geoR : Package for Geostatistical Data Analysis
An illustrative session

Paulo J. Ribeiro Jr. & Peter J. Diggle
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The package **geoR** provides functions for geostatistical data analysis using the software **R**.
This document illustrates some (**but not all**) of the capabilities of the package.

The objective is to familiarise the reader with the **geoR**'s commands for data analysis and show some of the grahical outputs which can be produced.
The commands used here are just illustrative, providing basic examples of the package handling.
We did not attempt to perform a definitive analysis of this data.

In what follows the **R** commands are shown in

```
typewriter fonts like this.
```

Typically, default arguments are used for the function calls and the user is encouraged to inspect other argumets of the functions. For example, to see all the arguments for the function `variog` type:

```
args(variog)
```

You can click to download the file geoRintro.R with the commands shown in this page.

We refer to the **geoR** documentation for more details on the functions included in **geoR**.

---

1. STARTING A SESSION AND LOADING DATA

After starting an **R** session, load **geoR** with the command:

```
library(geoR)
```

If the installation directory for the package is the default location for **R** packages, type:

```
library(geoR, lib.loc="PATH_TO_geoR")
```

where `"PATH_TO_geoR"` is the path to the directory where **geoR** was installed. If the package is loaded correctly the following message will be displayed:

```
--------------------------------------------
geoR: functions for geostatistical analysis
geoR version 1.1-8 is now loaded
--------------------------------------------
```

Typically, data are stored as an object (a list) of the class `"geodata"`.
An object of this class contains at least the coordinates of data locations and the data values.

Click for information on how to import data from an ASCII file.
We refer to the documentation for the functions `as.geodata` and `read.geodata` for more information on how to import/convert data and on the definitions for the class `"geodata"`.

For the examples included in this document we use the data set `s100` included in the **geoR** distribution.
To load this data type:

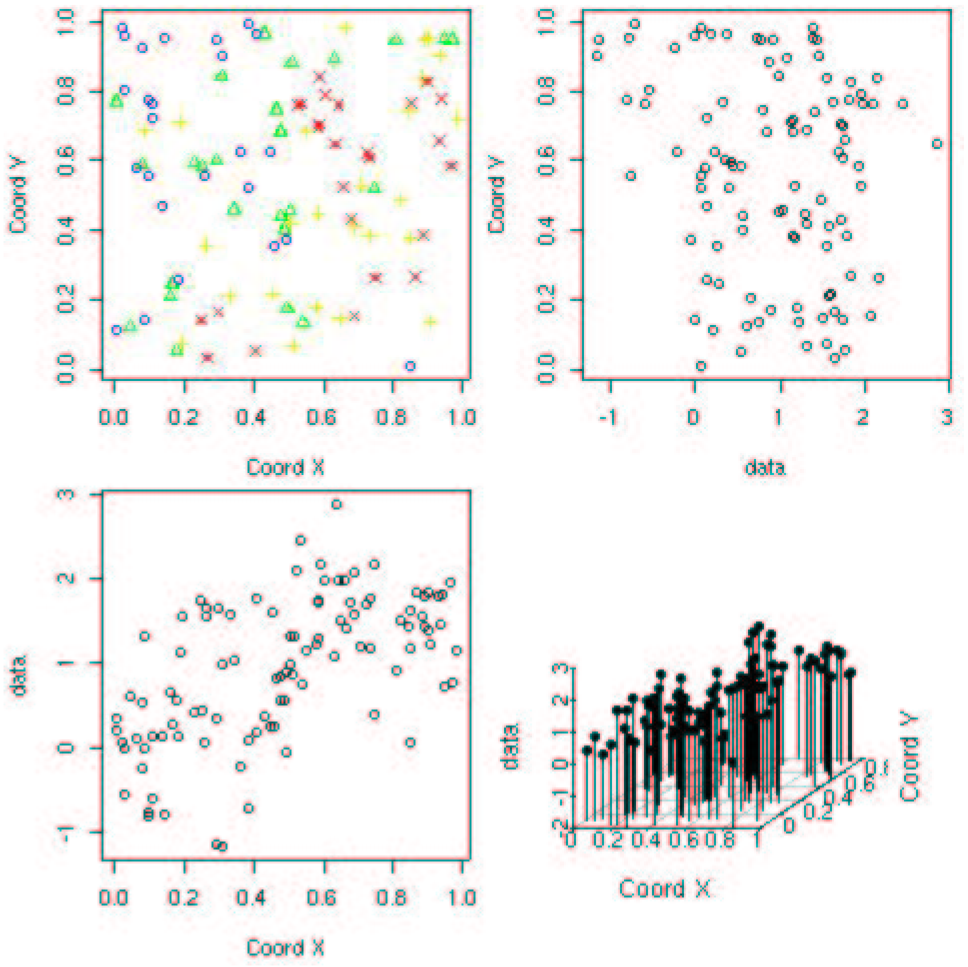
```
data(s100)
```

2. EXPLORATORY TOOLS

1. Plotting data locations and values

The function plot.geodata shows a 2 x 2 display with data locations (top plots) and data *versus* coordinates (bottom plots). For an object of the class "geodata" the plot is produced by the command:

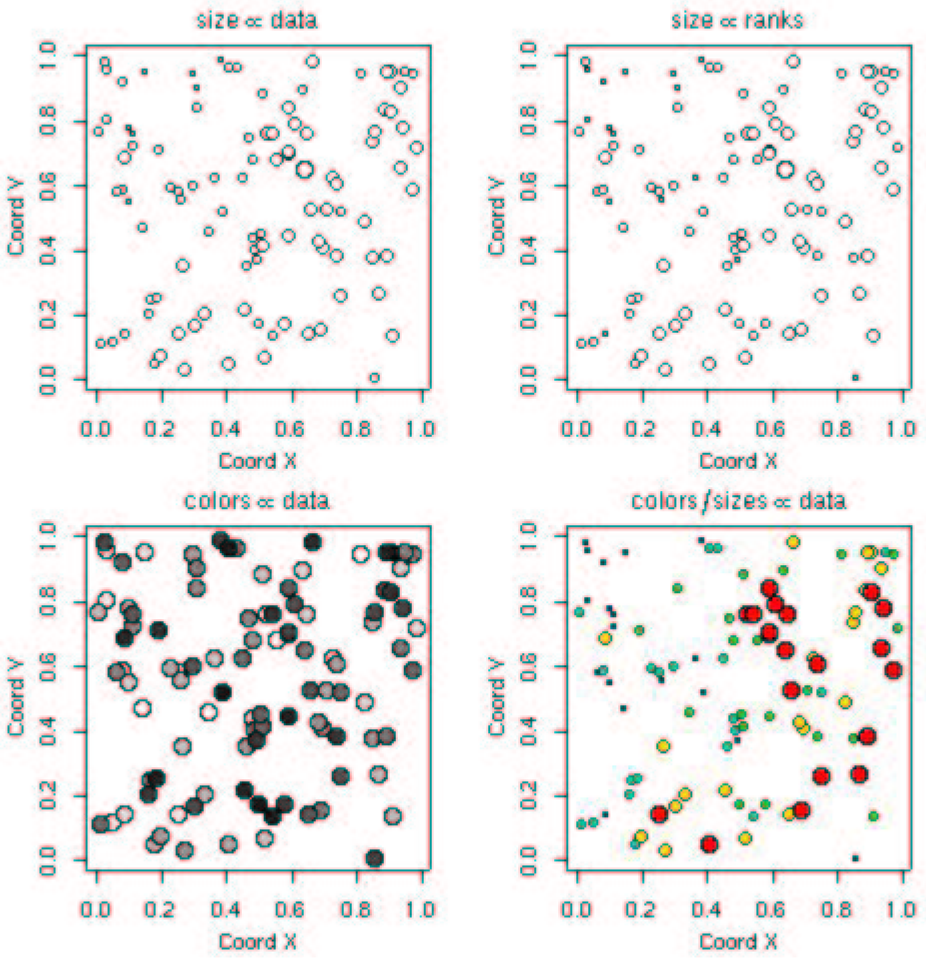
```
plot(s100)
```



Notice that the top-right plot is produced using the package **scaterplot3d** If this package is not installed a histogram of the data will replace this plot.

The function points.geodata produces a plot showing the data locations. Alternatively, points indicating the data locations can be added to a current plot.
There are options to specify point sizes, patterns and colors, which can be set to be proportional to the data values or specified quantiles.
Some examples of graphical outputs are illustrated by the commands and corresponding plots as shown below.
We start saving the current graphical parameters.

