Hierarchical Modelling for Large Spatial Datasets

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The Big $n$ issue

Univariate spatial regression

$$Y = X\beta + w + \epsilon,$$

- Estimation involves $(\sigma^2 R(\phi) + \tau^2 I)^{-1}$, which is $n \times n$.
- Matrix computations occur in each MCMC iteration.
- Known as the “Big-N problem” in geostatistics.
- Approach: Use a model $Y = X\beta + Zw^* + \epsilon$. But what $Z$?
Consider “knots” $\mathcal{I}^* = \{s_1^*, \ldots, s_n^*\}$ with $n^* \ll n$.

Let $w^* = \{w(s_i^*)\}_{i=1}^{n^*}$

$Z(\theta) = \{\text{cov}(w(s_i), w(s_j^*))\}'\{\text{var}(w^*)\}^{-1}$ is $n \times n^*$.

**Predictive process regression model**

$$Y = X\beta + Z(\theta)w^* + \epsilon,$$

Fitting requires only $n^* \times n^*$ matrix computations ($n^* \ll n$).

**Key attraction:** The above arises as a process model:

$\tilde{w}(s) \sim GP(0, \sigma_w^2 \tilde{\rho}(\cdot; \phi))$ instead of $w(s)$.

$\tilde{\rho}(s_1, s_2; \phi) = \text{cov}(w(s_1), w^*)\text{var}(w^*)^{-1}\text{cov}(w^*, w(s_2))$
Knots: A “Knotty” problem??

- Knot selection: Regular grid? More knots near locations we have sampled more?

- Formal spatial design paradigm: maximize information metrics (Zhu and Stein, 2006; Diggle & Lophaven, 2006)

- Geometric considerations: space-filling designs (Royle & Nychka, 1998); various clustering algorithms

- Compare performance of estimation of range and smoothness by varying knot size.

- Stein (2007, 2008): method may not work for fine-scale spatial data

- Still a popular choice – seamlessly adapts to multivariate and spatiotemporal settings.
Selection of knots

The graph shows a relationship between two variables: knots and $\tau^2$. The $x$-axis represents the number of knots, ranging from 0 to 200, while the $y$-axis represents $\tau^2$, ranging from 0 to 25. The data points are plotted with error bars, indicating variability or uncertainty in the measurements. The trend of the data suggests a decreasing $\tau^2$ value as the number of knots increases.
A rectified predictive process is defined as

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

where

$$\tilde{\epsilon}(s) \overset{indep}{\sim} N(0, \sigma_w^2(1 - r(s, \phi)' R^{-1}(\phi) r(s, \phi))).$$

Maximum likelihood estimates of $\tau^2$:

<table>
<thead>
<tr>
<th># of Knots</th>
<th>Predictive Process</th>
<th>Rectified Predictive Process</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.56941</td>
<td>1.00786</td>
</tr>
<tr>
<td>36</td>
<td>1.65688</td>
<td>1.15386</td>
</tr>
<tr>
<td>64</td>
<td>1.45169</td>
<td>1.08358</td>
</tr>
<tr>
<td>100</td>
<td>1.37916</td>
<td>1.09657</td>
</tr>
<tr>
<td>225</td>
<td>1.27391</td>
<td>1.08985</td>
</tr>
<tr>
<td>400</td>
<td>1.22429</td>
<td>1.09489</td>
</tr>
<tr>
<td>625</td>
<td>1.21127</td>
<td>1.09998</td>
</tr>
<tr>
<td>exact</td>
<td>1.14414</td>
<td>1.14414</td>
</tr>
</tbody>
</table>
Illustration from:


Univariate random effects models


*Quantitative genetics*: studies the inheritance of polygenic traits, focusing upon estimation of additive genetic variance, $\sigma^2_a$, and the heritability $h^2 = \sigma^2_a / \sigma^2_{Tot}$, where the $\sigma^2_{Tot}$ represents the total genetic and unexplained variation.

A high heritability, $h^2$, should result in a larger selection response (i.e., a higher probability for genetic gain in future generations).
Observed trees

Data overview:
- established in 1971 (by Skogforsk)
- partial diallel design of 52 parent trees
- 8,160 planted randomly on 2.2m squares
- 1997 reinventory of 4,970 surviving trees, height, DBH, branch angle, etc.
Genetic effects model:

\[ Y_i = \mathbf{x}_i^T \beta + a_i + d_i + \epsilon_i, \]

- \( a = [a_i]_{i=1}^n \sim MVN(0, \sigma_a^2 A) \)
- \( d = [d_i]_{i=1}^n \sim MVN(0, \sigma_d^2 D) \)
- \( \epsilon = [\epsilon_i]_{i=1}^n \sim N(0, \tau^2 I_n) \)

