Model Selection for Geostatistical Models

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Model Selection for Geostatistical Models

\[ Z(s) = \beta_0 + X_1(s)\beta_1 + \cdots + X_p(s)\beta_p + \delta(s) \]

- Which explanatory variables should be included?
- What is the form of \( \delta(s) \)?
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Model Selection for Geostatistical Models

Problem: How does one choose the “best” set of covariates and family of covariance functions?

Potential Objectives of Model Selection

1. Choose the correct model (consistency)
   - There exists a “true” finite-dimensional model.
   - If not a finite-dimensional model, at least include the key explanatory variables.

2. Choose the model that is best for prediction (efficiency)
   - Find a model that predicts well at un-observed locations.

3. Choose the model that maximizes data compression.
   - Find a model that summarizes the data in the most compact fashion.
The Geostatistical Model

Let \( Z = (Z(s_1), \ldots, Z(s_n))' \) be a partial realization of a random field \( Z(s) \), where \( s \in D \), a fixed finite area under study.

A model for the random field at any location \( s \) is given by

\[
Z(s) = X'(s)\beta + \delta(s),
\]

where

- \( X(s) = (1, X_1(s), \ldots, X_p(s))' \) is a vector of explanatory variables observed at location \( s \),
- \( \beta \) is a \( p + 1 \) vector of unknown coefficients
- We assume that the error process \( \delta(s) \) is a stationary, isotropic Gaussian process with mean zero and covariance function

\[
\text{Cov}(\delta(s), \delta(t)) = \sigma^2 \rho(||s - t||, \theta),
\]

where \( \sigma^2 \) is the variance of the process, \( \rho(\cdot, \theta) \) is an isotropic correlation function, and \( || \cdot || \) denotes Euclidean distance.
Autocorrelation Functions

Some of the standard autocorrelation functions:

1. **Exponential**
   \[
   \rho(d) = \exp\left(\frac{-d}{\theta_1}\right)
   \]

2. **Gaussian**
   \[
   \rho(d) = \exp\left(\frac{-d^2}{\theta_2^2}\right)
   \]

3. **Matern**
   \[
   \rho(d) = \frac{1}{2^{\theta_2-1}\Gamma(\theta_2)} \left(\frac{2d\sqrt{\theta_2}}{\theta_1}\right)^{\theta_2} \mathcal{K}_{\theta_2}\left(\frac{2d\sqrt{\theta_2}}{\theta_1}\right), \quad \theta_1 > 0, \theta_2 > 0,
   \]
   where \(\mathcal{K}_{\theta_2}(\cdot)\) is the modified Bessel function.

   - Range parameter, \(\theta_1\), controls the rate of decay of the correlation between observations as distance increases.
   - Smoothness parameter, \(\theta_2\), controls the smoothness of the random field.
AIC for Spatial Models

Background on AIC

Burnham and Anderson (1998), and McQuarrie and Tsai (1998)

Suppose

- \( Z \sim f_T \)
- \( \{ f(\cdot; \psi), \psi \in \Psi \} \) is a family of candidate probability density functions

The Kullback-Leibler information between \( f(\cdot; \psi) \) and \( f_T \)

\[ I(\psi) = \int -2 \log \left( \frac{f(z | \psi)}{f_T(z)} \right) f_T(z) dz. \]

- distance between \( f(\cdot; \psi) \) and \( f_T \)
- similar to the notion of relative entropy
- loss of information when \( f(\cdot; \psi) \) is used instead of \( f_T \).
AIC for Spatial Models

By Jensen’s inequality,

\[ I(\psi) \geq 0 \quad \text{if and only if} \quad f(z; \psi) = f_T(z) \quad \text{a.e.} \ [f_T] \]

Basic idea: minimize the Kullback-Leibler index

\[ \Delta(\psi) = \int -2 \log (f(z | \psi)) f_T(z) d\mathbf{z} \]

\[ = E_T(-2 \log L_Z(\psi)) , \]

where \( L_Z(\psi) \) is the likelihood based on the data \( \mathbf{Z} \).
Model Selection and Spatial Correlation

Traditional approach to model selection:

1. Select explanatory variables to model the large scale variation.
2. Estimate parameters using residuals from model in step 1.
3. Iterate.

