Model Selection for Geostatistical Models

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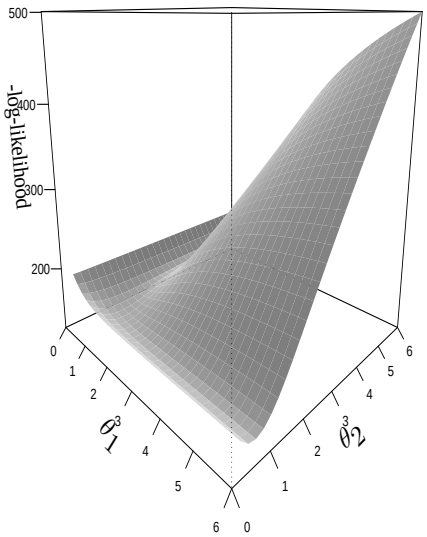
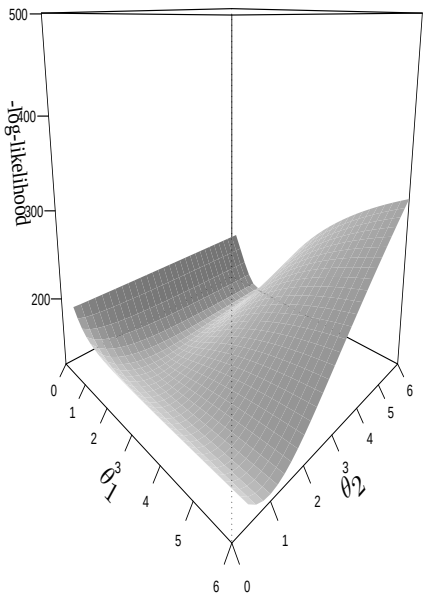
paper: `www.stat.colostate.edu/~jah/papers/spavarsel.pdf`
software: `www.stat.colostate.edu/~jah/software/matern.R`

NULL Model



True Model



Model Selection for Geostatistical Models

MOTIVATION

- Many investigators have looked at model selection but not in context of geostatistical models.
- We will show that ignoring the spatial dependence in the error structure can have a profound effect on the model selected.

Consider a problem where we observe some response Z at n locations such that $\boldsymbol{Z} = (Z(s_1), \ldots, Z(s_n))'$.

- At each location we also observe $p-1$ explanatory variables, *i.e.*, at location s we observe $X_1(s), \ldots, X_{p-1}(s)$.

A linear model for Z is given by

$$Z(s) = \beta_0 + X_1(s)\beta_1 + \cdots + X_{p-1}(s)\beta_{p-1} + \delta(s).$$

- Which explanatory variables should be included?
- What is the form of the model for $\delta(s)$?

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 or interpolation (efficiency).
   - Find a model that predicts well at unobserved 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 $\mathbf{Z} = (Z(s_1), \ldots, Z(s_n))'$ be a partial realization of a random field $\mathbf{Z}(s)$, where $s \in D$, a fixed finite area under study.

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

$$Z(s) = \mathbf{X}'(s)\boldsymbol{\beta} + \delta(s),$$

where

- $\mathbf{X}(s) = (1, X_1(s), \ldots, X_{p-1}(s))'$ is a p-vector of explanatory variables observed at location s,
- $\boldsymbol{\beta}$ is a p-vector of unknown coefficients, and
- $\delta(s)$ is the unobserved regression error at location s.

We assume that the error process $\delta(s)$ is a stationary, isotropic Gaussian process with mean zero and covariance function

$$\text{Cov}(\delta(s), \delta(t)) = \sigma^2 \rho(d, \boldsymbol{\theta}),$$

where

- σ^2 is the variance of the process,
- $d = ||s - t||$ is the Euclidean distance between locations s and t, and
- $\rho(\cdot, \boldsymbol{\theta})$ is an isotropic correlation function depending on a k dimensional parameter vector $\boldsymbol{\theta}$.