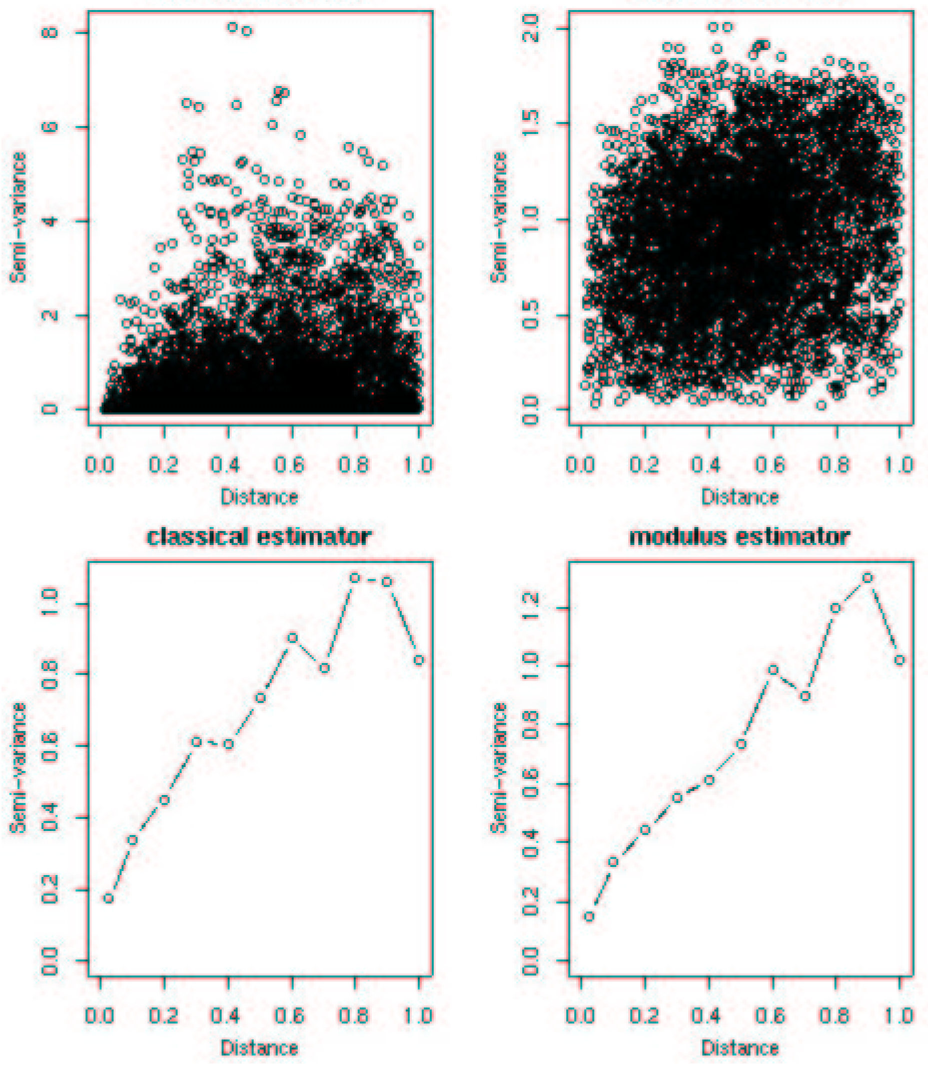
```
par.ori <- par(no.readonly = TRUE)
par(mfrow = c(2,2))
points(s100, xlab = "Coord X", ylab = "Coord Y")
points(s100, xlab = "Coord X", ylab = "Coord Y", pt.divide = "rank.prop")
points(s100, xlab = "Coord X", ylab = "Coord Y", cex.max = 1.7,
      col = gray(seq(1, 0.1, l=100)), pt.divide = "equal")
points(s100, pt.divide = "quintile", xlab = "Coord X", ylab = "Coord Y")
```



