

# Introduction to Bayes and non-Bayes spatial statistics

#### Gabriel Huerta

Department of Mathematics and Statistics University of New Mexico http://www.stat.unm.edu/~ghuerta/geoRcode.txt



## **General Concepts**

- Spatial Statistics are methods and techniques for the analyses of geo-referenced data.
- Aplications in diverses areas like atmospheric sciences, climatology, ecology, real estate, etc.
- Example: Study temperature and precipitation through,
  - daily measurements from monitoring stations;
  - a mean surface that considers changes in elevation or trends by location.



## **General Concepts**

Interested on summaries of the data, but also in:

- modeling trends and correlations,
- estimating underlying parameters,
- comparing diverse model,
- prediction of observations at non-observed sites.

#### Some notation

The basic format for geostatistical data is

$$(x_i, y_i); i = 1, 2, ..., n.$$

- $x_i$  represents some spatial location (2-D, 3-D).
- $y_i$  is a response variable corresponding to  $x_i$ .
- The values of  $x_i$  belong to a domain A.
- The x<sub>i</sub>'s could define fixed stations, a grid on A or points generated by a stochastic process.



## Example: Elevations data

- $y_i$  elevation on a surface with 52 locations  $(x_i's)$  on a square A (side 6.7 units).
- Use R packages, geoR and geoRgIm from http://www.r-project.org.
- In Windows go to "Packages", "Install" and search geoR

```
require(geoR)
data(elevation)
help(elevation)
points(elevation, cex.min=2,cex.max=2,col="gray")
summary(elevation)
plot(elevation, lowess=T)
```



## Example: Elevations data

**Goal:** Build a *continuous* map of elevations on *A*.

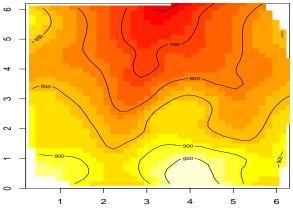
- Useful to produce images and contours.
- Download and call akima: library(akima).

```
library(akima)
int=interp.new(elevation$coords[,1],elevation$coords[,2]
,elevation$data)
image(int,xlim=range(elevation$coords[,1]),
ylim=range(elevation$coords[,2]))
contour(int,add=T)
```

Akima provides a linear interpolation. Does not permit formal predictions.



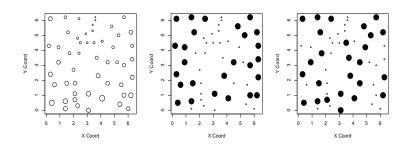
## Interpolation with akima



## Exploratory analysis of the data

```
par(mfrow=c(1,3))
points(elevation, cex.max=2.5)
points(elevation, trend="1st", pt.div=2, abs=T, cex.max=2.5)
points(elevation, trend="2nd", pt.div=2, abs=T, cex.max=2.5)
```

- Size proportional to magnitude of observations.
- Not simple to visualize the impact on spatial correlations.



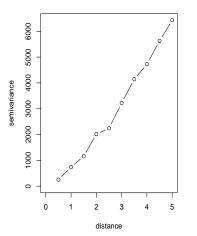
## **Empirical Variogram**

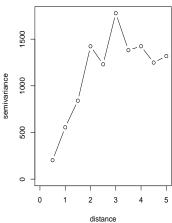
- Measure to study spatial correlations in terms of distance.
- For a set  $(x_i, y_i)$ , i = 1, 2, ..., n, the empirical semi-variogram ordinates:  $v_{ij} = \frac{1}{2}(y_i y_j)^2$ .
- If  $y_i's$  have a constant mean and variance,  $E(v_{ij}) = \sigma^2 \{1 \rho(x_i, x_j)\}$  where  $\rho(x_i, x_j)$  is the correlation between  $y_i$  and  $y_j$ ;  $\sigma^2$  is the variance of  $y_i$ .
- If  $y_i$  arises from a *stationary* process,  $\rho(x_i, x_j)$  depends on the distance between  $x_i$  and  $x_j$ .
- $E(v_{ij}) \approx \sigma^2$ , if  $u_{ij} = ||x_i x_j|| \to \infty$ .