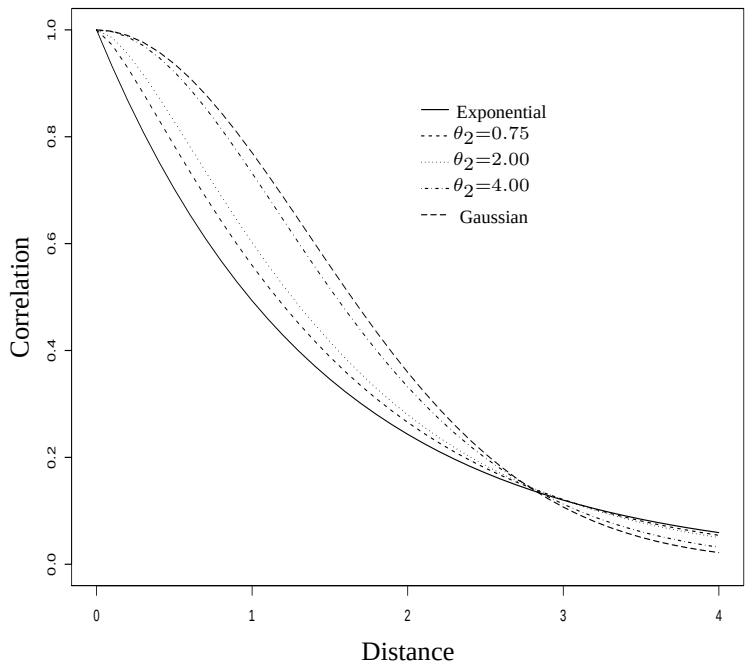
Matérn Autocorrelation Function

The Matérn autocorrelation function is defined as

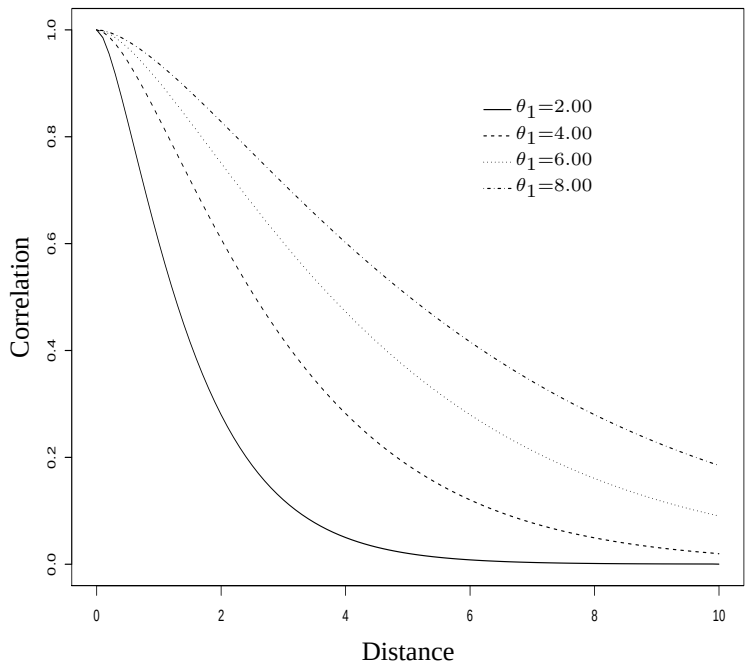
$$\rho(d, \boldsymbol{\theta}) = \frac{1}{2^{\theta_2 - 1}\Gamma(\theta_2)} \left(\frac{2d\sqrt{\theta_2}}{\theta_1} \right)^{\theta_2} \mathcal{K}_{\theta_2} \left(\frac{2d\sqrt{\theta_2}}{\theta_1} \right), \qquad \theta_1, \theta_2 > 0,$$

where $\mathcal{K}_{\theta_2}(\cdot)$ is the modified Bessel function.

Fixed range parameter, $\theta_1 = 4.00$



Fixed smoothness parameter, $\theta_2 = 1.00$



Estimation

Parameter estimation can proceed using one of several likelihood based approaches or a Bayesian approach. Here we consider the former.

