Course content

1. Kriging
   1. Gaussian regression
   2. Simple kriging
   3. Ordinary and universal kriging
   4. Effect of estimated covariance
   5. Bayesian kriging

2. Spatial covariance
   1. Isotropic covariance in $\mathbb{R}^2$
   2. Covariance families
   3. Parametric estimation
   4. Nonparametric models
   5. Fourier analysis
   6. Covariance on a sphere
3. Nonstationary structures I: deformations
1. Linear deformations
2. Thin-plate splines
3. Classical estimation
4. Bayesian estimation
5. Other deformations

4. Markov random fields
1. The Markov property
2. Hammersley-Clifford
3. Ising model
4. Gaussian MRF
5. Conditional autoregression
6. The non-lattice case

5. Nonstationary structures II: linear combinations etc.
1. Moving window kriging
2. Integrated white noise
3. Spectral methods
4. Testing for nonstationarity
5. Wavelet methods

6. Space-time models
1. Mean surface
2. Separability
3. A simple non-separable model
4. Stationary space-time processes
5. Space-time covariance models
6. Testing for separability
7. The Le-Zidek approach
### 7. Statistics, data and deterministic models
1. The kriging approach
2. Bayesian hierarchical models
3. Bayesian melding
4. Data assimilation
5. Model approximation

### 8. Statistics of compositions
1. An algebra for compositions
2. The logistic normal distribution
3. Source apportionment
4. Analysis of variance
5. A space-time model

### 9. Wavelet tools
1. Basic wavelet theory
2. Multiscale analysis
3. Longterm memory models
4. Wavelet analysis of trends

### 10. Setting air quality standards
1. Bayesian model averaging
2. Standards as hypothesis tests
3. Potential network bias
4. Maxima of spatial processes
5. Operational evaluation of air quality standards
Programs

R
  geoR
  fields
  spBayes
  RandomFields

GMRFLib: a C-library for fast and exact simulation of Gaussian Markov random fields

Course requirements

Submit at least 8 homework problems (3 can be replaced by an approved project)
Submit at least three lab reports

Every other Thursday will be a lab day.
Virtual lab machine (get Remote Desktop Connection)
Office hours

MTh 10-11 B213 Padelford
Skype name: guttorp

Homework solutions and lab reports must be submitted electronically

Kriging

NRCSE
**Research goals in environmental research**

Calculate pollution fields for health effect studies

Assess deterministic models against data

Interpret and set environmental standards

Improve understanding of complicated systems

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**The geostatistical model**

Gaussian process $Z(s), s \in D \subseteq R^2$

$\mu(s)=EZ(s)$ $\text{Var} Z(s) < \infty$

$Z$ is **strictly stationary** if

$Z(s_1), ..., Z(s_k))=Z(s_1 + h), ..., Z(s_k + h))$

$Z$ is **weakly stationary** if

$\mu(s) = \mu$ $\text{Cov}(Z(s_1), Z(s_2)) = C(s_1 - s_2)$

$Z$ is **isotropic** if weakly stationary and

$C(s_1 - s_2) = C_0(\|s_1 - s_2\|)$
The problem

Given observations at n locations
\[ Z(s_1), \ldots, Z(s_n) \]
estimate
\[ Z(s_0) \] (the process at an unobserved location)
or
\[ \int_A Z(s) \, d\nu(s) \] (an average of the process)

In the environmental context often time series of observations at the locations.

Some history

Regression (Bravais, Galton, Bartlett)
Mining engineers (Krige 1951, Matheron, 60s)
Spatial models (Whittle, 1954)
Forestry (Matérn, 1960)
Objective analysis (Gandin, 1961)
More recent work Cressie (1993), Stein (1999)
A Gaussian formula

If \( \begin{pmatrix} X \\ Y \end{pmatrix} \sim N \left( \begin{pmatrix} \mu_X \\ \mu_Y \end{pmatrix}, \begin{pmatrix} \Sigma_{XX} & \Sigma_{XY} \\ \Sigma_{YX} & \Sigma_{YY} \end{pmatrix} \right) \)

then \( (Y \mid X) \sim N(\mu_Y + \Sigma_{YX}\Sigma_{XX}^{-1}(X - \mu_X), \Sigma_{YY} - \Sigma_{YX}\Sigma_{XX}^{-1}\Sigma_{XY}) \)

Simple kriging

Let \( X = (Z(s_1), \ldots, Z(s_n))^T \), \( Y = Z(s_0) \), so that
\[
\begin{align*}
\mu_x &= \mu_{1,n}, & \mu_y &= \mu,
\Sigma_{xx} &= [C(s_i - s_j)], & \Sigma_{yy} &= C(0), \text{ and} \\
\Sigma_{yx} &= [C(s_i - s_0)].
\end{align*}
\]

Then
\[
p(X) = \tilde{Z}(s_0) = \mu + [C(s_i - s_0)]^T \left[ C(s_i - s_j) \right]^{-1} (X - \mu_{1,n})
\]

This is the best unbiased linear predictor when \( \mu \) and \( C \) are known (simple kriging).