\( A \) and \( D \) are fixed relationship matrices (See e.g., Henderson, 1985; Lynch and Walsh, 1998)

Note, genetic variance is further partitioned into additive and the non-additive dominance component \( \sigma_d^2 \).
Genetic effects model:

$$Y_i = x_i^T \beta + a_i + d_i + \epsilon_i,$$

- Common feature is systematic heterogeneity among observational units (i.e., violation of $\epsilon \sim N(0, \tau^2 I_n)$)
- Spatial heterogeneity arises from:
  - soil characteristics
  - micro-climates
  - light availability
- Residual correlation among units as a function of distance and/or direction = erroneous parameter estimates (e.g., biased $h^2$)
Genetic model results

Parameter credible intervals, 50% (2.5%, 97.5%) for the non-spatial models Scots pine trial.

<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td>$\beta$</td>
<td>72.53 (69.66, 75.08)</td>
<td>72.27 (70.04, 74.57)</td>
</tr>
<tr>
<td>$\sigma_a^2$</td>
<td>31.94 (18.30, 49.85)</td>
<td>25.23 (14.12, 43.96)</td>
</tr>
<tr>
<td>$\sigma_d^2$</td>
<td>-</td>
<td>22.37 (11.24, 40.11)</td>
</tr>
<tr>
<td>$\tau^2$</td>
<td>133.60 (121.18, 144.70)</td>
<td>116.14 (100.51, 127.76)</td>
</tr>
<tr>
<td>$h^2$</td>
<td>0.19 (0.12, 0.28)</td>
<td>0.15 (0.09, 0.26)</td>
</tr>
</tbody>
</table>
Genetic model results, cont’d.

So, \( \epsilon \sim N(0, \tau^2 I_n) \). Consider a spatial model.
Previous approaches to accommodating residual spatial dependence:

- **Manipulate the mean function**
  - constructing covariates using residuals from neighboring units (see e.g., Wilkinson et al., 1983; Besag and Kempton, 1986; Williams, 1986)

- **Geostatistical**
  - spatial process formed $AR(1)_{col} \otimes AR(1)_{row}$ (Martin, 1990; Cullis et al., 1998)
  - classical geostatistical method (Zimmerman and Harville, 1991)

All are computationally feasible, but **ad hoc and/or restrictive** from a modeling perspective.
Spatial model for genetic trials:

\[ Y(s_i) = x^T(s_i)\beta + a_i + d_i + w(s_i) + \epsilon_i, \]

- \( a = [a_i]_{i=1}^n \sim MVN(0, \sigma_a^2 A) \)
- \( d = [d_i]_{i=1}^n \sim MVN(0, \sigma_d^2 D) \)
- \( w = [w(s_i)]_{i=1}^n \sim MVN(0, \sigma_w^2 C(\theta)) \)
- \( \epsilon = [\epsilon_i]_{i=1}^n \sim N(0, \tau^2 I_n) \)

Tools used to estimate parameters:
- Markov chain Monte Carlo (MCMC) - iterative
  - Gibbs sampler \((\beta, a, d, w)\)
  - Metropolis-Hastings and Slice samplers \((\theta)\)

Here MCMC is computationally infeasible because of Big-N!
Trick to sample genetic effects:

Gibbs draw for random effects, e.g., $a| \cdot \sim MN(\mu_a|., \Sigma_a|.)$, where calculating $\Sigma_a|.| = \left[ \frac{1}{\sigma_a^2} A^{-1} + \frac{I_n}{\tau^2} \right]^{-1}$ is computationally expensive!

However $A$ and $D$ are known, so use initial spectral decomposition i.e., $A^{-1} = P^T \Lambda^{-1} P$.

Thus, $\Sigma_a|.| = P^T \left( \frac{1}{\sigma_a^2} \Lambda^{-1} + \frac{1}{\tau^2} I \right)^{-1} P$ to achieve computational benefits.
Unfortunately, this *trick* does not work for $\mathbf{w}$. Rather, we proposed the knot-based *predictive process*.

**Corresponding predictive process model:**

$$Y(s_i) = \mathbf{x}^T(s_i)\beta + a_i + d_i + \tilde{w}(s_i) + \epsilon_i,$$

where, $\tilde{w}(s_i) = \mathbf{c}(s_i; \theta)^T C(\theta)^{-1}(\theta) \mathbf{w}^*$