2. Empirical variograms

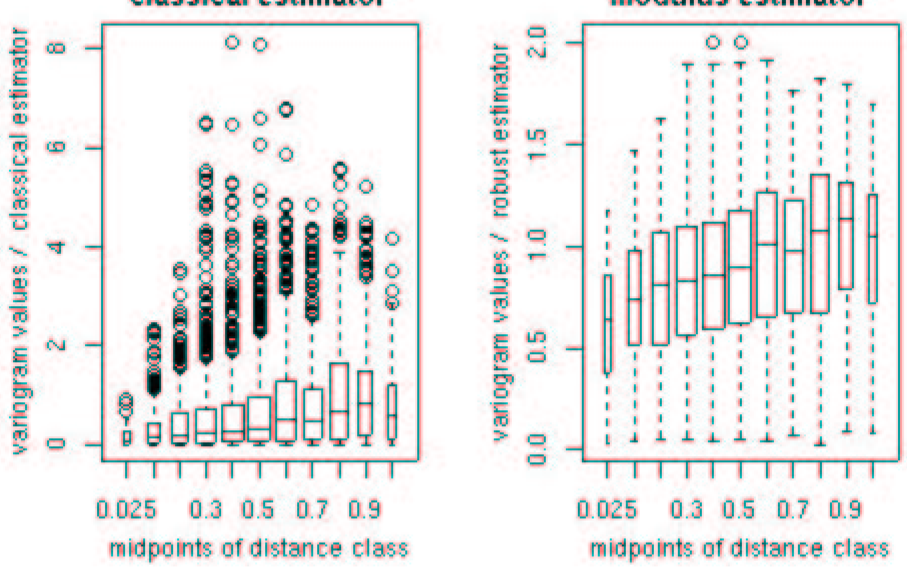
Empirical variograms are calculated using the function variog. There are options for the *classical* or *modulus* estimator.
Results can be returned as variogram clouds, binned or smoothed variograms.

```
cloud1 <- variog(s100, option = "cloud", max.dist=1)
cloud2 <- variog(s100, option = "cloud", estimator.type = "modulus", max.dist=1)
bin1 <- variog(s100, uvec=seq(0,1,l=11))
bin2  <- variog(s100, uvec=seq(0,1,l=11), estimator.type= "modulus")

par(mfrow=c(2,2))
plot(cloud1, main = "classical estimator")
plot(cloud2, main = "modulus estimator")
plot(bin1, main = "classical estimator")
plot(bin2, main = "modulus estimator")
par(par.ori)
```



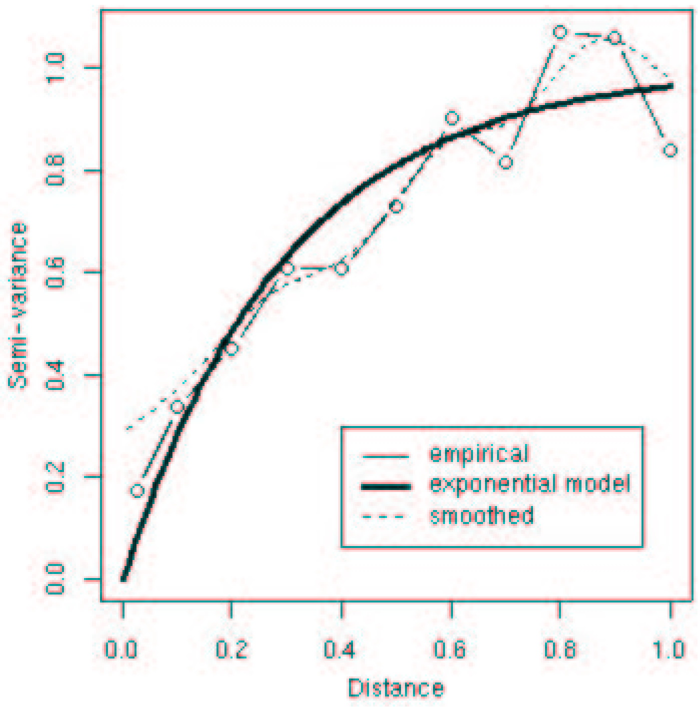
Furthermore, the points of the variogram clouds can be grouped into classes of distances ("bins") and displayed with a box-plot for each bin.

```
bin1 <- variog(s100,uvec = seq(0,1,l=11), bin.cloud = T)
bin2 <- variog(s100,uvec = seq(0,1,l=11), estimator.type = "modulus", bin.cloud = T)

par(mfrow = c(1,2))
plot(bin1, bin.cloud = T, main = "classical estimator")
plot(bin2, bin.cloud = T, main = "modulus estimator")
par(par.ori)
```



Theoretical and empirical variograms can be plotted and visually compared. For example, the figure below shows the theoretical variogram model used to simulate the data s100 and two estimated variograms.

