Linear geostatistical models

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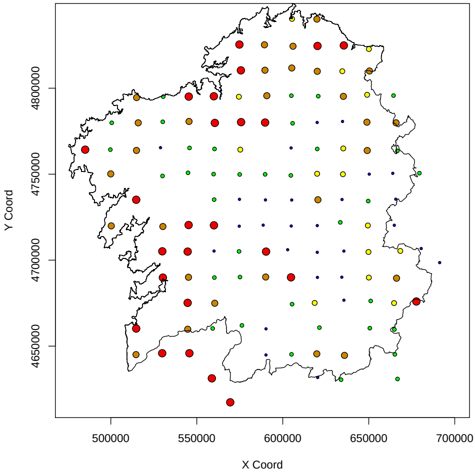
Where we observe matters



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- How do we choose $\rho(\cdot)$?
- Example: $\rho(u) = \exp\{-u/\phi\}$

The theoretical variogram (continued)

$$v(u) = \tau^2 + \sigma^2(1 - \rho(u))$$

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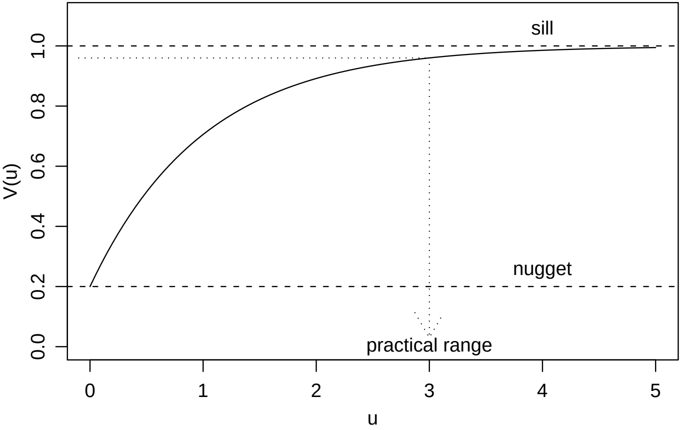

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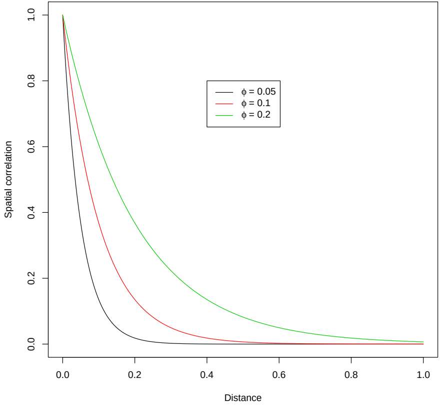

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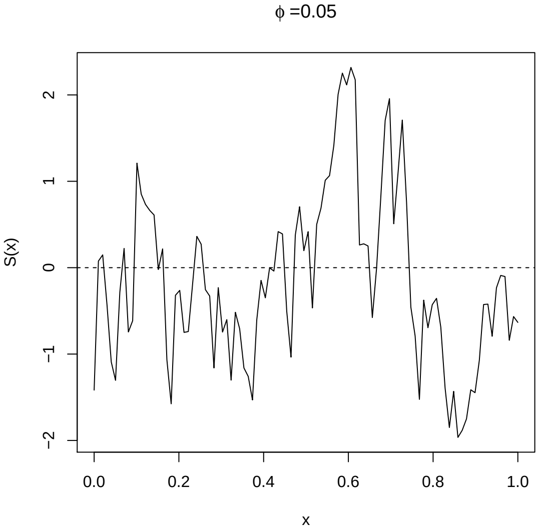

