Spatial Variability: Classical vs. Bayesian Kriging

Tobias Doppler

PhD Seminar

Bayesian Networks and Bayesian Hierarchical Analysis in Engineering

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Eawag: Swiss Federal Institute of Aquatic Science and Technology

Content

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2. Very Short history of kriging
3. General introduction
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6. Example Swiss rainfall data
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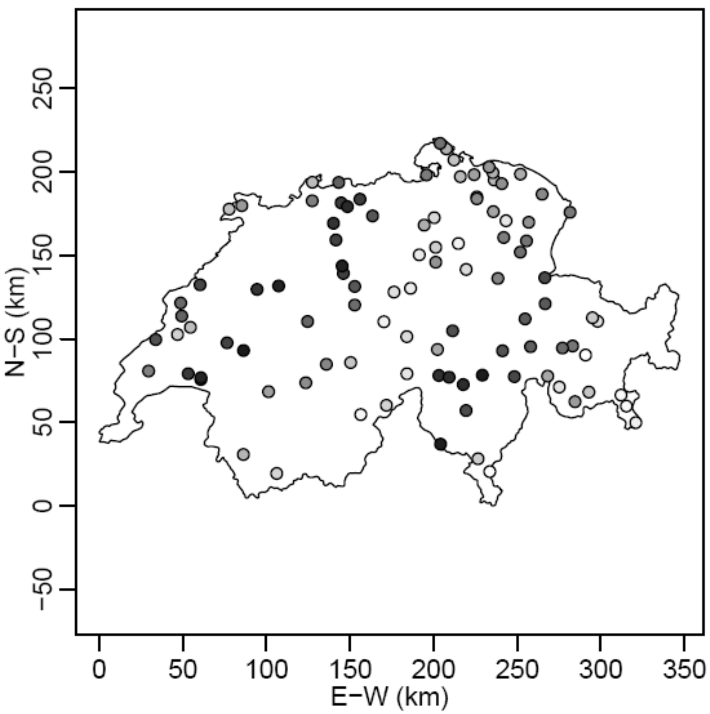
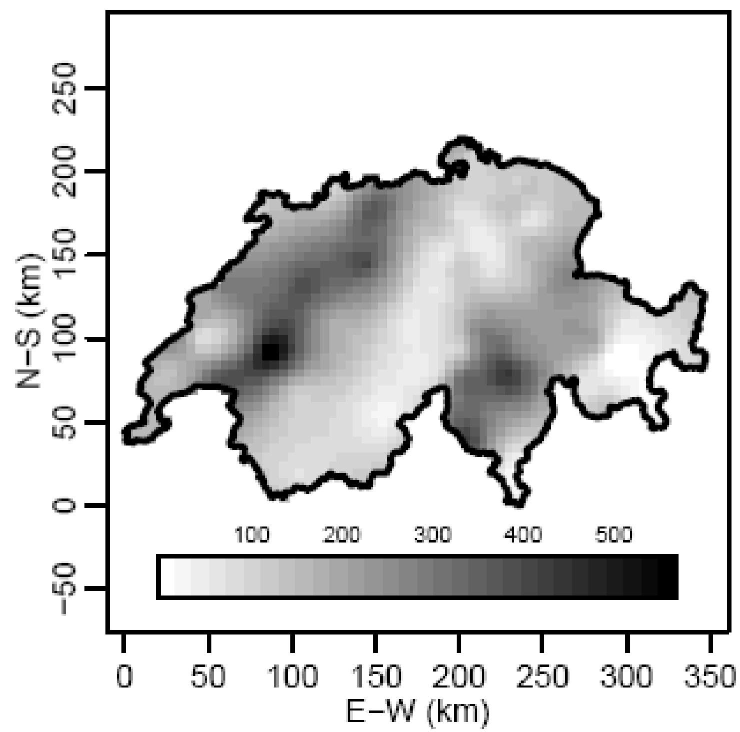
What is Kriging ?

Kriging is a group of geostatistical techniques to interpolate the value of a random field at an unobserved location from observations of its value at nearby locations.
(Wikipedia, Nov. 2009)



Kriging



Example: Rainfall data in Switzerland (From Diggle et al 2003)

History

Daniel Gerhardus Krige: South African Mining Engineer (*1919)

Master Thesis
2 Papers 1951/52
Basis for Kriging

Georges François Paul Marie Matheron: French Mathematician and Geologist (1930 – 2000)
Translated Kriges Papers
Formalized the Approach

Who uses Kriging?

- Mining
- Hydrogeology
- Natural resources
- Environmental science
- Remote sensing
- Black box modelling in computer experiments

(Wikipedia Nov. 2009)

Typs of Kriging

Simple kriging assumes a known constant trend: $\mu(x) = 0$.

Ordinary kriging assumes an unknown constant trend: $\mu(x) = \mu$.

Universal kriging assumes a general linear trend model

IRFk-kriging assumes $\mu(x)$ to be an unknown polynomial in x.

Indicator kriging uses indicator functions instead of the process itself, in order to estimate transition probabilities.

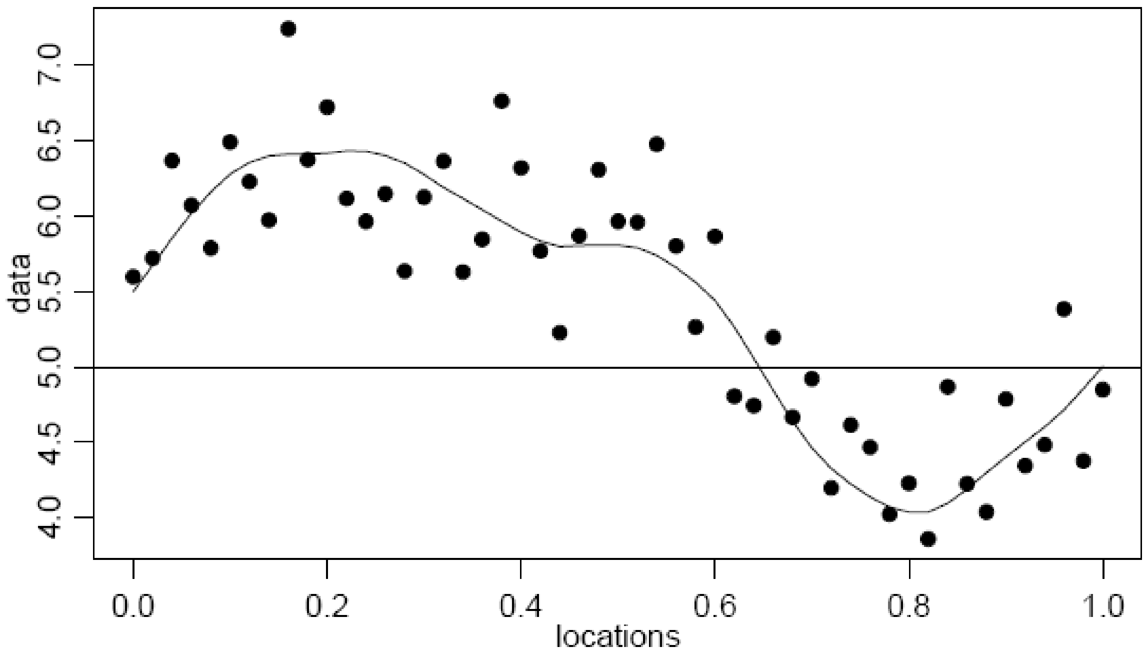
Disjunctive kriging is a nonlinear generalisation of kriging.