The log-likelihood of the parameters $\left(\boldsymbol{\theta}, \boldsymbol{\beta}, \sigma^2\right)$ given the data, $\boldsymbol{Z}$, is

$$\log L_{\boldsymbol{Z}}\left(\boldsymbol{\beta}, \boldsymbol{\theta}, \sigma^2\right) \propto -\frac{1}{2}\log\left|\sigma^2\boldsymbol{\Omega}\right| - \frac{1}{2\sigma^2}\left(\boldsymbol{Z}-\boldsymbol{X}\boldsymbol{\beta}\right)'\boldsymbol{\Omega}^{-1}\left(\boldsymbol{Z}-\boldsymbol{X}\boldsymbol{\beta}\right),$$

where $\boldsymbol{\Omega} = [\rho(d, \boldsymbol{\theta})]$ represents the matrix of correlations between all pairs of observations.

Estimation can proceed via an iterative maximum (profile) likelihood approach or via a restricted maximum likelihood (REML) approach.

- Although REML estimates often have more desirable sampling properties, their performance for model selection is not clear.

The resulting log *profile* likelihood is

$$\ell_{profile}(\boldsymbol{\theta}; \hat{\boldsymbol{\beta}}, \hat{\sigma}^2, \boldsymbol{Z}) = -\frac{1}{2}\log|\boldsymbol{\Omega}| - \frac{n}{2}\log\left(\hat{\sigma}^2\right) - \frac{n}{2},$$

where

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{\Omega}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Omega}^{-1}\boldsymbol{Z} \quad \text{and} \quad \hat{\sigma}^2 = \frac{1}{n}(\boldsymbol{Z}-\boldsymbol{X}\hat{\boldsymbol{\beta}})'\boldsymbol{\Omega}^{-1}(\boldsymbol{Z}-\boldsymbol{X}\hat{\boldsymbol{\beta}}).$$

AIC for Geospatial Models

Suppose

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

The Kullback-Leibler information between $f(\cdot;\psi)$ and f_T is defined by

$$I(\psi) = \int -2\log\left(\frac{f(\boldsymbol{z};\psi)}{f_T(\boldsymbol{z})}\right) f_T(\boldsymbol{z})d\boldsymbol{z}.$$

- Measures the distance between $f(\cdot;\psi)$ and f_T.
- Quantifies the loss of information when $f(\cdot;\psi)$ is used as the model for the data instead of f_T.

The quantity

$$AICC = -2\log L_Z(\hat{\beta},\hat{\theta},\hat{\sigma}^2) + 2n\frac{p+k+1}{n-p-k-2},$$

referred to as the corrected AIC, is an approximately unbiased estimate of the expected Kullback-Leibler information.

Model Selection and Spatial Correlation

Traditional approach to model selection:

1. Select explanatory variables to model the large scale variation.
   - Select the best set of explanatory variables *without* considering the dependence between locations.
2. Estimate correlation function parameters using residuals from model in step 1.
3. Re-estimate regression parameters using GLS.
4. Iterate steps 2 and 3.

Limitations:

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

Proposed Solution – Fit all candidate models assuming dependence between locations and select the model(s) with the smallest spatial AICC.

Model Selection: Simulation Set-up

Simulations: Compare model selection performance of AICC for independent error regression model and geostatistical model.