- The graph of  $v_{ij}$  versus the distances  $u_{ij}$  defines the variogram.
- For better interpretability, the  $v'_{ij}s$  are averaged over a 'band' of distances.

```
plot (variog(elevation, uvec=seq(0,5,by=0.5)), type="b")
res1.v <- variog(elevation, trend="1st",
uvec=seq(0,5,by=0.5))
plot(res1.v,type="b")</pre>
```





#### Statistical Model

- Defined as:  $Y_i = S(x_i) + Z_i$ ; i = 1, 2, ..., n.
  - The  $Z_i's$  are mutually independent  $N(0, \tau^2)$ .
  - $S(x_i)$  its a realization of a *Gaussian Process*.
- A Gaussian process is such that the joint distribution of (S<sub>1</sub>, S<sub>2</sub>,..., S<sub>k</sub>) follows a *Multivariate Normal* with some mean y covariance.
- S(x) is a Gaussian Stationary process of mean  $\mu$ , variance  $\sigma^2 = Var(S(x))$  and correlation  $\rho(u) = Corr(S(x), S(x'))$  where u = ||x x'||.
- $\tau^2$  is a measure error and represents "micro-scale" errors.



#### Statistical model

- Selection of  $\rho(u)$  requires a carefull exploration of the variogram.
- $\rho(u)$  can adopt a parametric form (Matérn class):

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

- $K_{\kappa}(\cdot)$  is the modified *Bessel* function of order  $\kappa$ .
- $\bullet$   $\phi$  is a range parameter.
- Determines the rate in which the correlation decays to 0.

#### **Estimation**

- The parameters,  $\tau^2$ ,  $\mu$ ,  $\sigma^2$ ,  $\kappa$  and  $\phi$  are unknown.
- Estimation via numerical Maximum Likelihood.
- Initial values for  $\sigma^2$ ,  $\phi$  are needed.

```
m10=likfit(elevation, ini=c(3000,2), cov.model="matern"
,kappa=1.5)
m10
likfit: estimated model parameters:
    beta tausq sigmasq phi
" 848.316" "48.138" "3510.233" "1.198"
Practical Range with cor=0.05 for
asymptotic range: 5.685412
likfit: maximised log-likelihood = -242.1
```



- $\hat{\mu} = 848.3$ ,  $\hat{\tau^2} = 48.1$ ,  $\hat{\sigma^2} = 3510.2$ ,  $\hat{\phi} = 1.2$
- The exploratory analysis of the data suggests a model,

$$\mu(\mathbf{x}) = \beta_0 + \beta_1 \mathbf{x}_1 + \beta_2 \mathbf{x}_2$$

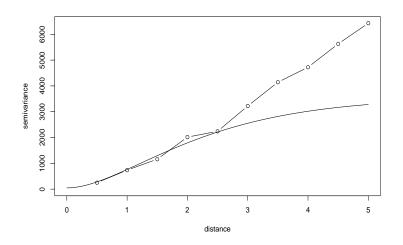
```
m11=likfit(elevation,trend="1st",ini=c(1300,2),
  cov.model="matern",kappa=1.5)
m11
likfit: estimated model parameters:
   beta0 beta1 beta2 tausq sigmasq phi
" 912.48" "-4.99" "-16.46" "34.89" "1693.13" "0.81"
Practical Range with cor=0.05 for asymptotic
range: 3.824244
likfit: maximised log-likelihood = -240.1
```

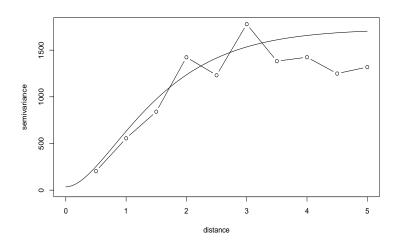
## Comparison of Variograms

- To evaluate fit, compare empirical variogram to the theoretically estimated variogram.
- For a stationary process  $Y_i = S(x_i) + Z_i$ , the variogram is:

$$V_Y(u) = \frac{1}{2} Var\{S(x) - S(x - u)\} = \tau^2 + \sigma^2\{1 - \rho(u)\}$$

```
plot (variog(elevation, uvec=seq(0,5,by=0.5)),
type="b")
lines.variomodel(seq(0,5,by=0.5),
cov.pars=c(m10$sigmasq,m10$phi),
cov.model="mat",kap=1.5,nug=m10$tausq)
```





## **Spatial Prediction**

- Also known as Kriging.
  - Prediction with minimum mean square error.
  - Estimated parameters are treated as true.
- For observations  $y = (y_1, ..., y_n)$  and a spatial point x, the predictor  $\hat{S}(x)$  is such that minimizes

$$E(\hat{S}(x) - S(x))^2$$



## **Spatial Prediction**

• Then,  $\hat{S}(x) = E(S(x)|y)$  and so

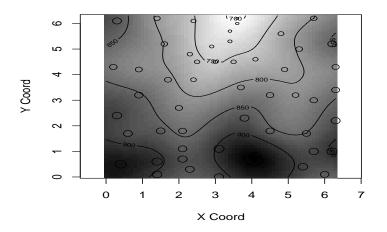
$$\hat{S}(x) = \mu + \sum_{i=1}^{n} w_i(x)(y_i - \mu)$$