The prediction variance is
\[
m_i = C(0) - [C(s_i - s_0)]^T \left[ C(s_i - s_j) \right]^{-1} [C(s_i - s_0)]
\]
Some variants

*Ordinary kriging (unknown \( \mu \))*

\[
p(X) = \hat{Z}(s_0) = \hat{\mu} + [C(s_i - s_0)]^{-1} [C(s_i - s_i)]^{-1} (X - \hat{\mu} 1_n)
\]

where

\[
\hat{\mu} = \left(1_n^T \left[ C(s_i - s_i) \right]^{-1} 1_n \right)^{-1} 1_n^T \left[ C(s_i - s_i) \right]^{-1} X
\]

*Universal kriging (\( \mu(s) = A(s) \beta \) for some spatial variable \( A \))*

\[
\hat{\beta} = (\left[ A(s_i) \right]^T \left[ C(s_i - s_i) \right]^{-1} \left[ A(s_i) \right])^{-1} \\
\left[ A(s_i) \right]^T \left[ C(s_i - s_i) \right]^{-1} X
\]

Still optimal for known \( C \).

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**Universal kriging variance**

\[
E(\hat{Z}(s_0) - Z(s_0))^2 = m_1 + \\
\left( A(s_o) - [A(s_i)]^T [C(s_i - s_i)]^{-1} [C(s_i - s_o)] \right)^T \\
\left( [A(s_i)]^T [C(s_i - s_i)]^{-1} [A(s_i)] \right)^{-1} \\
\times \left( [A(s_i)]^T [C(s_i - s_i)]^{-1} [A(s_i)] \right)^{-1} \\
\times \left( A(s_o) - [A(s_i)]^T [C(s_i - s_i)]^{-1} [C(s_i - s_o)] \right)
\]

variability due to estimating \( \beta \)
Some other kriging variants

Indicator kriging
\[ 1(Z(s_0) > c) \]

Block kriging
\[ \int_{\Lambda} Z(s) \, ds \]

Co-kriging
Using a covariate to improve kriging

Disjunctive kriging
A nonlinear version of kriging: expand the field into CONS and co-krige these

The (semi)variogram
\[ \gamma(||h||) = \frac{1}{2} \text{Var}(Z(s + h) - Z(s)) = C(0) - C(||h||) \]

Intrinsic stationarity
Weaker assumption (C(0) needs not exist)

Kriging predictions can be expressed in terms of the variogram instead of the covariance.
Ordinary kriging

\[ \hat{Z}(s_0) = \sum_{i=1}^{n} \lambda_i Z(s_i) \]

where

\[ \lambda^T = \left( \gamma + 1^{\top} \Gamma^{-1} \gamma \right)^T \Gamma^{-1} \]

\[ \gamma = (\gamma(s_0 - s_1, ..., \gamma(s_0 - s_n))^T \]

\[ \Gamma_{ij} = \gamma(s_i - s_j) \]

and kriging variance

\[ m_i(s_0) = 2 \sum_{i=1}^{n} \lambda_i \gamma(s_0 - s_i) - \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \lambda_j \gamma(s_i - s_j) \]

An example

Ozone data from NE USA (median of daily one hour maxima June–August 1974, ppb)
Fitted variogram

\[ \gamma(t) = e^{2t} + s^2 \]

Kriging surface
Kriging standard error

A better combination
**Effect of estimated covariance structure**

The usual geostatistical method is to consider the covariance known. When it is estimated
- the predictor $p_2(X) = p(X; \hat{\theta}(X))$ is not linear
- nor is it optimal
- the “plug-in” estimate $m_1(\hat{\theta}(X))$ of the variability often has too low mean

Let $m_2(\theta) = E_{\theta}(p_2(X) - \mu)^2$. Is $m_1(\hat{\theta})$ a good estimate of $m_2(\theta)$?

**Some results**

1. Under Gaussianity, $m_2(\theta) \geq m_1(\theta)$ with equality iff $p_2(X) = p(X; \theta)$ a.s.
2. Under Gaussianity, if $\hat{\theta}$ is sufficient, and if the covariance is linear in $\theta$, then
   $$E_{\theta} m_1(\hat{\theta}) = m_2(\theta) - 2(m_2(\theta) - m_1(\theta))$$
3. An unbiased estimator of $m_2(\theta)$ is
   $$2 \hat{m} - m_1(\hat{\theta})$$
   where $\hat{m}$ is an unbiased estimator of $m_1(\theta)$. 
Better prediction variance estimator

(Zimmerman and Cressie, 1992)

\[ m_2(\theta) = m_1(\theta) + \text{tr} \left( \text{Cov}_\theta(\hat{\theta}) \left[ \frac{\partial p(X; \theta)}{\partial \theta} \right] \right) \]

(Taylor expansion)
\[ \text{Var}(Z(s_0; \hat{\theta})) = m_1(\hat{\theta}) + 2 \text{tr} \left[ \text{cov}(\hat{\theta}) \cdot \text{cov}(\nabla Z(s_0; \hat{\theta})) \right] \]

(often approx. unbiased)

A Bayesian prediction analysis takes account of all sources of variability (Le and Zidek, 1992)