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

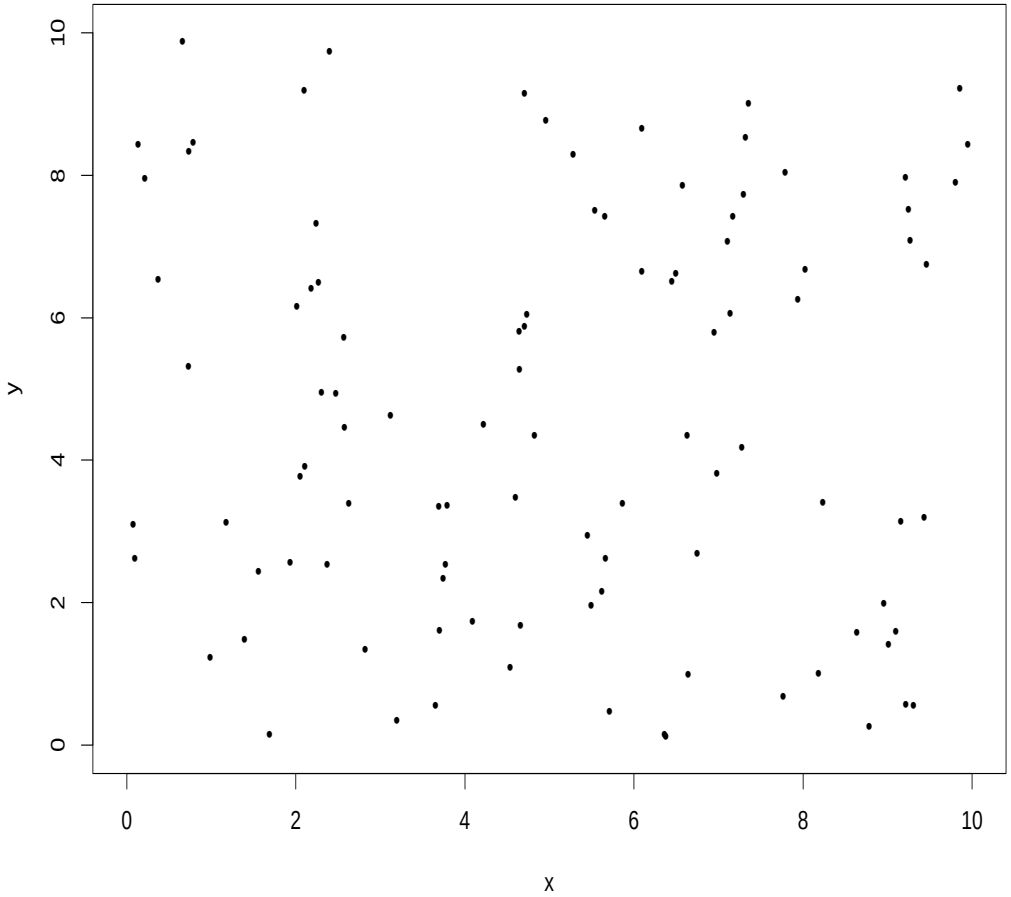
2. **Explanatory Variables:** Five possible explanatory variables such that $X_1, X_2, X_3, X_4, X_5 \overset{iid}{\sim} \sqrt{\frac{10}{12}}\, t_{12}$.

3. **Response:**
$$\boldsymbol{Z} = 2 + 0.75\boldsymbol{X}_1 + 0.50\boldsymbol{X}_2 + 0.25\boldsymbol{X}_3 + \boldsymbol{\delta},$$
where $\boldsymbol{\delta}$ is a Gaussian random field with mean zero, $\sigma^2 = 50$, and autocorrelation Matérn 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. **AICC:** Computed for $2^5 = 32$ possible models per replicate.

Model Selection: Random Pattern Sampling Design



Model Selection: Simulation Results for the Random Pattern

- Independent AICC and Spatial AICC 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.
- The two methods agree only 17 times over the 500 simulations (3.4%).

Variables in Model	Spatial AICC	Independent AICC
$\boldsymbol{X}_1, \boldsymbol{X}_2, \boldsymbol{X}_3$	56.0	2.4
$\boldsymbol{X}_1, \boldsymbol{X}_2, \boldsymbol{X}_3, \boldsymbol{X}_5$	14.4	0.2
$\boldsymbol{X}_1, \boldsymbol{X}_2, \boldsymbol{X}_3, \boldsymbol{X}_4$	10.8	0.2
$\boldsymbol{X}_1, \boldsymbol{X}_2$	10.2	8.4
Intercept only	0.0	26.8
$\boldsymbol{X}_1$	0.4	14.2
$\boldsymbol{X}_2$	0.0	13.8

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.