Lognormal kriging interpolates positive data by means of logarithms.

(Wikipedia, November 2009)

Basic Assumptions & Notation

- Locations $x=x_1,x_2,\ldots,x_n$ with measurements $y=y_1,y_2,\ldots,y_n$
- y is a realization of a random field Y (measurement process)
- There is an unobserved stochastic process S (signal process)



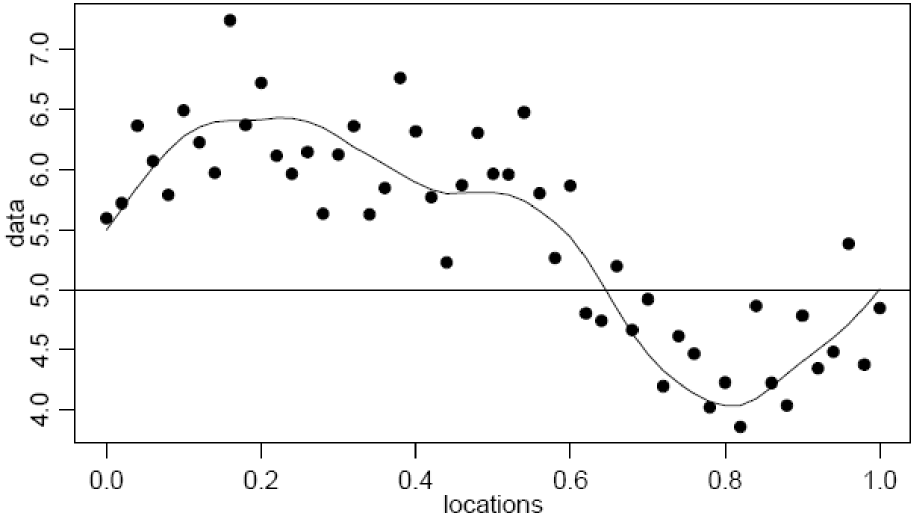
Gaussian Model

- S is a stationary gaussian process with:
  - $E(S(x)) = \mu$, $Var(S(x)) = \sigma^2$
  - Correlation function $\rho(u) = corr(S(x),S(x'))$ with $u = |x-x'|$

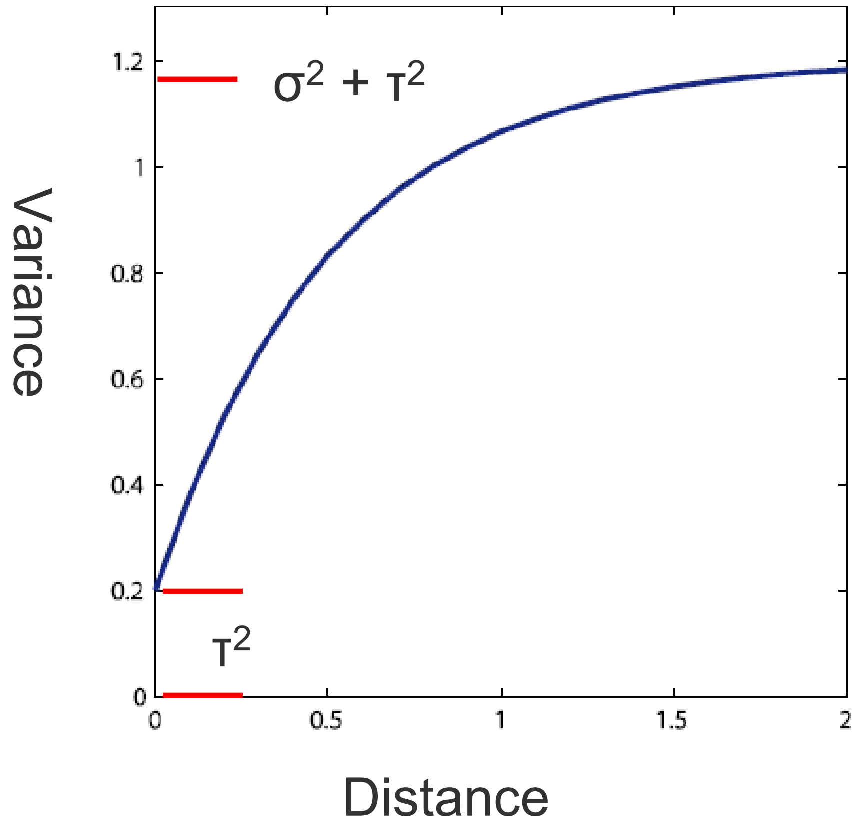
- Conditional distribution of Y_i given S is gaussian with
  - $E(Y_i) = S(x_i)$, $Var(Y_i) = \tau^2$
  - Y_i are mutually independent