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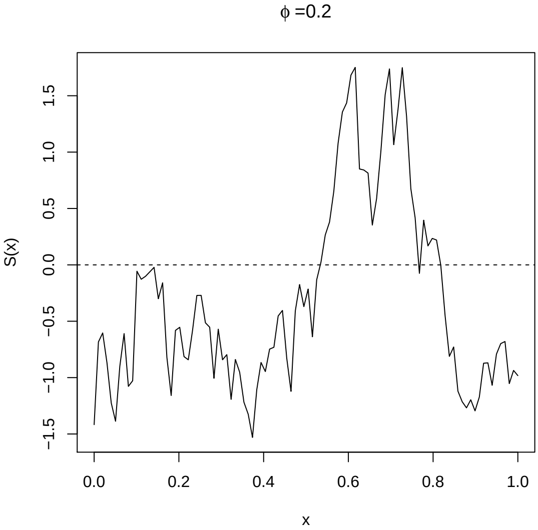

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- Often sufficient to choose amongst $\kappa = 0.5, 1.5, 2.5$

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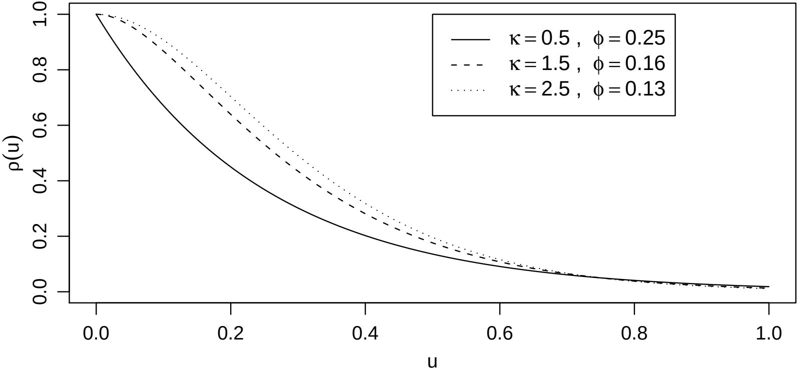

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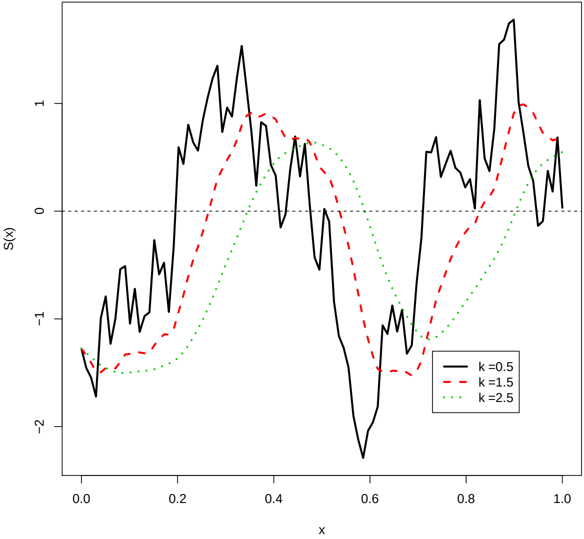

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Y_i &= \alpha + S(x_i) + Z(x_i) \\
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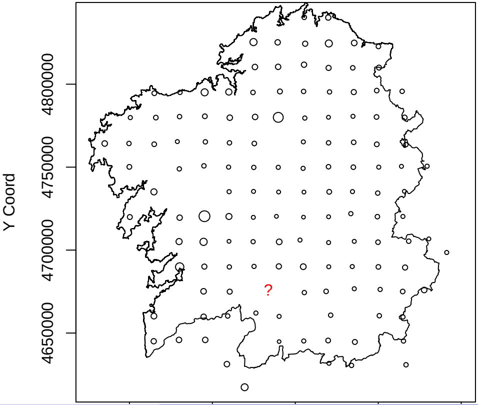
If $u^* < u_{min}$ then $Z(x_i)$ is pure noise.

The canonical geostatistical problem

Given a set of measurements $Y_i : i = 1, \ldots, n$ at locations x_i in a spatial region A, presumed to be (noisy) measurements of a spatially continuous phenomenon $S(x_i)$, what can we say about the realisation of $S(x)$ throughout A?