Limitations:

- Ignores potential confounding between explanatory variables and correlation in spatial process
- Ignoring autocorrelation function can mask importance of explanatory variables

Simulations: Compare model selection performance of AIC for independent error regression model and geostatistical model
Model Selection: Simulation Set-up

1. **Sampling Design:** 100 locations simulated in a random pattern.

2. **Explanatory Variables:** Five possible explanatory variables:
   \[ X_1, X_2, X_3, X_4, X_5 \sim \sqrt{\frac{12}{10}} t_{12} \]

3. **Response:**
   \[ Z = 2 + 0.75X_1 + 0.50X_2 + 0.25X_3 + \delta, \]
   where \( \delta \) is a Gaussian random field with mean zero, \( \sigma^2 = 50 \), and autocorrelation Matern with parameters \( \theta_1 = 4 \) and \( \theta_2 = 1 \).

4. **Replicates:** 500 replicates were simulated with a new Gaussian random field generated for each replication.

5. **AIC:** Computed for \( 2^5 = 32 \) possible models per replicate
Model Selection: Random Pattern Sampling Design
Independent AIC and Spatial AIC report the percentage of simulations that each model was selected.

Of the 32 possible models, the results given here include only those with 10% or more support for one of the models.

<table>
<thead>
<tr>
<th>Variables in Model</th>
<th>Spatial AIC</th>
<th>Independent AIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_1, X_2, X_3$</td>
<td>46</td>
<td>0</td>
</tr>
<tr>
<td>$X_1, X_2$</td>
<td>18</td>
<td>6</td>
</tr>
<tr>
<td>$X_1, X_2, X_3, X_5$</td>
<td>11</td>
<td>0</td>
</tr>
<tr>
<td>Intercept only</td>
<td>0</td>
<td>37</td>
</tr>
<tr>
<td>$X_1$</td>
<td>1</td>
<td>18</td>
</tr>
<tr>
<td>$X_2$</td>
<td>0</td>
<td>12</td>
</tr>
</tbody>
</table>
Model Selection: Independent model AIC Values

![Model Selection Diagram](image-url)
Model Selection: Spatial model AIC Values
Sampling Patterns

Highly Clustered

Lightly Clustered

Random Pattern

Regular Pattern

Grid Design
Model Selection: Effect of Sampling Design

Summary of model selection results for 5 different sampling patterns

<table>
<thead>
<tr>
<th>Variables in Model</th>
<th>Highly Clustered</th>
<th>Lightly Clustered</th>
<th>Random</th>
<th>Regular Pattern</th>
<th>Grid Design</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_1, X_2, X_3$</td>
<td>73</td>
<td>65</td>
<td>46</td>
<td>43</td>
<td>16</td>
</tr>
<tr>
<td>$X_1, X_2$</td>
<td>0</td>
<td>2</td>
<td>18</td>
<td>21</td>
<td>35</td>
</tr>
<tr>
<td>$X_1, X_2, X_3, X_4$</td>
<td>12</td>
<td>13</td>
<td>8</td>
<td>8</td>
<td>3</td>
</tr>
<tr>
<td>$X_1, X_2, X_3, X_4$</td>
<td>10</td>
<td>13</td>
<td>11</td>
<td>7</td>
<td>7</td>
</tr>
</tbody>
</table>

- Each column reports the percentage of simulations that each model was selected.
- Of the 32 possible models, the results given here include only those with 10% or more support for at least one of the sampling patterns.
Prediction

Efficient prediction

- Time series (Shibata (1980), Brockwell and Davis (1991)). AIC is an efficient order selection procedure for autoregressive models.
- Regression (see McQuarrie and Tsai (1998)).
- Other notions of efficiency, e.g., Kullback-Leibler efficiency and $L_2$ efficiency (see McQuarrie and Tsai (1998)).
Prediction: Prediction Error