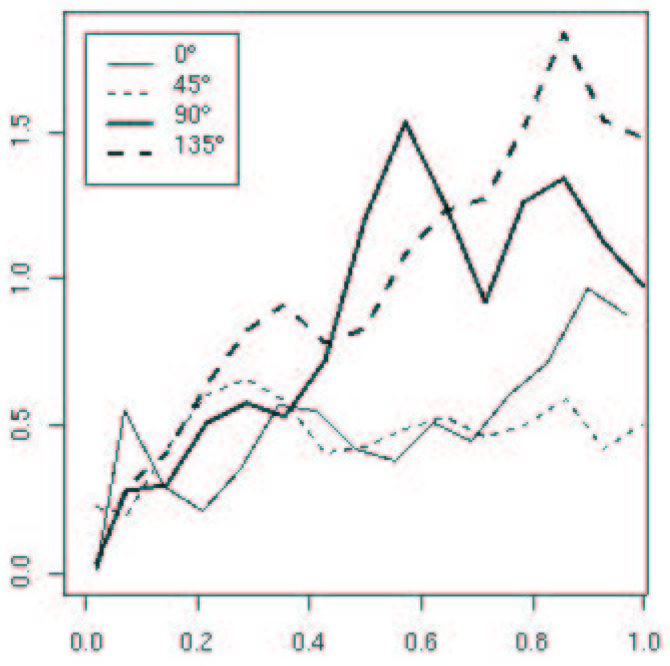
```
bin1 <- variog(s100, uvec = seq(0,1,l=11))
plot(bin1)
lines.variomodel(list(nugget = 0, cov.pars = c(1,0.3), max.dist = 1, cov.model = "exp"), lwd = 3)
smooth <- variog(s100, option = "smooth", max.dist = 1, n.points = 100, kernel = "normal", band = 0.2)
lines(smooth, type ="l", lty = 2)
legend(0.4, 0.3, c("empirical", "exponential model", "smoothed"), lty = c(1,1,2), lwd = c(1,3,1))
```



Directional variograms can also be computed by the function variog using the arguments direction and tolerance. For example, to compute a variogram for the direction 60 degrees with the default tolerance angle (22.5 degrees) the command would be:

```
vario60 <- variog(s100, max.dist = 1, direction=pi/3)
```

```
vario.4 <- variog4(s100, max.dist = 1)
plot(vario.4, lwd=2)
```



3. PARAMETER ESTIMATION

Model parameters can be estimated by using:

- *least squares fit of empirical variograms*: with options for ordinary (OLS) and weighted (WLS) least squares
- *likelihood based methods*: with options for maximum likelihood (ML) and restricted maximum likelihood (REML)

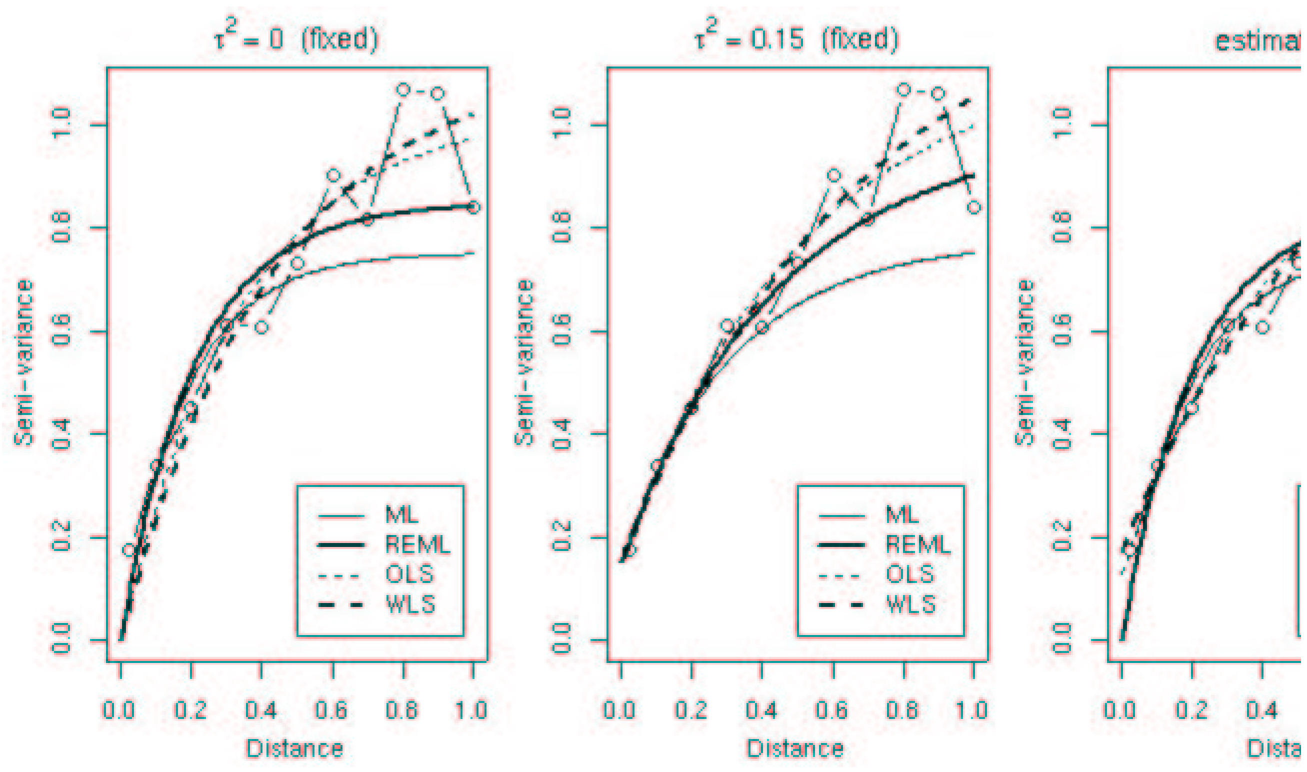
Bayesian methods are also implemented and will be presented in Section 5.