$Y_i = S(x_i) + Z_i$: i=1,…,n

$Z_1,\ldots,Z_n$ are independent
With $Z_i \sim N(0, \tau2)$



Presentation of Katharina: Variograms



Correlation Functions

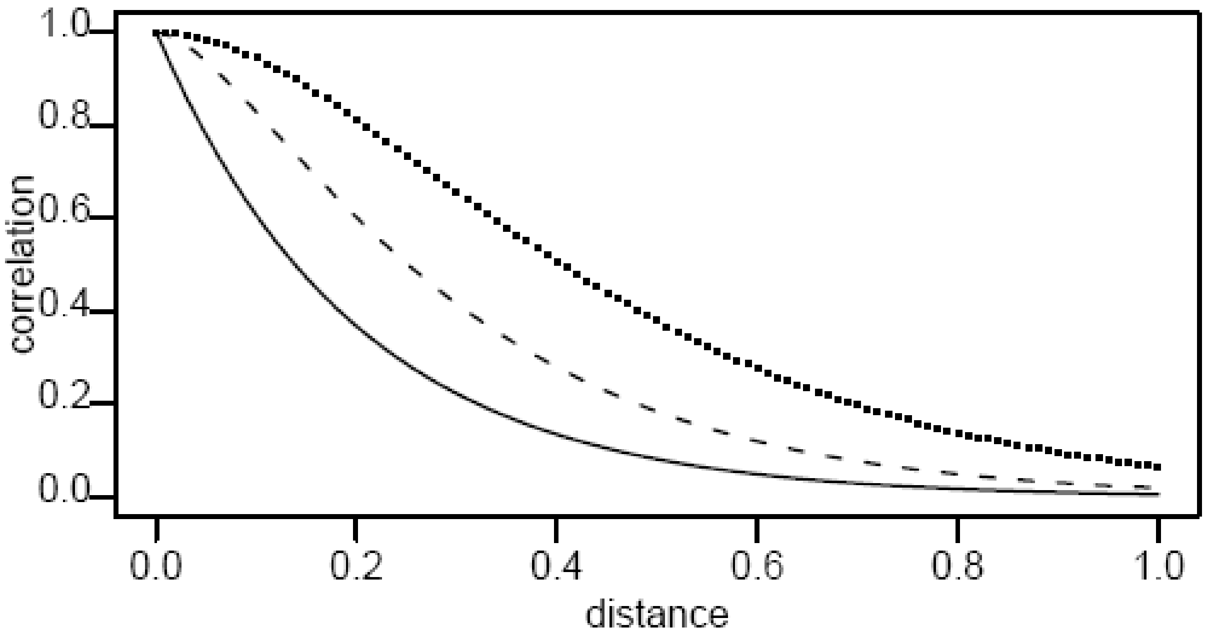


FIGURE 1.4. The Matérn correlation function with $\phi = 0.2$ and $\kappa = 1$ (solid line), $\kappa = 1.5$ (dashed line) and $\kappa = 2$ (dotted line).

$$\rho(u) = \{2^{\kappa-1}\Gamma(\kappa)\}^{-1}(u/\phi)^{\kappa}K_{\kappa}(u/\phi)$$

Gaussian Model

The distribution of Y is multivariate Gaussian

$Y \sim N(\mu\mathbf{1}, \sigma^2 R + \tau^2 I)$

R = correlation matrix

I = identity matrix

1 = vector of 1

$$\begin{bmatrix} \sigma^2\rho(u_{1,1})+\tau^2 & \sigma^2\rho(u_{1,2})+\tau^2 & \cdots \\ \sigma^2\rho(u_{2,1})+\tau^2 & \sigma^2\rho(u_{2,2})+\tau^2 & \cdots \\ \vdots & & \end{bmatrix}$$

$u_{i,j} = | x_i - x_j |$

Correlation Functions

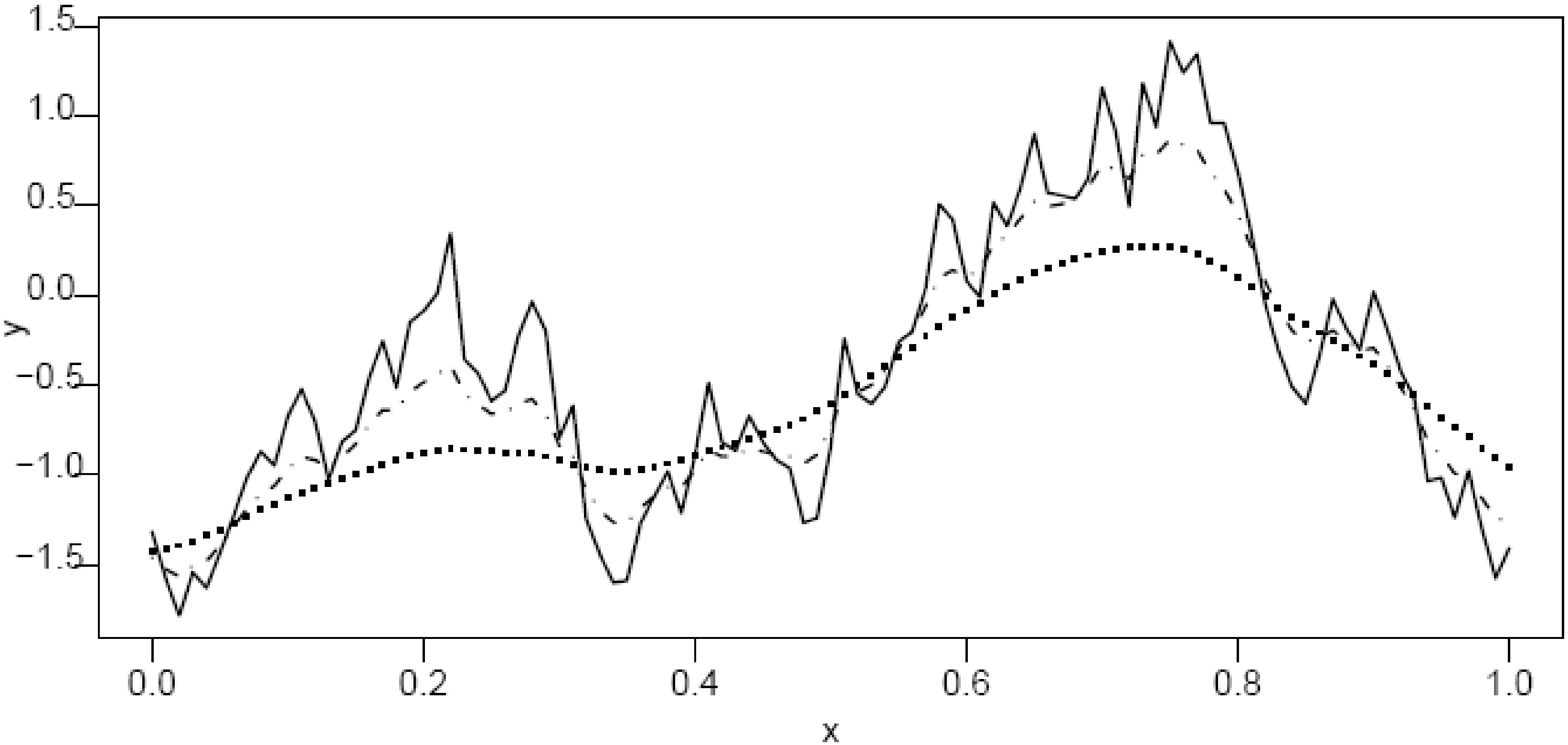


FIGURE 1.7. Simulations of Gaussian processes with Matérn correlation functions, using $\phi = 0.2$ and $\kappa = 0.5$ (solid line), $\kappa = 1$ (dashed line) or $\kappa = 2$ (dotted line).

