi_2)} (\|t - s\| \phi_1)^{\phi_2} \kappa_{\phi_2}(\|t - s\|; \phi_1) \]

\[ \phi_1 \rightarrow \text{controls how fast correlation decays} \]

\[ \phi_2 \rightarrow \text{controls smoothness of the spatial surface} \]
Hierarchical Gaussian process models

Full rank model

- $T = \{t_1, t_2, \ldots, t_n\}$ are locations where data is observed
- $y(t_i)$ is outcome at the $i^{th}$ location, $y = (y(t_1), y(t_2), \ldots, y(t_n))^\top$
- $y = X\beta + Zw + \epsilon, \epsilon \sim N(0, \tau^2 I)$
- $w = (w(t_1), w(t_2), \ldots, w(t_n))^\top$ are spatial random effects
- $w \sim N(0, K_\theta)$, $K_\theta$ is a valid spatial covariance matrix
- Priors on $\{\beta, \tau^2, \theta\}$
Computation issues

- Storage: $n^2$ pairwise distances to compute $K_\theta$
- $K_\theta$ is dense; solve $K_\theta x = b$ and need $\det(K_\theta)$
- Complexity: roughly $O(n^3)$ flops; computationally infeasible for large datasets
Burgeoning literature on spatial big data

- Low-rank approaches (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; Lemos et al., 2011; Guhaniyogi et al., 2011, 2013; Salazar et al., 2013)

- Covariance tapering (Furrer et al. 2006; Zhang and Du, 2007; Du et al. 2009; Kaufman et al., 2009)

- Spectral domain: (Fuentes 2007; Paciorek, 2007)

- Approximation using GMRFs: INLA (Rue et al. 2009; Lindgren et al., 2011)

- Nearest-neighbor models (processes) (Vecchia 1988; Stein et al. 2004; Gramacy et al. 2014; Stroud et al 2014; Datta et al., 2015)
Low-rank models: hierarchical approach

\[ N(w^* \mid 0, K^*_\theta) \times N(y \mid B_\theta w^*, D) \]

- \( y \) is \( n \times 1 \) and \( n \) is large
- \( w^* \) is \( r \times 1 \), where \( r << n \); so \( K^*_\theta \) is \( r \times r \)
- \( B_\theta \) is \( n \times r \) is a matrix of “basis” functions
- \( D \) is \( n \times n \), but easy to invert (e.g. diagonal)
- Derive \( \text{var}(y) \) (or \( \text{var}(w^* \mid y) \)) in two ways to obtain

\[
(D + B_\theta K^*_\theta B_\theta^\top)^{-1} = D^{-1} - D^{-1} B_\theta (K^*_\theta^{-1} + B_\theta^\top D^{-1} B_\theta)^{-1} B_\theta^\top D^{-1}.
\]

- This is the famous Sherman-Woodbury-Morrison formula.
- Modeling: specifying \( w^* \) and \( B_\theta \).
Gaussian predictive process (Banerjee et al., *JRSS-B*, 2008)

- Start with a parent Gaussian process $w(s) \sim GP(0, K_\theta(\cdot, \cdot))$
- Fix a set of “knots” $s_1, s_2, \ldots, s_r$, and let $K^*_\theta = \{K_\theta(s_i, s_j)\}$
- Then, $w^* = (w(s_1), w(s_2), \ldots, w(s_r))^\top \sim N(0, K^*_\theta)$
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- Then, \( w^* = (w(s_1), w(s_2), \ldots, w(s_r))^\top \sim N(0, K_\theta^*) \)
- Predictive process: \( \tilde{w}(s) = E[w(s) \mid w^*] = b_\theta(s)^\top w^* \)
- Orthogonal decomposition:
  \[
  \text{var}\{w(s)\} = \text{var}\{\tilde{w}(s)\} + \text{var}\{w(s) - \tilde{w}(s)\}
  \]
- Approximate residual process with a sparse process (Sang et al. 2011)
Figure: Comparing full GP vs low-rank GP with 2000 locations
Sparse Gaussian Processes

- Introduce (auxiliary) random effects to achieve computational benefits.
- Let $\mathcal{S} = \{s_1, s_2, \ldots, s_k\}$ be a “reference” set of points.
  \[
  \text{Spatial random effects: } (w(s_1), w(s_2), \ldots, w(s_k))^\top \sim N(0, \tilde{K}_\theta),
  \]
  \[
  \text{Spatial process: } w(t) = \sum_{i=1}^{k} a_i(t)w(s_i) + \eta(t).
  \]

1. Example: $\eta(t) \overset{ind}{\sim} N(0, \tau^2(t))$.
2. Example: $a_i(t) \neq 0 \text{ ONLY IF } t \text{ is a “neighbor” of } s_i$.