The nugget effect parameter can be estimated or set to a fixed value. The same applies for smoothness, anisotropy and transformation parameters. Options for taking trends into account are also included. Trends can be specified as polynomial functions of the coordinates and/or linear functions of given covariates.

The commands below shows models fitted by different methods with options for fixed or estimated nugget parameter. Features not illustrated here include estimation of trends, anisotropy, smoothness and Box-Cox transformation parameter.

```
# Fitting models with nugget fixed to zero
ml <- likfit(s100, ini = c(1,0.5), fix.nugget = T)
reml <- likfit(s100, ini = c(1,0.5), fix.nugget = T, method = "RML")
ols <- variofit(bin1, ini = c(1,0.5), fix.nugget = T, weights="equal")
wls <- variofit(bin1, ini = c(1,0.5), fix.nugget = T)

# Fitting models with a fixed value for the nugget
ml.fn <- likfit(s100, ini = c(1,0.5), fix.nugget = T, nugget = 0.15)
reml.fn <- likfit(s100, ini = c(1,0.5), fix.nugget = T, nugget = 0.15, method = "RML")
ols.fn <- variofit(bin1,ini = c(1,0.5), fix.nugget = T, nugget = 0.15, weights="equal")
wls.fn <- variofit(bin1, ini = c(1,0.5), fix.nugget = T, nugget = 0.15)

# Fitting models estimated nugget
ml.n <- likfit(s100, ini = c(1,0.5), nug = 0.5)
reml.n <- likfit(s100, ini = c(1,0.5), nug = 0.5, method = "RML")
ols.n <- variofit(bin1, ini = c(1,0.5), nugget=0.5, weights="equal")
wls.n <- variofit(bin1, ini = c(1,0.5), nugget=0.5)
```

```
# Now, plotting fitted models against empirical variogram
par(mfrow = c(1,3))
plot(bin1, main = expression(paste(tau^2 == 0, "  (fixed)")))
lines(ml, max.dist = 1)
lines(reml, lwd = 2, max.dist = 1)
lines(ols, lty = 2, max.dist = 1)
lines(wls, lty = 2, lwd = 2, max.dist = 1)
legend(0.5, 0.3, legend = c("ML", "REML", "OLS", "WLS"), lty = c(1,1,2,2), lwd = c(1,2,1,2))

plot(bin1, main = expression(paste(tau^2 == 0.15, "  (fixed)")))
lines(ml.fn, max.dist = 1)
lines(reml.fn, lwd = 2, max.dist = 1)
lines(ols.fn, lty = 2, max.dist = 1)
lines(wls.fn, lty = 2, lwd = 2, max.dist = 1)
legend(0.5, 0.3, legend = c("ML", "REML", "OLS", "WLS"), lty = c(1,1,2,2), lwd = c(1,2,1,2))

plot(bin1, main = expression(paste("estimated  ", tau^2)))
lines(ml.n, max.dist = 1)
lines(reml.n, lwd = 2, max.dist = 1)
lines(ols.n, lty = 2, max.dist = 1)
lines(wls.n, lty =2, lwd = 2, max.dist = 1)
legend(0.5, 0.3, legend = c("ML", "REML", "OLS", "WLS"), lty = c(1,1,2,2), lwd = c(1,2,1,2))

par(par.ori)
```