Prediction under the Gaussian Model

Target of prediction $T = S(x_0)$

Gaussian Model => joint distribution of T and Y is multivariate normal

Conditional distribution T | Y=y is gaussian with

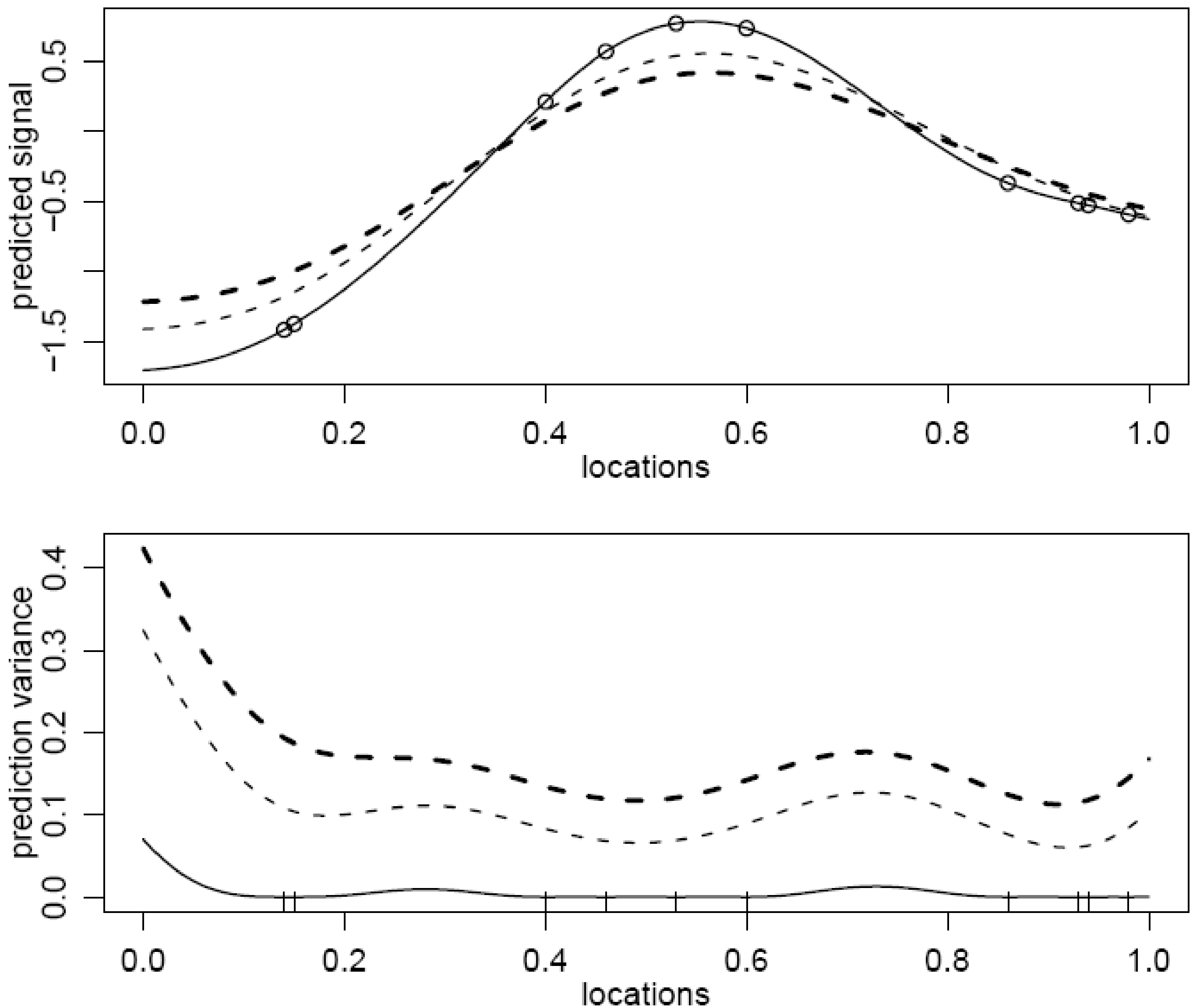
Mean = $\check{T} = \mu + \sigma^2 \mathbf{r}^T (\tau^2 I + \sigma^2 R)^{-1} (y - \mu\mathbf{1})$

$\mathrm{Var}(T \mid y) = \sigma^2 - \sigma^2 \mathbf{r}^T (\tau^2 I + \sigma^2 R)^{-1} \sigma^2 \mathbf{r}$

r = correlation vector

=> Simple Kriging uses $\check{T}$ as predictor at any location x_0

Prediction under the Gaussian Model



Prediction with GLSM

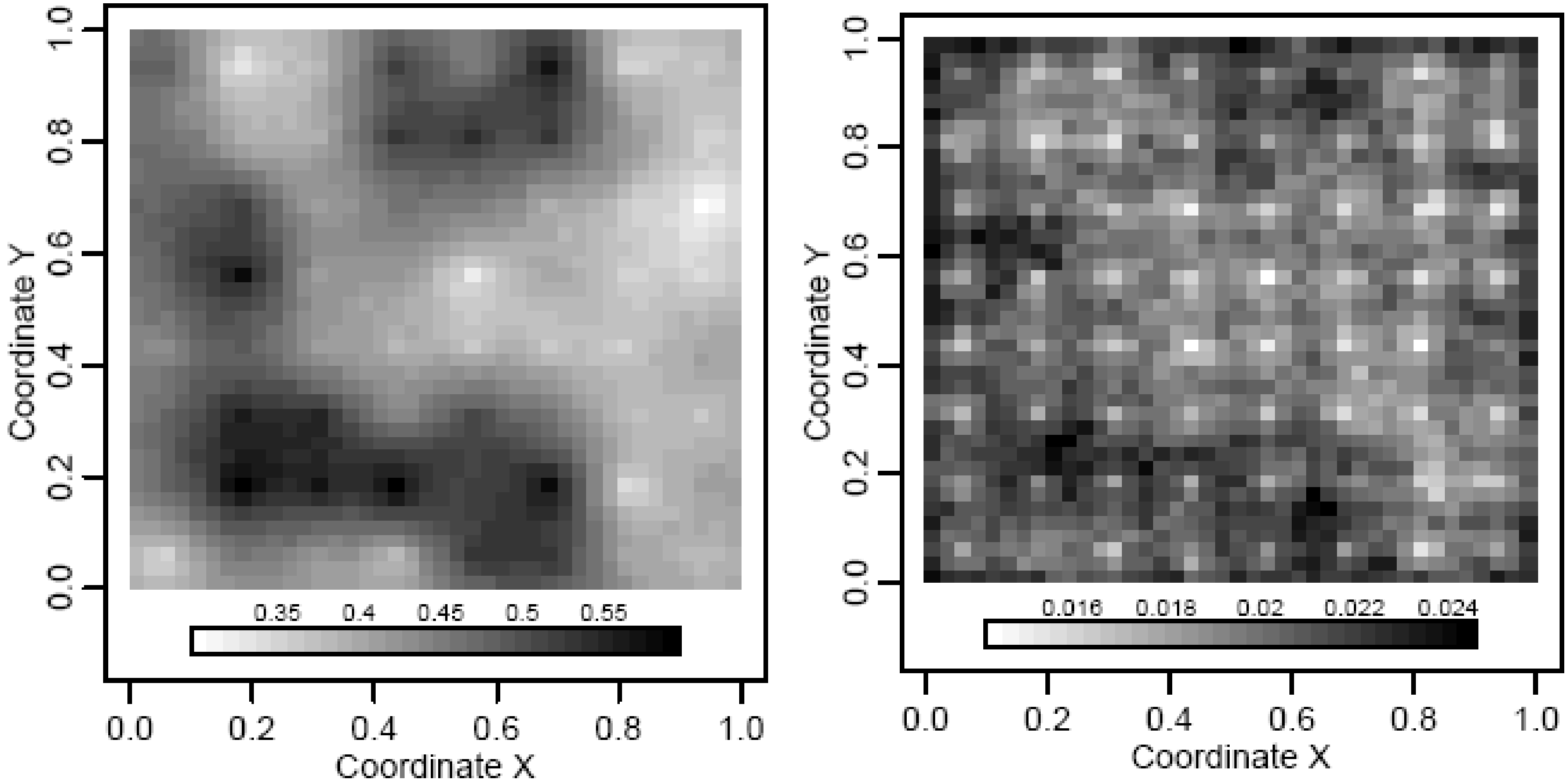


FIGURE 1.19. Left: predicted values at the grid points. Right: prediction variances.