- Three pieces to the puzzle:
  1. How do we construct $\tilde{K}_\theta^{-1}$ to be sparse and $\det(\tilde{K}_\theta)$ to be cheap?
  2. How do we define “neighbors” for arbitrary points $t$?
  3. How do we choose nonzero $a_i(t)$’s? Ensure good approx. to full GP?
Sparse Gaussian Processes

Simple method of introducing sparsity (e.g. graphical models)

- Write a joint density \( p(w) = p(w_1, w_2, \ldots, w_n) \) as:

\[
p(w_1)p(w_2 | w_1)p(w_3 | w_1, w_2) \cdots p(w_n | w_1, w_2, \ldots, w_{n-1})
\]

- Example: For Gaussian distributions:

\[
w_1 = 0 + \eta_1; \\
w_i = a_{i1}w_1 + a_{i2}w_2 + \cdots + a_{i,i-1}w_{i-1} + \eta_i; \quad i = 2, 3, \ldots, n
\]

\[\implies w = Aw + \eta; \quad \eta \sim N(0, D)\]

- Making some \( a_{ij} = 0 \) introduces conditional independence

- Equivalent to \( w \sim N(0, K_\theta) \) and \( \text{chol}(K_\theta^{-1}) = LDL^\top \), then additional zeroes in lower-triangular \( L \).
Sparse likelihood approximations (Vecchia, 1988; Stein et al., 2004)

- With $w_i \equiv w(s_i)$, write a GP joint density $p(w) = p(w_1, w_2, \ldots, w_n)$ as:

  $$p(w_1)p(w_2 | w_1)p(w_3 | w_1, w_2) \cdots p(w_n | w_1, w_2, \ldots, w_{n-1})$$

- Use “screening effect” to impose conditional independence and obtain:

  $$\tilde{p}(w) = p(w_1)p(w_2 | w_1)p(w_3 | w_1, w_2)p(w_4 | w_1, w_3) \cdots p(w_n | w_{i_n}, w_{j_n})$$

- If $w \sim \mathcal{N}(0, K_\theta)$, then $\tilde{p}(w) = \mathcal{N}(w | 0, \tilde{K}_\theta)$

- $\tilde{K}_\theta^{-1}$ is sparser than $K_\theta^{-1}$. 
Sparse Gaussian Processes

Two crucial facts

1. $\tilde{p}(w)$ is a valid joint density from the model $w \sim N(0, \tilde{K}_\theta)$
2. $\tilde{K}_\theta^{-1}$ depends on $K_\theta$ and is sparse with at most $nm^2$ non-zero entries

Figure: Sparse precision matrices from neighbor-based approximation
Extension to a Nearest-neighbor GP (Datta et al., JASA, 2015)

- Fix any “reference” set $S = \{s_1, s_2, \ldots, s_k\}$

$$N(s_i) = \begin{cases} 
  \text{empty set for } i = 1 \\ 
  \{s_1, s_2, \ldots, s_{i-1}\} \text{ for } 2 \leq i \leq m \\ 
  m \text{ nearest neighbors of } s_i \text{ among } \{s_1, s_2, \ldots, s_{i-1}\} \text{ for } i > m
\end{cases}$$

- Model $w_S \sim N(0, \tilde{K}_\theta)$ (“Vecchia prior”)

- For any $t$ outside $S$, define $N(t)$ as the set of $m$-nearest neighbors of $t$ in $S$

- Construct $w(t) = \sum_{i=1}^{k} a_i(t)w(s_i) + \eta(t)$ with $a_i(t) = 0$ if $s_i \notin N(t)$.

- Nonzero $a_i(t)$’s are specified according to $p(w(t) \mid w_{N(t)})$. 
For $T = \{t_1, t_2, \ldots, t_n\}$ outside $S$, we define

$$
\tilde{p}(w_T \mid w_S) = \prod_{i=1}^{n} p(w(t_i) \mid w_{N(t_i)}) .
$$

Generalize to any finite $T$ as follows:

$$
\tilde{p}(w_T) = \int \tilde{p}(w_S)\tilde{p}(w_T \setminus S \mid w_S) \prod_{\{i \mid s_i \in S \setminus T\}} d(w(s_i))
$$

Example: Model $\tilde{p}(w_S)\tilde{p}(w_T \mid w_S) = N(w_S \mid 0, \tilde{K}_\theta) \times N(w_T \mid A_T w_S, D_T)$

A very convenient choice in practice: $S = T$, i.e., take set of observed locations as reference set.
Hierarchical NNGP model

NNGP used as a sparsity inducing prior for hierarchical models.