Getting initial parameter estimates

- Widely used, but not recommended except for initial analysis.
- $\theta = (\sigma^2, \phi, \tau^2)$
- Weighted least squares criterion:

$$W(\theta) = \sum_k n_k [\hat{v}(u_k) - v(u_k; \theta)]^2$$

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- Arbitrary binning and upper limit for u_k.
- Standard errors not available.

Maximum likelihood estimation

Maximum likelihood estimation

- Multivariate Gaussian distribution: $Y \sim MVN(D\beta, \sigma^2 + \tau^2 I)$.
  - D matrix of covariates: $[D]_{ik} = d_k(x_i)$
  - R matrix of spatial correlation: $[R]_{ij} = \rho(u_{ij})$, with $u_{ij} = \|x_i - x_j\|$.

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- Fitting process
  1. Initialise β, e.g. using ordinary least squares.
  2. Initialise θ, e.g. using the empirical variogram
  3. Maximize

     $$l(\theta) = \log\{f(y; \beta, \theta)\}$$

     where $f(\cdot; \beta; \theta)$ denotes the density of the multivariate Gaussian distribution.

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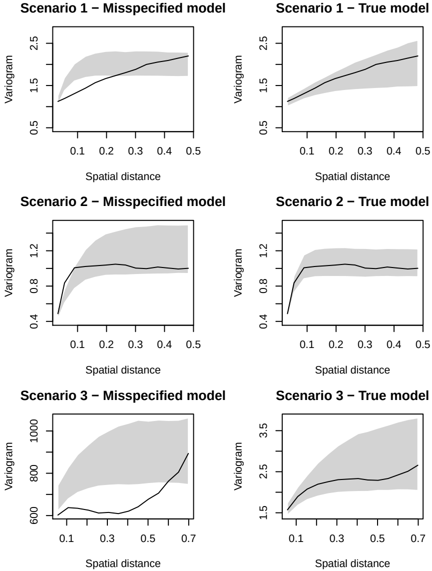
The generated 95% bandwidth from the last step indicates the band of variation for the variogram under the assumed model.

Examples



Scenario 1 − Misspecified model
Scenario 1 − True model
Scenario 2 − Misspecified model
Scenario 2 − True model
Scenario 3 − Misspecified model
Scenario 3 − True model
Variogram
Spatial distance
0.5
1.5
2.5
0.1 0.2 0.3 0.4 0.5
0.4
0.8
1.2
600
800
1000
1.5
2.5
3.5
0.1 0.3 0.5 0.7

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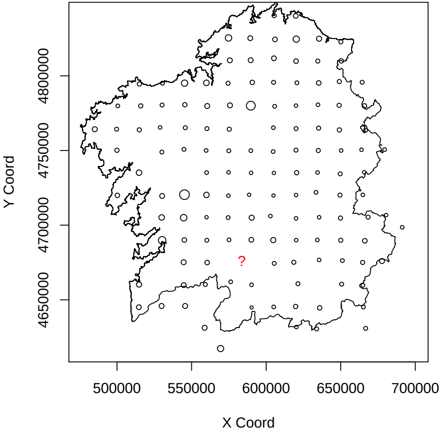


Prediction

The answer to any prediction problem is a probability distribution

Peter McCullagh, FRS

- $T =$ any quantity of scientific interest
- $Y =$ data that can tell us something about T.

The predictive distribution of T is the conditional probability distribution of T given Y

Geostatistical prediction

Let $S^* = \{S(x_1^*), ..., S(x_M^*)\}$ for any set of locations $\{x_1^*, ..., x_M^*\}$

- $Y \sim$ multivariate Normal
- for the Gaussian linear model $S^*|Y \sim$ multivariate Normal
- hence simulate samples of S^* conditional on Y
- corresponding $T^* = \mathcal{T}(S^*)$ are samples from predictive distribution of T