Extensions of Gaussian Model

Anisotropy -> Coordinate transformation (rotation and streching)

Relationship between mean and variance -> Box-Cox Transformation of the data

$$\tilde{y}_i = h_\lambda(y_i) = \begin{cases} (y_i^\lambda - 1)/\lambda & \text{if } \lambda \neq 0 \\ \log y_i & \text{if } \lambda = 0, \end{cases}$$

But models can get too complex:

Over-complex models together with small datasets lead to poor identifiability of model parameters

Plug-in prediction / bayesian inference

Standard approach in geostatistics: Plug-in predicion with **fitted parameters**

Suggestion of Diggle et al: Plug-in predicion with **maximum likelihood estimates** of the parameters

Or use **bayesian inference**

Likelihood Function

Describes the likelihood of a certain parameterset given a model and measured data

Log likelihood function for the gaussian model:

$$
\begin{aligned}
l(\beta, \tau^2, \sigma^2, \phi, \kappa) \quad &\propto \quad -0.5\{\log|(\sigma^2 R + \tau^2 I)| \\
&\quad +(y - F\beta)^{\mathrm{T}}(\sigma^2 R + \tau^2 I)^{-1}(y - F\beta)\}
\end{aligned}
$$

Bayesian inference

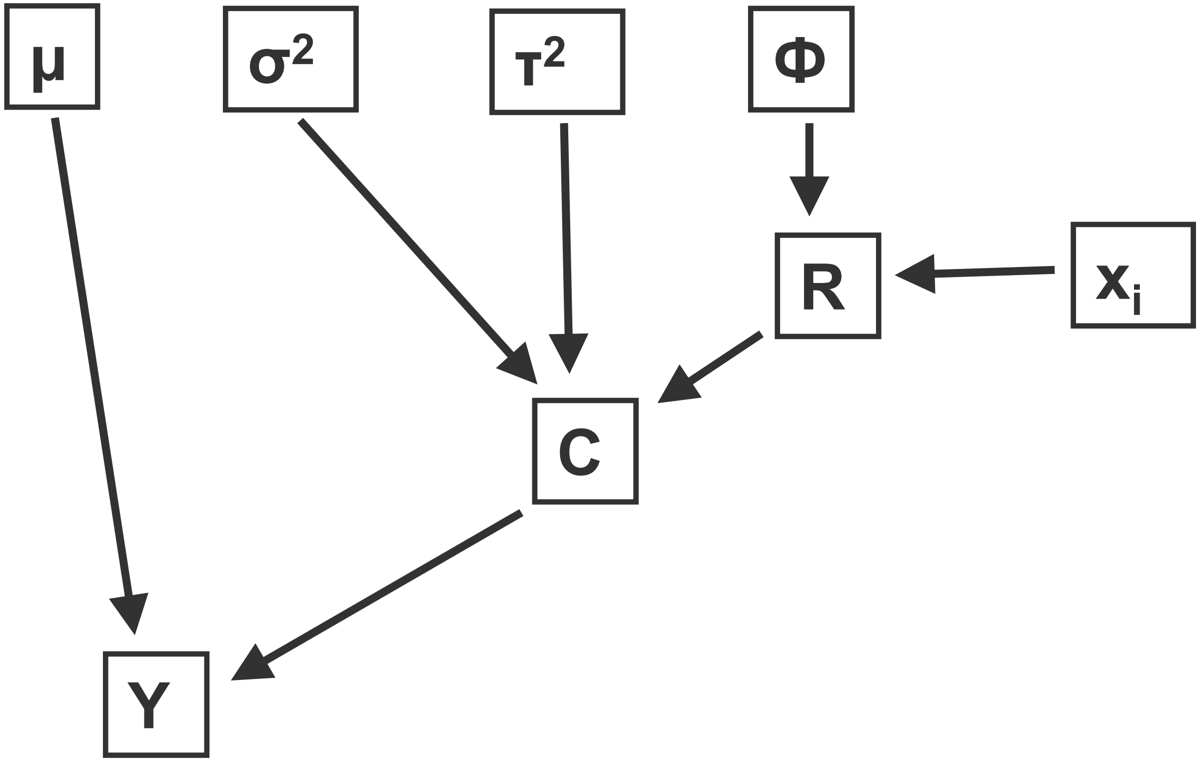
We need:

- Prior distribution of parameters
- Likelihood function

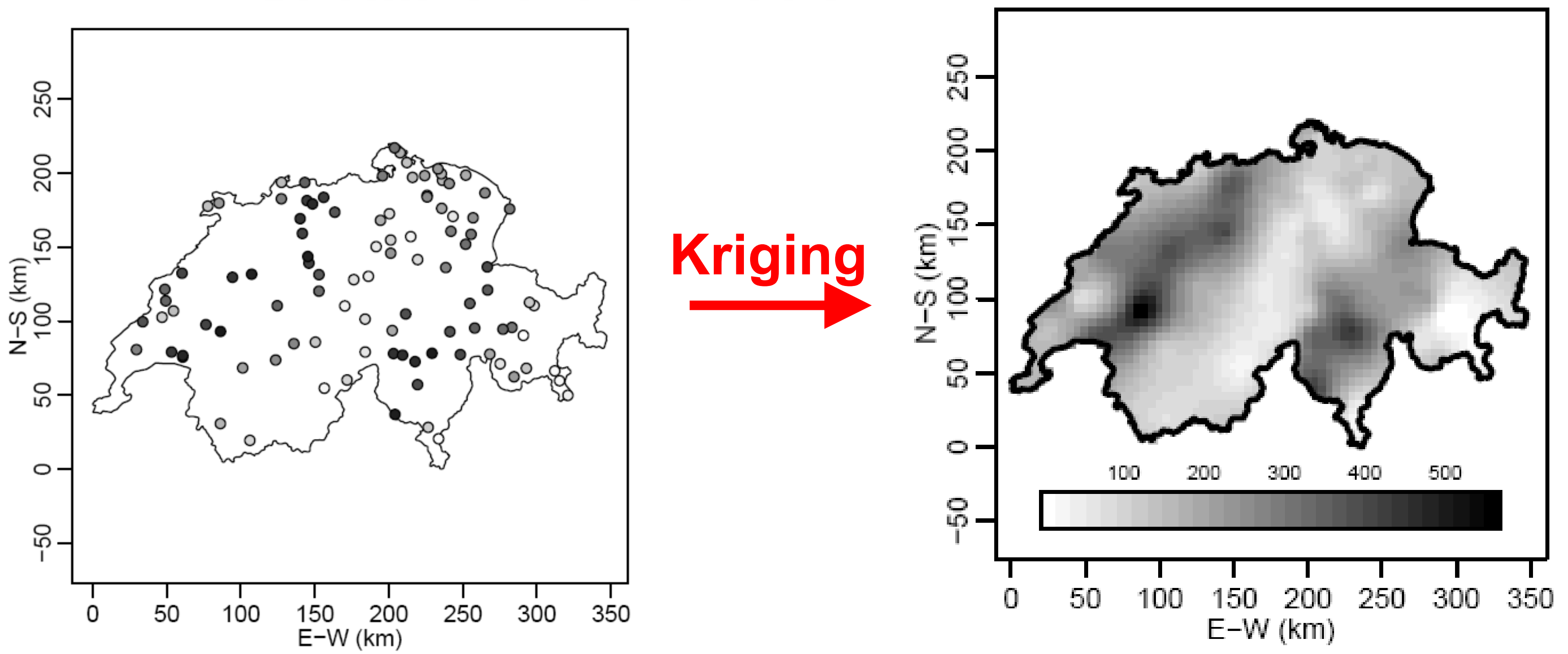
We get:

- Posterior distribution of the parameters

Bayesian Net



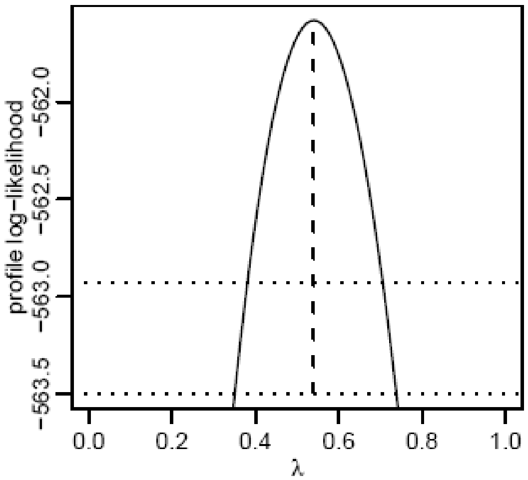
Example: Swiss Rainfall Data



Transformed gaussian model (Box-Cox transformed data) with Mathérn correlation structure.

Example: Swiss Rainfall Data

Estimates of λ (transformation parameter) and κ (one of the correlation parameters) by maximum likelihood estimation



κ	$\hat{\lambda}$	$\log \hat{L}$
0.5	0.496	-564.857
1	0.540	-561.579
2	0.561	-563.115

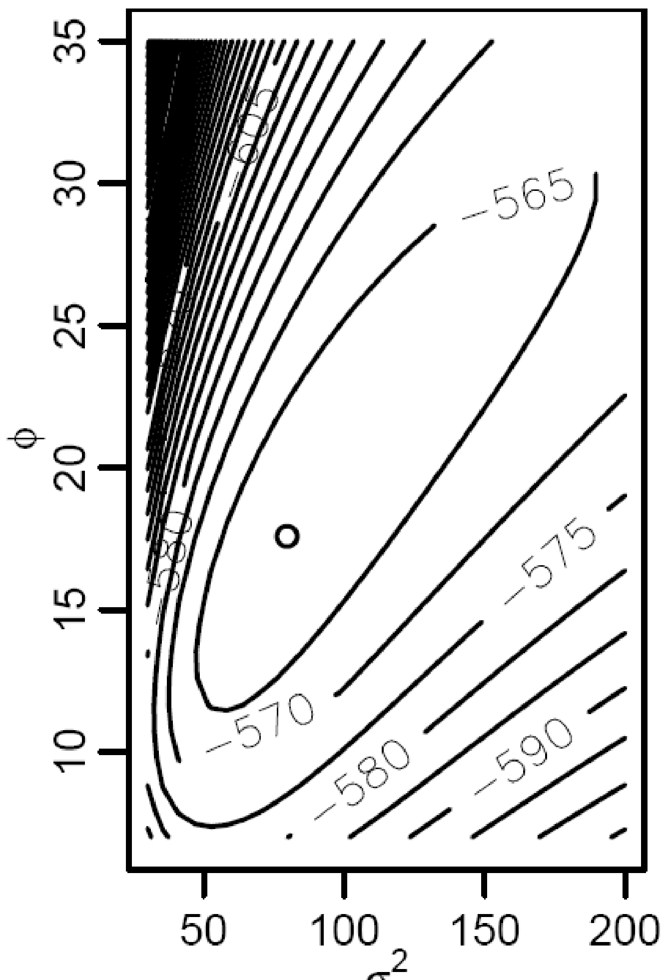
λ = 0.5

κ	$\hat{\beta}$	$\hat{\sigma}^2$	$\hat{\phi}$	$\hat{\tau}^2$	$\log \hat{L}$
0.5	21.205	83.865	42.388	0	-564.858
1.0	22.426	79.694	17.583	0	-561.664
2.0	23.099	72.698	8.358	0	-563.292