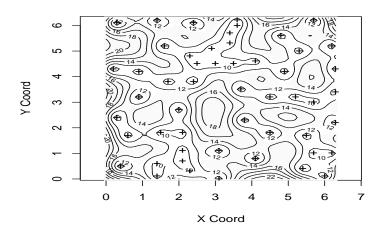
- $w_i(x)$  depend on  $\sigma^2$ ,  $\tau^2$  and  $\phi$ .
- Considers the standard error of prediction

$$SE(x) = \sqrt{Var\{S(x)|y\}}$$

#### Prediction in GeoR

```
locs=pred_grid(c(0,6.3),c(0,6.3),by=0.1)
KC=krige.control(type="sk",obj.mod=m10)
sk=krige.conv(elevation, krige=KC,loc=locs)
# spatial maps of predictions
pred.lim=range(c(sk$pred,skt$pred)
sd.lim=range(c(sk$kr,skt$kr))
image(sk,col=gray(seq(1,0,l=51)),zlim=pred.lim)
contour(sk,add=T,nlev=6)
points(elevation,add=TRUE,cex.max=2)
```





#### **Correlation Functions**

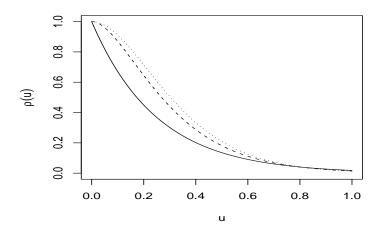
Matérn Family:

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

- If  $\kappa = 0.5$ ,  $\rho(u) = exp(-u/\phi)$ , Exponential model (continuous, non differentiable at 0).
- If  $\kappa \to \infty$ ,  $\rho(u) \to exp\{-(u/\phi)^2\}$ , Gaussian model (infinitely differentiable).
- Practical Range : u value where  $\rho(u) = 0.05$ .

```
x=seq(0,1,l=101)
plot(x,cov.spatial(x,cov.model="mat",kappa=0.5,
cov.pars=c(1,0.25)),type="l")
```



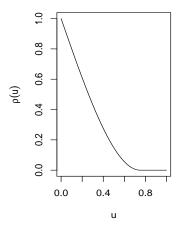


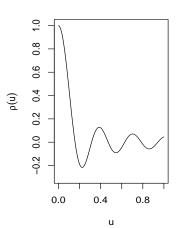
#### Other families

- Power Exponential:  $\rho(u) = exp(-(u/\phi)^{\kappa}), 0 < \kappa \le 2$  (monotone decreasing).
- Spherical:  $\rho(u) = 1 \frac{3}{2}(u/\phi) + \frac{1}{2}(u/\phi)^3$ ;  $0 \le u \le \phi$ ;  $\rho(u) = 0$ ;  $u > \phi$ .
- Non-monotone:  $\rho(u) = (u/\phi)^{-1} \sin(u/\phi)$ ;  $\phi > 0$

```
x=seq(0,1,l=101)
plot(x,cov.spatial(x,cov.model="spherical",
cov.pars=c(1,0.75)),type="1")
plot(x,cov.spatial(x,cov.model="wave",
cov.pars=c(1,0.05)),type="1")
```



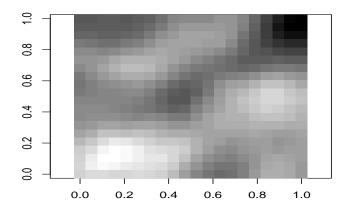




#### Simulation of a Gaussian Process

- Could be done through the R-function grf.
- Could use a regular grid or random points.
- One specifies the model and its parameters.

```
image(grf(20^2,grid="reg",cov.pars=c(1,0.13),
cov.model="mat",kappa=2.5),
col=gray(seq(1,0,1=51)),xlab=" ", ylab=" ")
```



## Bayesian Analysis in Spatial Statistics

- Takes into account uncertainty in parameters.
- Does not solely depend on a point estimator  $\hat{\theta}$ .
- Elegant solution that requires Monte Carlo simulation (MCMC) and priors.
- If *S* is the spatial process; *Y* is the data:

$$p(Y, S, \theta) = p(\theta)p(S|\theta)p(Y|S, \theta)$$

- $p(\theta)$  represents a prior distribution on  $\theta$ .
- The predictive distribution,

$$p(S|Y) = \int p(S|Y,\theta)p(\theta|Y)d\theta.$$

• Conditional predictions are 'integrated' respect to the posterior  $p(\theta|Y)$ .