Minimum mean square error prediction

Model

- $[S^*]$ = probability distribution of underlying spatial process
- $[Y|S^*]$ = probability distribution of data conditional on underlying spatial process
- Bayes' theorem then gives us the predictive distribution $[S^*|Y]$

Mean square error

- $\hat{T} = t(Y)$ is a point predictor
- $\text{MSE}(\hat{T}) = \mathrm{E}[(\hat{T} - T)^2]$ is the mean square error

Theorem

1. $MSE(\hat{T})$ takes its minimum value when $\hat{T} = \mathrm{E}(T|Y)$.
2. $\mathrm{Var}(T|Y)$ estimates the achieved mean square error

Simple and ordinary kriging

$$Y \sim \mathrm{MVN}(\mu 1, \sigma^2 V)$$

$$V = R + (\tau^2/\sigma^2) \qquad R_{ij} = \rho(\|x_i - x_j\|)$$

Target for prediction is $T = S(x)$

Write $r = (r_1, ..., r_n)$ where

$$r_i = \rho(\|x - x_i\|)$$

Standard results on multivariate Normal then give $[T|Y]$ as multivariate Gaussian with mean and variance

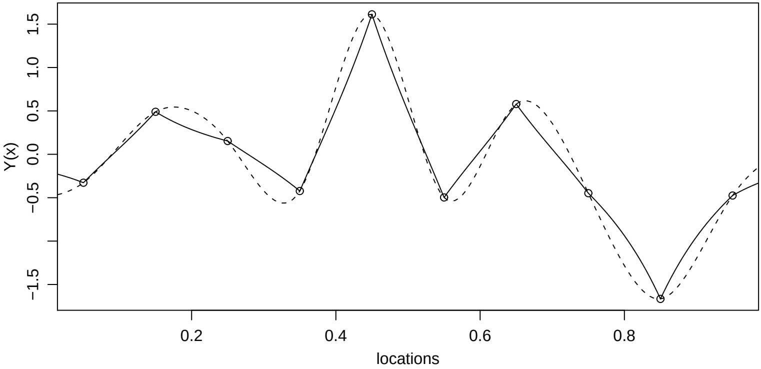
$$\hat{T} = \mu + r' V^{-1}(Y - \mu\mathbf{1})$$

$$\mathrm{Var}(T|Y) = \sigma^2(1 - r' V^{-1} r)$$

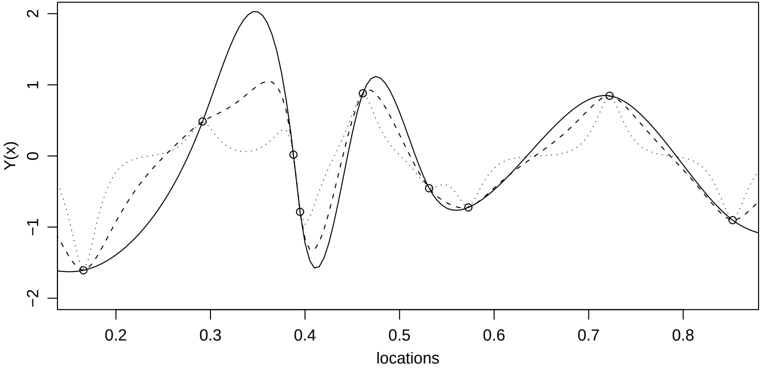
Simple kriging: $\hat{\mu} = \bar{Y}$ Ordinary kriging: $\hat{\mu} = (1' V^{-1} 1)^{-1} 1' V^{-1} Y$