κ = 1, τ^2 = 0

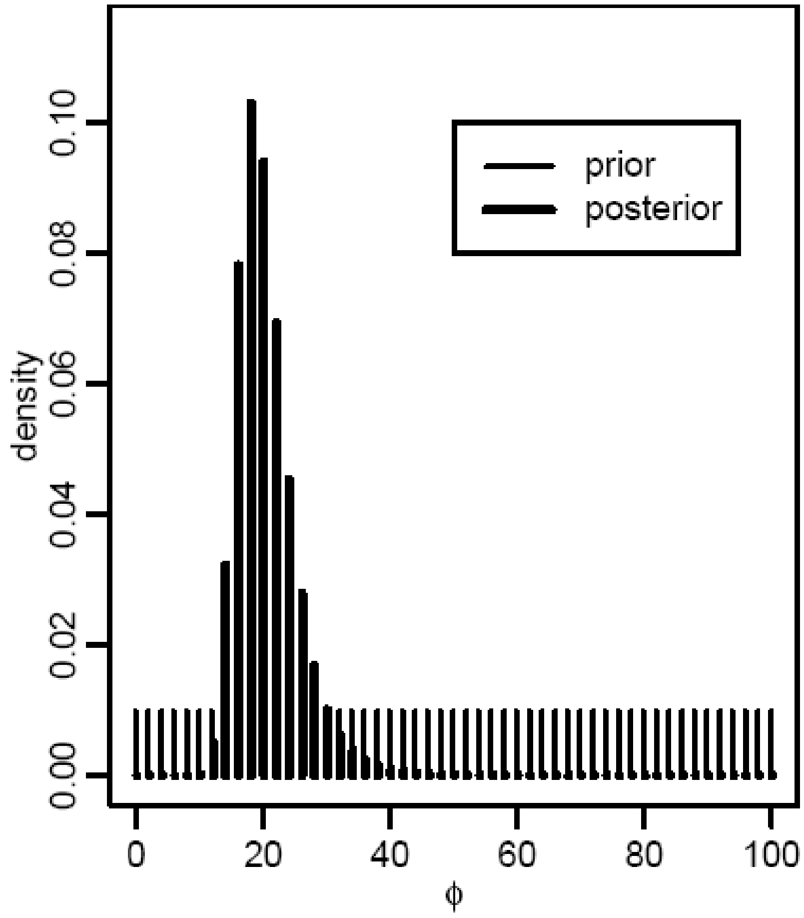
Example: Swiss Rainfall Data

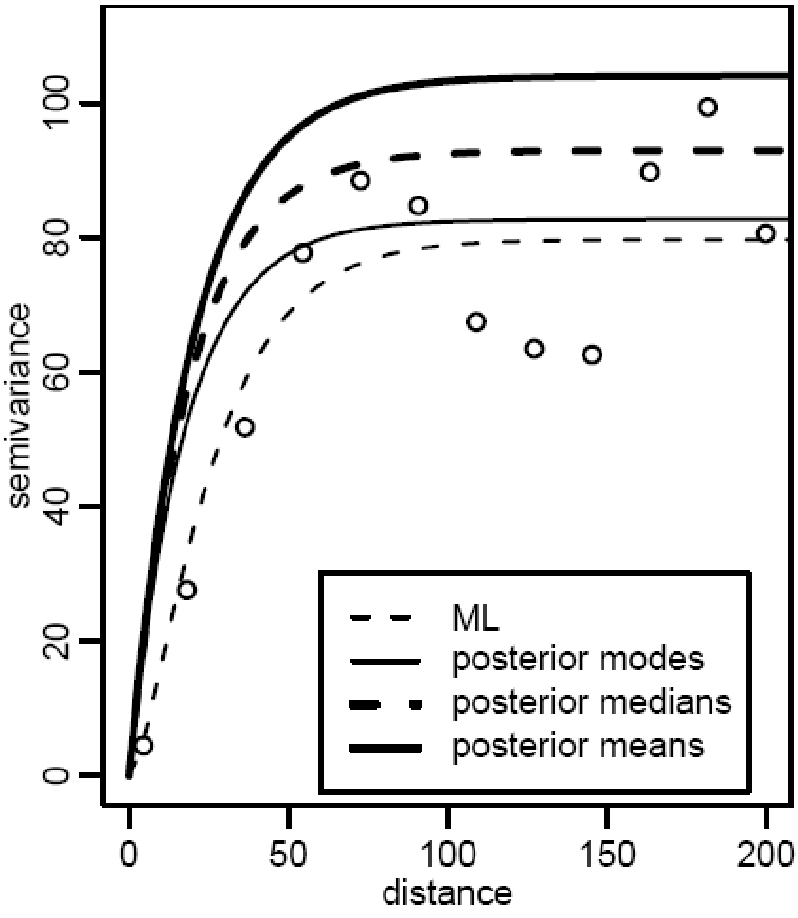
Likelihood function with λ = 0.5, κ = 1, τ^2 = 0



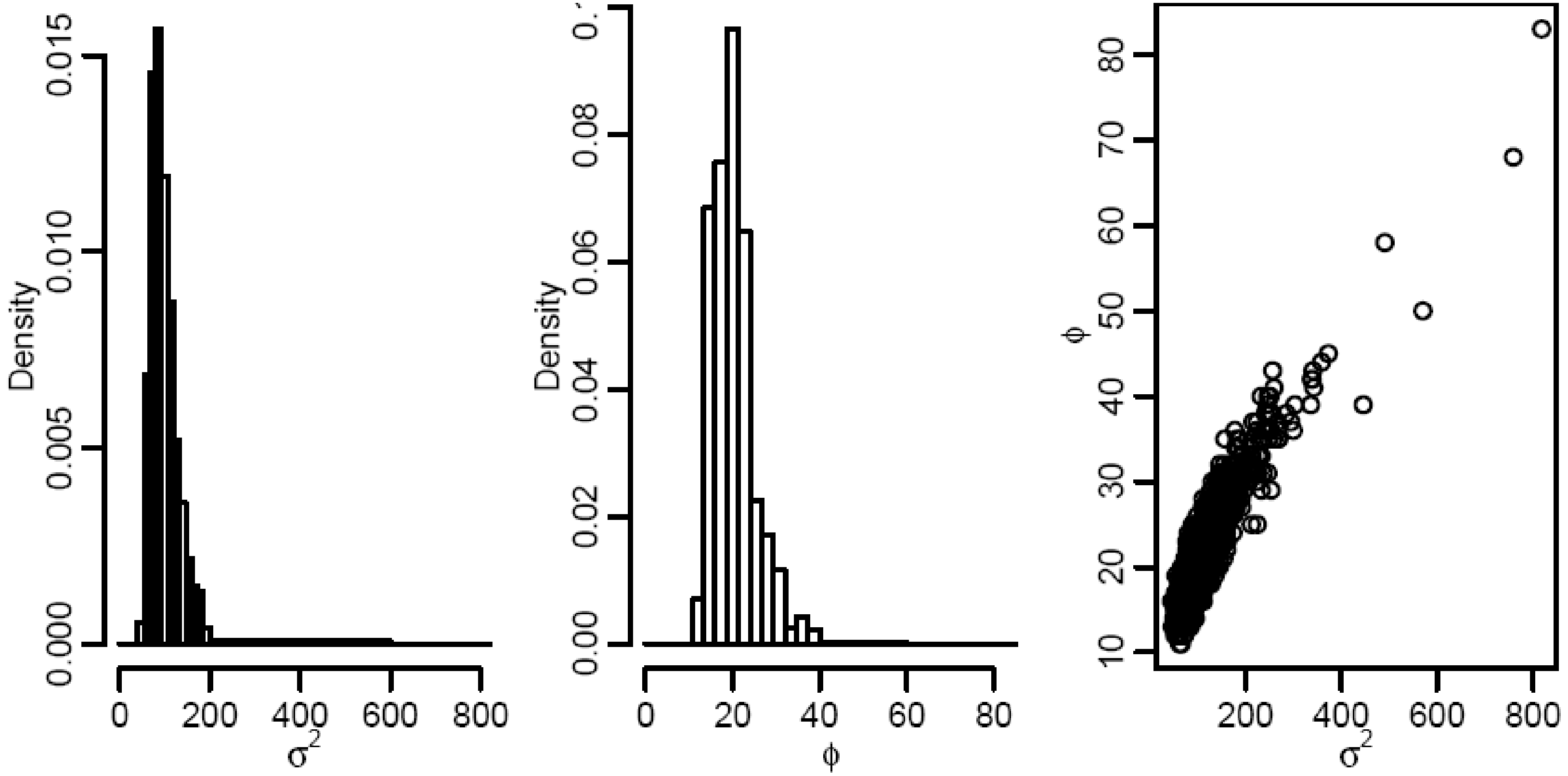
Example: Swiss Rainfall Data

Uniform discrete prior for Φ, Scaled-Inverse-χ^2 distribution for μ and σ^2





Example: Swiss Rainfall Data



Posterior distributions of Φ and σ^2

Software Implementation

All analysis shown were done in geoR and geoRglm (add on's to R) => mostly analytical solutions