Likelihood

\[
N(y | X\beta + Zw_T, \tau^2 I) \times N(w_T | A_T w_S, D_T) \times N(w_S | 0, \tilde{K}_\theta) \\
\times N(\beta | \mu_\beta, V_\beta) \times IG(\tau^2 | a_\tau, b_\tau) \times \pi(\theta)
\]

Gibbs’ sampler

- Conjugate full conditionals for $\beta, \tau^2$
- Sequential updates for full conditional of $w(t_i)$’s
- Metropolis step for updating $\theta$
Storage and computation

- **Never** needs to store $n \times n$ distance matrix. Stores $n$ small $m \times m$ matrices.
- Total flop count per iteration of Gibbs’ sampler is $O(nm^3)$ i.e linear in $n$.
- Scalable to massive datasets.
Simulation experiments

- 2500 locations on a unit square
- \( y(t_i) = \beta_0 + \beta_1 X(t_i) + w(t_i) + \epsilon(t_i) \)
- Single covariate generated from \( N(0, 1) \)
- Spatial effects generated from \( GP(0, \sigma^2 R(\nu, \phi)) \)
  - \( R(\nu, \phi) \) is Matern correlation function with smoothness \( \nu \) and decay \( \phi \)
- Candidate models: Full GP, Low rank GP (PPGP) with 64 knots and NNGP
Application to spatial datasets

Simulation experiments

(a) True w
(b) Full GP
(c) PPGP 64 knots
(d) NNGP, $m = 10$
(e) NNGP, $m = 20$

Figure: Univariate synthetic data analysis

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**Figure:** Choice of $m$ in NNGP models: Out-of-sample Root Mean Squared Prediction Error (RMSPE) and mean width between the upper and lower 95% posterior predictive credible intervals for a range of $m$ for the univariate synthetic data analysis.
### Table: Univariate synthetic data analysis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>True</th>
<th>$m = 10$</th>
<th>$m = 20$</th>
<th>Predictive Process 64 knots</th>
<th>Full Gaussian Process</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_0$</td>
<td>1</td>
<td>1.00 (0.62, 1.31)</td>
<td>1.03 (0.65, 1.34)</td>
<td>1.30 (0.54, 2.03)</td>
<td>1.03 (0.69, 1.34)</td>
</tr>
<tr>
<td>$\beta_1$</td>
<td>5</td>
<td>5.01 (4.99, 5.03)</td>
<td>5.01 (4.99, 5.03)</td>
<td>5.03 (4.99, 5.06)</td>
<td>5.01 (4.99, 5.03)</td>
</tr>
<tr>
<td>$\sigma^2$</td>
<td>1</td>
<td>0.96 (0.78, 1.23)</td>
<td>0.94 (0.77, 1.20)</td>
<td>1.29 (0.96, 2.00)</td>
<td>0.94 (0.76, 1.23)</td>
</tr>
<tr>
<td>$\tau^2$</td>
<td>0.1</td>
<td>0.10 (0.08, 0.13)</td>
<td>0.10 (0.08, 0.13)</td>
<td>0.08 (0.04, 0.13)</td>
<td>0.10 (0.08, 0.12)</td>
</tr>
<tr>
<td>$\phi$</td>
<td>12</td>
<td>12.93 (9.70, 16.77)</td>
<td>13.36 (9.99, 17.15)</td>
<td>5.61 (3.48, 8.09)</td>
<td>13.52 (9.92, 17.50)</td>
</tr>
</tbody>
</table>

- Parameter estimates for all models are similar
- **NNGP** performs at par with Full GP, **PPGP** performs worse
- **NNGP** yields huge computational gains

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Back to the Forest biomass dataset

- Number of spatial locations: \( n = 114,371 \)
- Full GP and PPGP storage requirements \( \gg \) 38 gigabytes available
- We use a hierarchical spatially varying coefficients NNGP model

**Model**

- \( \text{Biomass}(t) = (\beta_0 + \beta_0(t)) + (\beta_1 + \beta_1(t)) \text{NDVI}(t) + \epsilon(t) \)
- \( w(t) = (\beta_0(t), \beta_1(t))^{\top} \sim \text{Bivariate NNGP}(0, \tilde{K}_\theta(\cdot)), m = 5 \)
- Full inferential output: 46 hrs
Application to spatial datasets

Forest biomass analysis

(a) Observed biomass

(b) Fitted biomass

(c) $\beta_0(t)$

(d) $\beta_{\text{NDVI}}(t)$
Conclusions

- Unified platform for estimation, prediction and model comparison
- Easily extends to multivariate and spatial-temporal processes
- Posterior predictions, recovery of latent spatial surfaces
- Superior performance, massive computation and storage gains over existing models
- Possible extension to spatial GLMs
Thank you!