Summary methods have been written to summarize the resulting objects.
For example, for the model with estimated nugget fitted by maximum likelihood, typing:

```
ml.n
```

will produce the output:

```
likfit: estimated model parameters:
   beta   tausq sigmasq     phi
 0.7766  0.0000  0.7517  0.1827

likfit: maximised log-likelihood = -83.5696
```

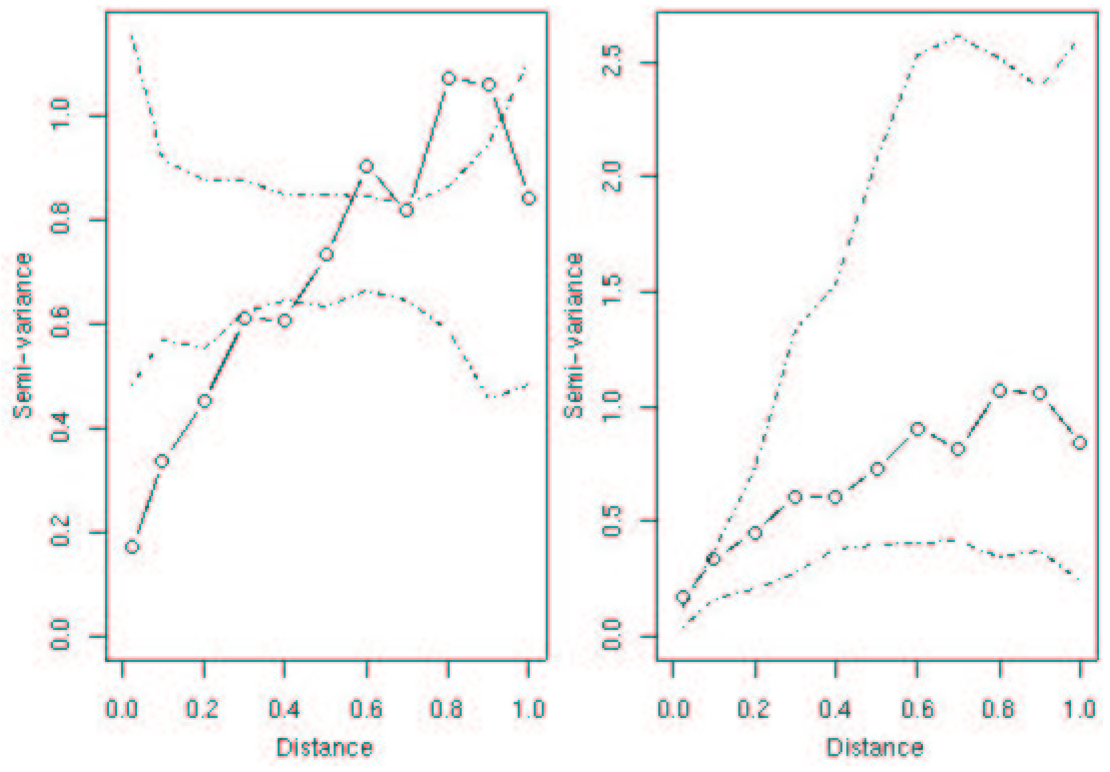
whilst a more detailed summary is obtained with:

```
summary(ml.n)

Summary of the parameter estimation
```

```
Estimation method: maximum likelihood

Parameters of the mean component (trend):
  beta
0.7766

Parameters of the spatial component:
   correlation function: exponential
      (estimated) variance parameter sigmasq (partial sill) =  0.7517
      (estimated) cor. fct. parameter phi (range parameter)  =  0.1827
   anisotropy parameters:
      (fixed) anisotropy angle = 0  ( 0 degrees )
      (fixed) anisotropy ratio = 1

Parameter of the error component:
      (estimated) nugget =  0

Transformation parameter:
      (fixed) Box-Cox parameter = 1 (no transformation)

Maximised Likelihood:
   log.L n.params      AIC      BIC
-83.5696   4.0000 -87.5696 -92.7799

Call:
likfit(geodata = s100, ini.cov.pars = c(0.5, 0.5), nugget = 0.5)
```

Two kinds of variogram *envelopes* can be computed by simulation and are illustrated in the next figure.
The plot on the left-hand side shows envelopes based on permutation of the data values across the data locations. The envelopes shown on the right-hand side are based on simulations from a given set of model parameters, in this example the parameter estimates from the *WLS* variogram fit.