GeoBugs is an extension for WinBugs => uses numerical techniques to sample from the distributions

GeoBugs: Model and Priors

Model

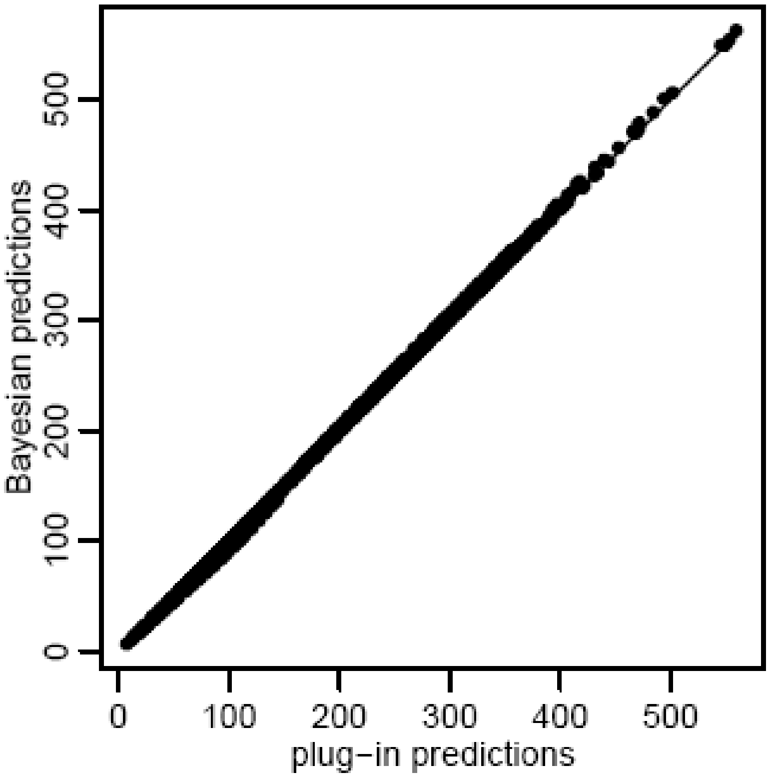
```
model {

 # Spatially structured multivariate normal likelihood
 height[1:N] ~ spatial.exp(mu[], x[], y[], tau, phi, kappa)        # exponential correlation function
 # height[1:N] ~ spatial.disc(mu[], x[], y[], tau, alpha)          # disc correlation function

 for(i in 1:N) {
    mu[i] <- beta
 }

 # Priors
 beta ~ dflat()
 tau ~ dgamma(0.001, 0.001)
 sigma2 <- 1/tau

 # priors for spatial.exp parameters
 phi ~ dunif(0.05, 20)         # prior range for correlation at min distance (0.2 x 50 ft) is 0.02 to 0.99
                               # prior range for correlation at max distance (8.3 x 50 ft) is 0 to 0.66
 kappa ~ dunif(0.05,1.95)

 # priors for spatial.disc parameter
 # alpha ~ dunif(0.25, 48)     # prior range for correlation at min distance (0.2 x 50 ft) is 0.07 to 0.96
                               # prior range for correlation at max distance (8.3 x 50 ft) is 0 to 0.63
```

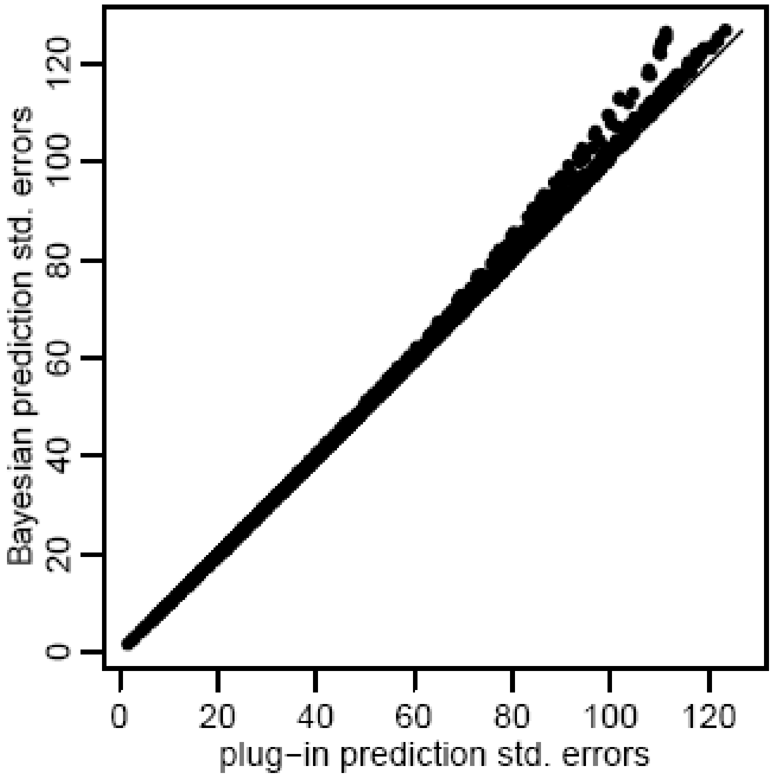
GeoBugs: Prediction

```
# Spatial prediction

# Single site prediction
for(j in 1:M) {
   height.pred[j] ~ spatial.unipred(beta, x.pred[j], y.pred[j], height[])
}

# Only use joint prediction for small subset of points, due to length of time it takes to run
for(j in 1:10) { mu.pred[j] <- beta }
height.pred.multi[1:10] ~ spatial.pred(mu.pred[], x.pred[1:10], y.pred[1:10], height[])

}
```

Bayesian vs plug-in: Differences and Similarities

- Often predicted values are similar
- Prediction Variances in bayesian predictions are often higher
- Differences are larger for non-linear targets (eg. Max value)
- Differences are lager for noisy data-sets





Advantages and Disadvantages of bayesian approach

+ Explicit handling of uncertainty
+ More honest assessment of prediction error

– Computationally more expensive
– Choice of prior can be important