Simulations:

- Performed model selection and estimation using 100 observations and evaluated prediction performance using 100 additional observations simulated as above.
- Evaluated predictive performance

Mean Square Prediction Error:

\[
\text{MSPE} = \frac{1}{100} \sum_{j=1}^{100} (Z_j - \hat{Z}_j)^2
\]

where \( \hat{Z}_j \) is the universal kriging predictor for the \( j^{th} \) prediction location using the true parameter values.
Prediction: MSPE
**Prediction: Predictive Coverage**

Predictive Coverage: for a 95% prediction interval, do 95% of the observed data fall in their corresponding prediction intervals?

**Simulations:**
For each of the 500 simulations, we compute predictive coverage. Then, over all 500 simulations, we examine:

- Mean predictive coverage
- Standard deviation of predictive coverage

<table>
<thead>
<tr>
<th>Model</th>
<th>Mean</th>
<th>Std Dev</th>
</tr>
</thead>
<tbody>
<tr>
<td>Independent error AIC</td>
<td>0.95</td>
<td>0.18</td>
</tr>
<tr>
<td>Spatial error AIC</td>
<td>0.92</td>
<td>0.25</td>
</tr>
</tbody>
</table>
Example: Lizard abundance

Abundance for the orange-throated whiptail lizard in southern California
Ver Hoef et al. (2001)

Data:

- 147 locations
- $Z = \log(\text{ave \# of lizards caught per day})$
- Explanatory variables: ant abundance (three levels), log(\% sandy soils), elevation, barerock indicator, \% cover, log(\% chapparal plants)
Example: Lizard abundance

- Explanatory variables:
  ant abundance (three levels), log(\% sandy soils), \% cover, elevation, barerock indicator, log(\% chapparal plants)

- 160 possible models

<table>
<thead>
<tr>
<th>Predictors</th>
<th>AIC</th>
<th>Spatial Rank</th>
<th>Ind Rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ant(_1), % sand</td>
<td>54.8</td>
<td>1</td>
<td>66</td>
</tr>
<tr>
<td>Ant(_1), Ants(_2), % sand</td>
<td>54.8</td>
<td>2</td>
<td>56</td>
</tr>
<tr>
<td>Ant(_1), % sand, % cover</td>
<td>55.7</td>
<td>3</td>
<td>59</td>
</tr>
<tr>
<td>Ant(_1), Ant(_2), % sand, % cover, elevation, barerock, % chaparral</td>
<td>92.2</td>
<td>41</td>
<td>1</td>
</tr>
<tr>
<td>Ant(_1), Ant(_2), % sand, % cover, elevation, barerock, % chaparral</td>
<td>95.5</td>
<td>33</td>
<td>2</td>
</tr>
<tr>
<td>Ant(_1), % sand, % cover, elevation, barerock,</td>
<td>95.7</td>
<td>38</td>
<td>3</td>
</tr>
</tbody>
</table>
Some Other Approaches to Model Selection and Prediction

- Bayesian Model Averaging
  - Model uncertainty is typically ignored in inference
  - Protect from over-confident inferences by averaging over models

- Minimum Description Length (MDL)
  - Goal: Find model that achieves maximum data compression.

  The code length (CL) of the data (Lee 2001) is the amount of memory required to store the data. Decomposition of CL:

  \[ CL(\text{"data"}) = CL(\text{"fitted model"}) + CL(\text{"data given fitted model"}). \]

  Here \( CL(\text{"fitted model"}) \) might be interpreted as the code length of the model parameters and \( CL(\text{"data given fitted model"}) \) as the code length of the residuals from the fitted model.
Conclusions

- Ignoring spatial correlation can influence model selection results for both covariate selection and prediction.
- Sampling patterns that offer observation pairs at small and larger distances may be advantageous for model selection.
- Preliminary results suggest that accounting for spatial correlation can have large effects on prediction errors, but perhaps smaller impacts on predictive coverage.