#### The Basic Model

Gaussian model with spatial 'trend':

$$Y \sim N(D\beta, \sigma^2 R(\phi) + \tau^2 I)$$

- $D\beta$  is a regression term.
- $\sigma^2$  is a spatial variance;  $\tau^2$  correspond to measurement error or micro-scale variability.
- $R_{ij} = \rho(||x_i x_j||, \phi)$  with  $\rho(\cdot)$  a correlation function.
- If  $\theta = (\beta, \sigma^2, \tau^2, \phi)$ , we need a prior  $p(\theta)$ , so the *posterior* is:

$$p(\theta|y) \propto f(y|\theta)p(\theta)$$

equivalent to  $p(\beta, \sigma^2, \tau^2, \phi | Y)$ .



Its typical to assume the parameters are independent:

$$p(\theta) = p(\beta)p(\sigma^2)p(\tau^2)p(\phi)$$

- Its common to adopt a *Multivariate Normal* on  $\beta$ , an *Inverse Gamma* on  $\sigma^2$  and  $\tau^2$ .
- For  $p(\phi)$  its usual to adopt a *Uniform* or *Inverse Gamma* prior.
- Non-informative:  $p(\beta) \propto 1$ , however  $\phi$  and at least one of  $\sigma^2$  or  $\tau^2$  must have an informative prior.
- Model requires use of Metropolis-Hastings or Slice Sampler.



## Alternative in geoR

Prior of the form

$$p(\beta, \sigma^2 | \phi, \nu^2) p(\phi, \nu^2)$$

with  $\nu^2 = \tau^2/\sigma^2$ ,  $p(\phi, \nu^2)$  a discrete distribution over a reasonable range.

The posterior distribution has a structure,

$$p(\beta, \sigma^2, \phi, \nu^2 | y) = p(\beta, \sigma^2 | y, \phi, \nu^2) p(\phi, \nu^2 | y)$$

The parameters are simulated iteratively.



• For a prediction of  $S^* = S(x^*)$  where  $x^*$  is an arbitrary site,

$$p(S^*|y) = \int p(S^*|\theta, y)p(\theta|y)d\theta.$$

• Method of composition: For each sample of  $p(\theta|y)$ , one simulates a sample from  $p(S^*|\theta, y)$ .

$$\theta_1, \theta_2, \dots, \theta_m \rightarrow S_1^*, S_2^*, \dots, S_m^*$$

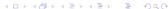
 The function krige.bayes() implements Bayesian inference on the Gaussian model.

- Its use is more simple through model.control, prior.control and output.control.
- A trend is specified with *trend.d* and *trend.l* for prediction.
- A discrete uniform is specified for  $\phi$  and  $\nu^2 = \tau^2/\sigma^2$ .
- For  $\beta$  and  $\sigma^2$ ,  $p(\beta, \sigma^2) \propto 1/\sigma^2$ .

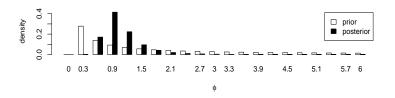
#### Elevation data

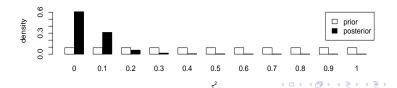
```
MC=model.control(trend.d="1st",trend.l
="1st",kappa=1.5)
PC=prior.control(phi.discrete=seq(0,6,1=21),
phi.prior="reciprocal",
tausq.rel.prior="unif",tausq.rel.discrete
=seq(0,1,1=11))
OC=output.control(n.post=1000,moments=T)
```

#### Now krige.bayes can be used:

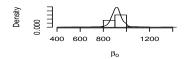


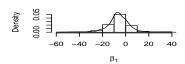
# Posterior distributions of $\phi$ and $\tau^2$ .