$\mathbf{w}^* = [w(s^*_i)]_{i=1}^m \sim \text{MVN}(\mathbf{0}, C^*(\theta))$ and $C^*(\theta) = [C(s^*_i, s^*_j; \theta)]_{i,j=1}^m$
\( \mathbf{w} \) can accommodate complex spatial dependence structures, E.g., anisotropic Matérn correlation function:

\[
\rho(s_i, s_j; \theta) = \left( \frac{1}{\Gamma(\nu)} \right)^{2^{\nu-1}} \left( 2 \sqrt{\nu d_{ij}} \right)^\nu \kappa_\nu \left( 2 \sqrt{\nu d_{ij}} \right),
\]

where \( d_{ij} = (s_i - s_j)^T \Sigma^{-1} (s_i - s_j) \), \( \Sigma = G(\psi) \Lambda^2 G^T(\psi) \). Thus, \( \theta = (\nu, \psi, \Lambda) \).
Genetic + spatial effects models

Candidate spatial models (i.e., specifications of $C^*(\theta)$):

1. $AR(1)_{col} \otimes AR(1)_{row}$
2. isotropic Matérn
3. anisotropic Matérn

Each model evaluated using 64, 144, and 256 knot grids.

Model choice using Deviance Information Criterion (DIC) (Spiegelhalter et al., 2002)
**Table:** Model comparisons using the DIC criterion for the Scots pine dataset.

<table>
<thead>
<tr>
<th>Model</th>
<th>$p_D$</th>
<th>DIC</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Non-spatial</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Add.</td>
<td>306.40</td>
<td>15,618.09</td>
</tr>
<tr>
<td>Add. Dom.</td>
<td>555.92</td>
<td>15,547.85</td>
</tr>
<tr>
<td><strong>Spatial Isotropic</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>64 Knots</td>
<td>639.77</td>
<td>14,877.51</td>
</tr>
<tr>
<td>144 Knots</td>
<td>739.61</td>
<td>14,814.89</td>
</tr>
<tr>
<td>256 Knots</td>
<td>802.29</td>
<td>14,771.64</td>
</tr>
<tr>
<td><strong>Spatial Anisotropic</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>64 Knots</td>
<td>678.82</td>
<td>14,884.13</td>
</tr>
<tr>
<td>144 Knots</td>
<td>748.89</td>
<td>14,823.90</td>
</tr>
<tr>
<td>256 Knots</td>
<td>806.46</td>
<td>14,781.53</td>
</tr>
</tbody>
</table>
Genetic + spatial effects models results

Parameter credible intervals, 50% (2.5%, 97.5%) for the isotropic Matérn and 64 and 256 knots Scots pine trial.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>64 Knots</th>
<th>256 Knots</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta$</td>
<td>72.53 (69.00, 76.05)</td>
<td>74.21 (69.66, 79.66)</td>
</tr>
<tr>
<td>$\sigma^2_a$</td>
<td>26.87 (17.14, 41.82)</td>
<td>33.03 (18.19, 53.69)</td>
</tr>
<tr>
<td>$\sigma^2_d$</td>
<td>11.69 (6.00, 34.27)</td>
<td>13.96 (7.65, 27.05)</td>
</tr>
<tr>
<td>$\sigma^2_w$</td>
<td>41.84 (23.71, 73.34)</td>
<td>50.36 (30.24, 88.10)</td>
</tr>
<tr>
<td>$\tau^2$</td>
<td>89.55 (72.11, 99.65)</td>
<td>80.75 (67.90, 96.16)</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.83 (0.31, 1.46)</td>
<td>0.47 (0.26, 1.28)</td>
</tr>
<tr>
<td>$\phi$</td>
<td>0.05 (0.02, 0.09)</td>
<td>0.04 (0.02, 0.09)</td>
</tr>
<tr>
<td>Eff. Range</td>
<td>71.00 (44.66, 127.93)</td>
<td>74.59 (45.22, 129.83)</td>
</tr>
<tr>
<td>$h^2$</td>
<td>0.21 (0.13, 0.31)</td>
<td>0.25 (0.15, 0.39)</td>
</tr>
</tbody>
</table>

- Decrease in $\tau^2$ due to removal of spatial variation, results in increase in $h^2$ (i.e., $\sim 0.25$ vs. $\sim 0.15$ with confounding).
Genetic + spatial effects models results, cont’d.

Genetic model residuals

$\tilde{w}(s)$, 64 knots

$\tilde{w}(s)$, 256 knots

*Predictive process* – balance model richness with computational feasibility (e.g., $4,970 \times 4,970$ vs. $64 \times 64$).
Summary

Challenge - to meet modeling needs:

- ensure computationally feasible
  - reduce algorithmic complexity = cheap tricks (e.g., spectral decomp. of $A$ prior to MCMC)
  - reduce dimensionality = predictive process

- maintain richness and flexibility
  - focus on the model **not** how to estimate the parameters = embrace new tools (MCMC) for estimating highly flexible hierarchical models

- truly acknowledge sources of uncertainty
  - propagate uncertainty through hierarchical structures (e.g., recognize uncertainty in $C(\theta)$)