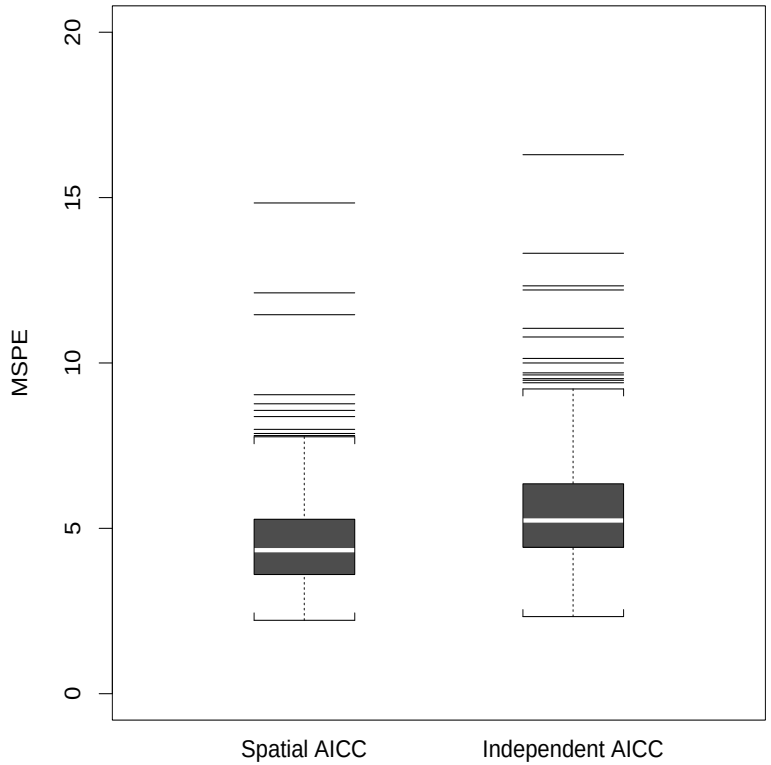
Mean Square Prediction Error:

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

where Z_j is the true value at location j and $\hat{Z}_j$ is the *universal kriging* predictor at location j using the maximum likelihood estimates of the parameter values, $(\hat{\beta}, \hat{\sigma}^2, \hat{\theta})$.

Prediction: Mean Square Prediction Error (MSPE)

- The mean MSPE for the spatial AICC is 16.9% smaller than that of the independent AICC.
- Spatial AICC reduces the mean MSPE by 39.6% if the noise is assumed to be independent.



Prediction: Predictive Coverage

For a 95% prediction interval, do 95% of the observed data fall in their corresponding prediction intervals?

Simulations:

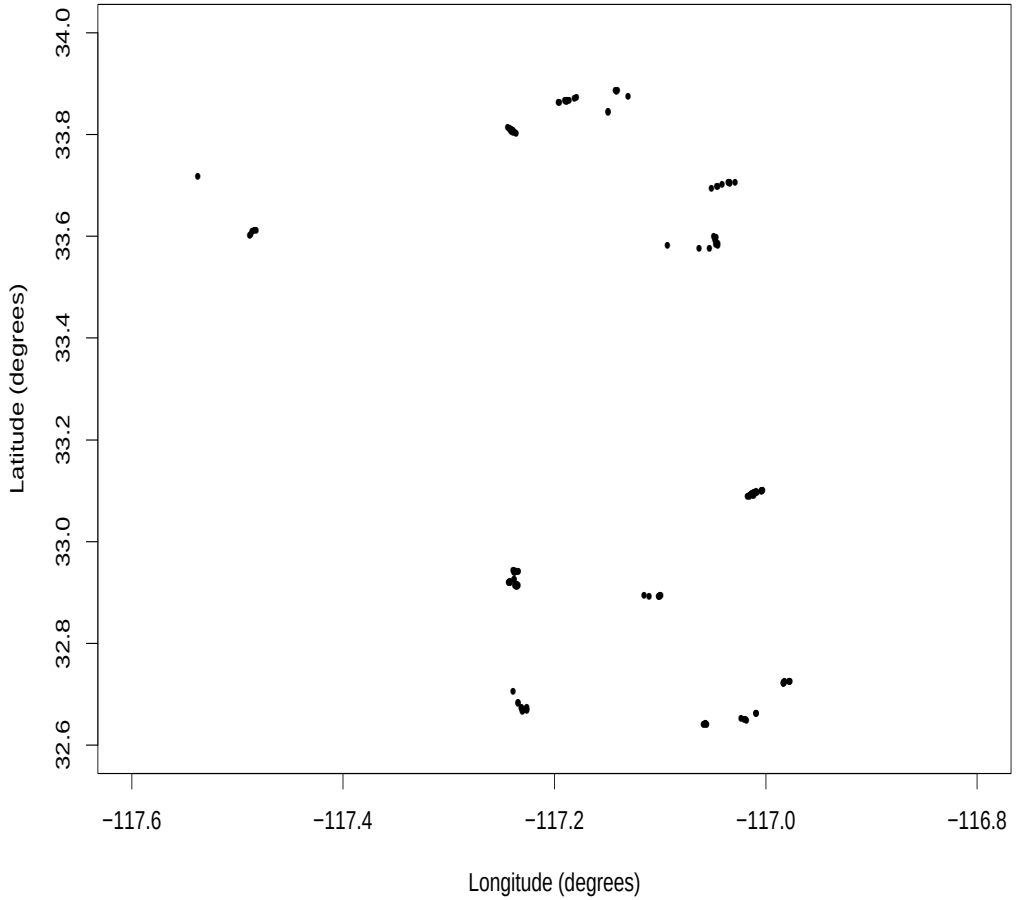
- For each of the 500 simulations, we compute predictive coverage and examine
  - the mean predictive coverage.
  - the standard error of predictive coverage.

Model Selection Procedure	Mean	Std Error
Independent AICC	0.95	0.008
Spatial AICC	0.92	0.011

Application: Lizard Abundance

- Applied the model selection strategy to the orange-throated whiptail lizard data set (Ver Hoef *et al.* (2001)).
  - Response variable is $\log$(lizard abundance) at 148 highly clustered sites throughout southern California.
  - Explanatory variables include a single catergorical variable and five continuous variables for a total of $5 \times 2^5 = 160$ unique models.
- The model selected coincides with that of Ver Hoef *et al.*
  - The selected model contains variables 1 and 4 only.
- Generated 100 simulated response data sets using the selected model and applied the spatial AICC model selection procedure.

Application: Sampling Pattern for the Lizard Abundance Study



Model Selection: Simulation Results for the Lizard Abundance Data

- Independent AICC and Spatial AICC report the percentage of simulations that each model was selected.
- Of the 160 possible models, the results given here include only those with 10% or more support for one of the models.

Variables in Model	Spatial AICC	Independent AICC
$\boldsymbol{X}_1, \boldsymbol{X}_4$	75.0	5.0
$\boldsymbol{X}_1, \boldsymbol{X}_4, \boldsymbol{X}_5, \boldsymbol{X}_8$	1.0	10.0

Conclusions

- We advise against ignoring spatial correlation when selecting explanatory variables.
  - Model choice for prediction should involve *joint* selection of the explanatory variables and the form of the autocorrelation function.
- The model selection methodology presented here can be easily adapted for use with other information criterion.
  - Bayesian Information Criterion (BIC).
  - Minimum Description Length (MDL).
- The sampling pattern can severely impact model selection (complete results not presented here).
  - Simulation studies demonstrate that this selection methodology is even more successful for lightly and heavily clustered sampling patterns.

Additional Ongoing Work

- Model Selection: We are investigating the asymptotic behavior of AIC as a function of *infill* and *expanding domain*.
- Geostatistics: We are looking at the impact of fitting (or failing to fit) a nugget parameter during modeling.

Paper, Software, & Acknowledgements

- We have made a copy of the paper and the simulation software available.
  - Paper: `www.stat.colostate.edu/~jah/papers/spavarsel.pdf`
    email: `merton@stat.colostate.edu`
  - Software: `www.stat.colostate.edu/~jah/software/matern.R`
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