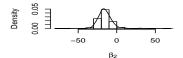


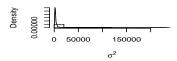


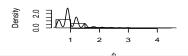
### Posterior distribution on parameters

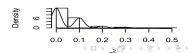






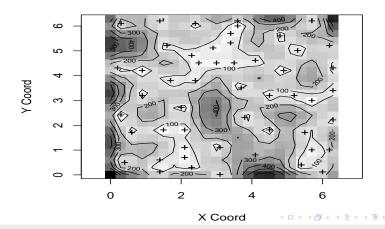




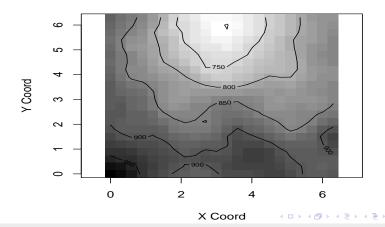


```
# Map of the mean of the predictive dist.
image(skb, col=gray(seg(1, 0, l=51)))
points (elevation, add=TRUE, cex.max=2)
# Map of the variance of the predictive dist.
image(skb, val="variance", col=gray(seg(1, 0, 1=51)),
main="prediccion var")
contour(skb, val="variance", add=T)
points(elevation$coords,pch="+")
# Sample of the predictive dist.
image(skb, val="simulation", col=gray(seg(1, 0, l=51)),
number.col=1, main="simulacion")
contour(skb, val="simulation", number.col=1, add=T)
```

# Map of the variance. Predictive distribution.



# Map of one sample. Predictive distribution.

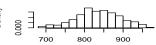


```
# Predictions for some points
names(skb$predictive)
dim(skb$predictive$simulations)
pred=skb$predictive$simulations
par(mfrow=c(3,2))
for(i in 1:6){hist(pred[,i],prob=T,xlab=" ",
main=paste("Prediction on",i)) }
names(skb$predictive)
```

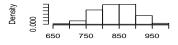
Prediccion en 1



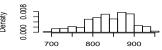
Prediccion en 2



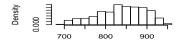
Prediccion en 3



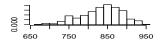
Prediccion en 4



Prediccion en 5



#### Prediccion en 6



## A generalized linear model (Poisson)

- The observations  $Y_i$ , i = 1, ..., n are counts on  $x_i$ .
- The  $Y_i's$  are conditionally independent,  $Y_i \sim Poisson(\mu_i)$ .

$$log(\mu_i) = \alpha + S(x_i) + Z_i.$$

- $S(\cdot)$  is a *Gaussian Process* with variance  $\sigma^2$  and correlation  $\rho(u)$
- The  $Z_i's$  are independent Normal  $N(0, \tau^2)$ .
- Induces spatial dependency through the parameters.
- Binomial case:  $log(p(x_i)/(1-p(x_i))) = \alpha + S(x_i)$ .

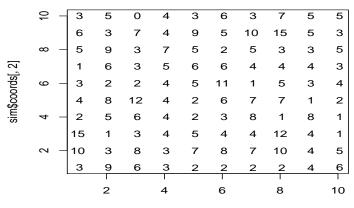


### Simulation of the generalized spatial process

 Through the function grf that simulates a Gaussian process plus noise.

```
sim <- grf(grid =expand.grid(x=seq(1,10,1 = 10),
    y =seq(1, 10, 1 = 10)),
    cov.pars = c(0.1, 0.2))
    attr(sim, "class") <- "geodata"
    sim$units.m <- c(rep(5, 100))
    sim$data <- rpois(100, lambda =
        sim$units.m*exp(sim$data))
plot(sim$coords[,1], sim$coords[,2], type = "n")
text(sim$coords[,1], sim$coords[,2], format(sim$data))</pre>
```

# Simulation of Poisson process



#### **Estimation and Predictions**

- Use pois.krige inside of geoRglm.
- Through conditional simulation with Gaussian process parameters fixed.
- Look for a 60% acceptance rate.

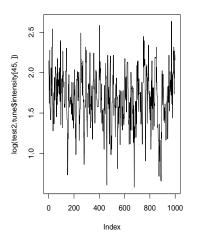
```
model2=krige.glm.control(cov.pars =c(1,1),beta = 1)
test2.tune=pois.krige(p50,krige=model2,
mcmc.input=list(S.scale=0.2,thin = 1))
```

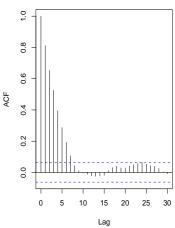
• The optimal value is around *S.scale* = 0.5.