Simple kriging: three examples

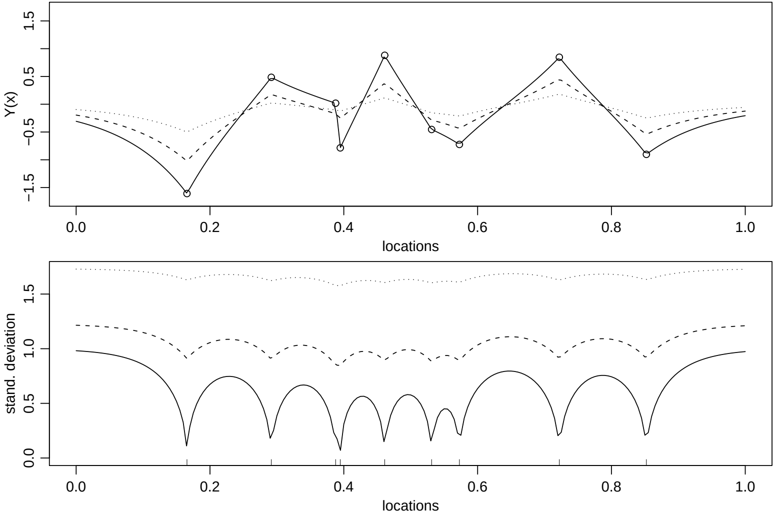
1. Varying κ (smoothness of $S(x)$)



2. Varying ϕ (range of spatial correlation



3. Varying τ^2/σ^2 (noise-to-signal ratio)



Trans-Gaussian models

- assume Gaussian model holds after point-wise transformation
- Box-Cox family is widely used

$$Y_i^* = h_\lambda(Y_i) = \begin{cases} (Y_i^\lambda - 1)/\lambda & \text{if } \lambda \neq 0 \\ \log(Y_i) & \text{if } \lambda = 0 \end{cases}$$

Example: log-Gaussian kriging

- $T(x) = \exp\{S(x)\} \quad \hat{T}(x) = \exp\{\hat{S}(x) + v(x)/2\}$
- $S_1, ..., S_m$ are a sample from $[S|Y]$
- $T_i = \exp(S_i) \Rightarrow T_1, ..., T_m$ are a sample from $[T|Y]$

Reminder: Predicting non-linear functionals

- minimum mean square error prediction is not invariant under non-linear transformation
- the complete answer to a prediction problem is the predictive distribution, $[T|Y]$
- Recommended strategy:
  - draw repeated samples from $[S^*|Y]$
  - calculate required summaries

Bayesian inference

Model specification

$$[Y, \theta] = [\theta][Y|\theta]$$

- $[Y|\theta]$ probability distribution of Y given parameter value θ
- $[\theta]$ prior probability distribution for θ
(before you collect any data)

Parameter estimation

- Bayes' Theorem gives posterior distribution for θ
(adding information from data)

$$[\theta|Y] = [Y|\theta][\theta]/[Y]$$

where $[Y] = \int [Y|\theta][\theta] d\theta$

Bayesian inference for geostatistical models

Model specification

$$[Y, S, \theta] = [\theta][S|\theta][Y|S, \theta]$$

- $[S]$ is an unobserved spatial stochastic process, representng the spatial phenomenon of scientifc interest

Parameter estimation

- integration gives likelihood function

$$[Y, \theta] = \int [Y, S, \theta] dS = [\theta][Y|\theta]$$

- as before, Bayes' Theorem gives posterior distribution

$$[\theta|Y] = [Y|\theta][\theta]/[Y]$$

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Bayesian inference for geostatistical models (2)

Prediction

S denotes the spatial process of interest at data-locations

S^* denotes the same process at data and prediction locations

- expand model specification to

$$[Y, S^*, \theta] = [\theta][S|\theta][Y|S, \theta][S^*|S, \theta]$$

- plug-in predictive distribution is

$$[S^*|Y, \hat{\theta}]$$

- Bayesian predictive distribution is

$$[S^*|Y] = \int [S^*|Y, \theta][\theta|Y]d\theta$$

- for any target $T = t(S^*)$, required predictive distribution $[T|Y]$ follows by direct calculation

Notes

- likelihood function is central to both classical and Bayesian inference
- Bayesian prediction is a weighted average of plug-in predictions, with different plug-in values of θ weighted according to their conditional probabilities given the observed data.
- Bayesian prediction is usually more conservative than plug-in prediction