#### Its necessary to study how the chain mixes.

#### Series log(test2.tune\$intensity[45, ])





Predictions of intensity at 2 points, (0.5,0.5) and (1,0.4).

```
test2=pois.krige(p50,locations=
  cbind(c(0.5,0.5),c(1,0.4)),
  krige=model2, mcmc.input
  =mcmc.control(S.scale = 0.5),
  output=output.glm.control(sim.predict = TRUE))
```

 Output includes predictions, variances of predictions and Monte Carlo errors.

```
test2$predict
test2$krige.var
test2$mcmc.error
```

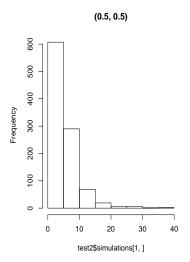
 The predictions of the intensity at 2 points are in test2\$simulations.

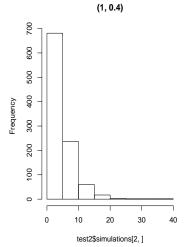
```
par(mfrow = c(1,2))
hist(test2$simulations[1,],main="(0.5, 0.5)")
hist(test2$simulations[2,],main ="(1, 0.4)")
```

For "beta" to follow a uniform distribution

```
model2.u=krige.glm.control(cov.pars = c(1,1),
beta = 1,type.krige = "ok")
test2.unif.beta =pois.krige(p50,krige =model2.u,
mcmc.input = list(S.scale = 0.5))
```







### Full Bayes Analysis

Implemented in the function pois.krige.bayes

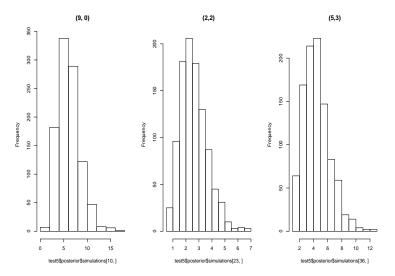
```
prior5=prior.glm.control(phi.prior="fixed", phi = 0.1)
mcmc5.tune=mcmc.control(S.scale = 0.01, thin = 1)
test5.tune=pois.krige.bayes(p50, prior =
   prior5, mcmc.input = mcmc5.tune)
```

S.scale parameter adjusted to improve acceptance rate.

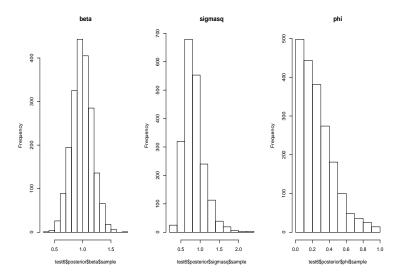
```
mcmc5=mcmc.control(S.scale = 0.075, thin = 100)
test5=pois.krige.bayes(p50, locations =
t(cbind(c(2.5,3),c(-6050,-3270))),
  prior = prior5, mcmc.input = mcmc5,
output = list(threshold=10,
quantile = c(0.05,0.99)))
```

- "Posterior" contains information about the posterior distribution of parameters and simulations at data points.
- "Predictive" contains information about predictions.
- "threshold=10" gives the probability that predictions are lower than 10.
- "quantiles" gives 0.05 and 0.99 quantiles of predictive (test5\$predictive, test5\$quantiles).

```
par(mfrow = c(1,3))
hist(test5$posterior$simulations[10,],main="(9, 0)")
hist(test5$posterior$simulations[23,],main="(2,2)")
hist(test5$posterior$simulations[36,],main="(5,3)")
```



```
# Example with uncertainty in other parameters
mcmc6.tune<-mcmc.control(S.scale=0.075, n.iter=2000,
thin=100, phi.scale = 0.01)
prior6<-prior.glm.control(phi.prior="uniform",</pre>
phi.discrete = seq(0.02,1, 0.02), tausq.rel = 0.05)
test6.tune <- pois.krige.bayes(p50,prior =
prior6, mcmc.input= mcmc6.tune)
#This may take some time.
mcmc6 <-mcmc.control(S.scale=0.075,</pre>
n.iter=400000,thin=200,burn.in=5000,
phi.scale=0.12, phi.start=0.5)
test6 <- pois.krige.bayes(p50,locations =
t(cbind(c(2.5,3.5),c(-60,-37))),
prior=prior6, mcmc.input=mcmc6)
# some posterior distributions.
par(mfrow=c(1,3))
hist(test6$posterior$beta$sample,main="beta")
hist(test6$posterior$sigmasg$sample,main="sigmasg")
```



#### References

- Diggle P.J. and Ribeiro P. J. (2007) Model-based Geostatistics, Springer-Verlag, New York.
- Banerjee, S, Carlin B. and Gelfand A. (2004) Hierarchical Modeling and Analysis for Spatial Data. Chapman and Hall/CRC