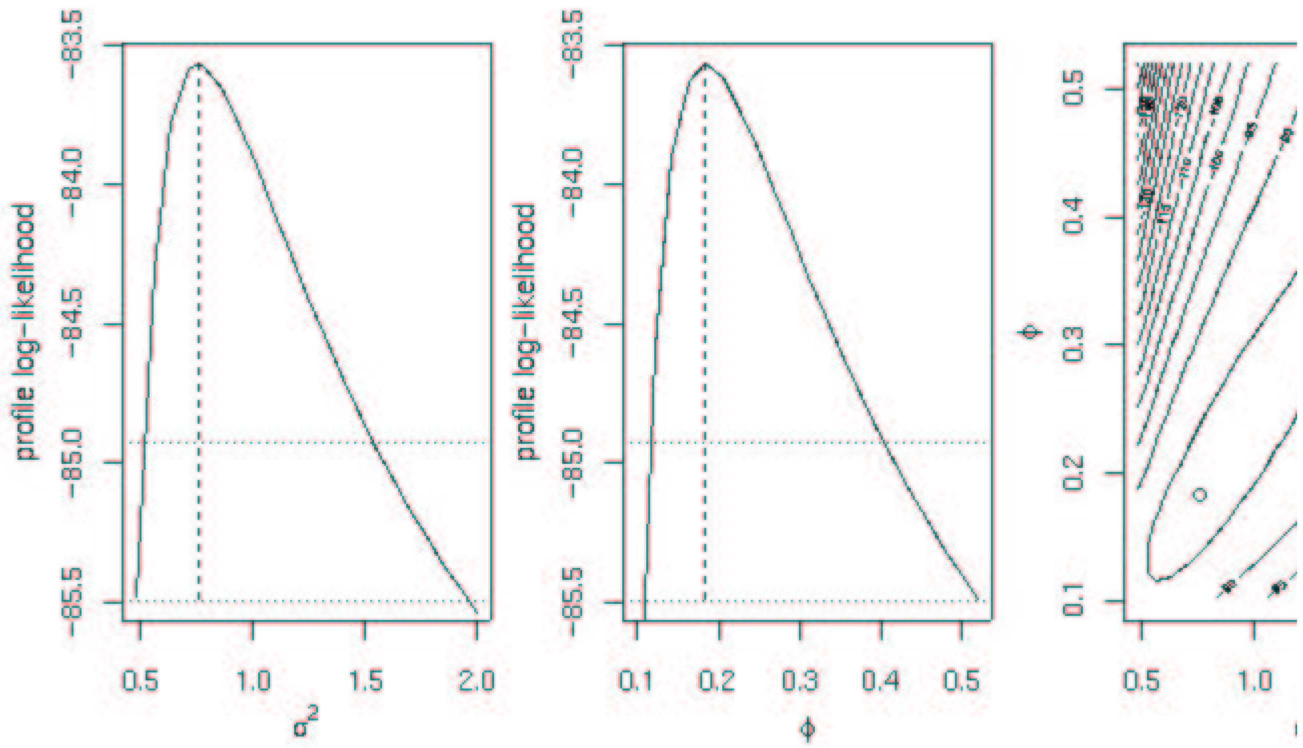
```
env.mc <- variog.mc.env(s100, obj.var=bin1)
env.model <- variog.model.env(s100, obj.var=bin1, model=wls)

par(mfrow=c(1,2))
plot(bin1, envelope=env.mc)
plot(bin1, envelope=env.model)
par(par.ori)
```



Profile likelihoods (1-D and 2-D) are computed by the function proflik. Here we show the profile likelihoods for the covariance parameters of the model without nugget effect previously fitted by likfit.

WARNING: RUNNING THE NEXT COMMAND CAN BE TIME-CONSUMING

```
prof <- proflik(ml, geodata = s100, sill.val = seq(0.48, 2, l=11),
            range.val = seq(0.1, 0.52, l=11), uni.only = FALSE)

par(mfrow=c(1,3))
plot(prof, nlevels=16)
par(par.ori)
```



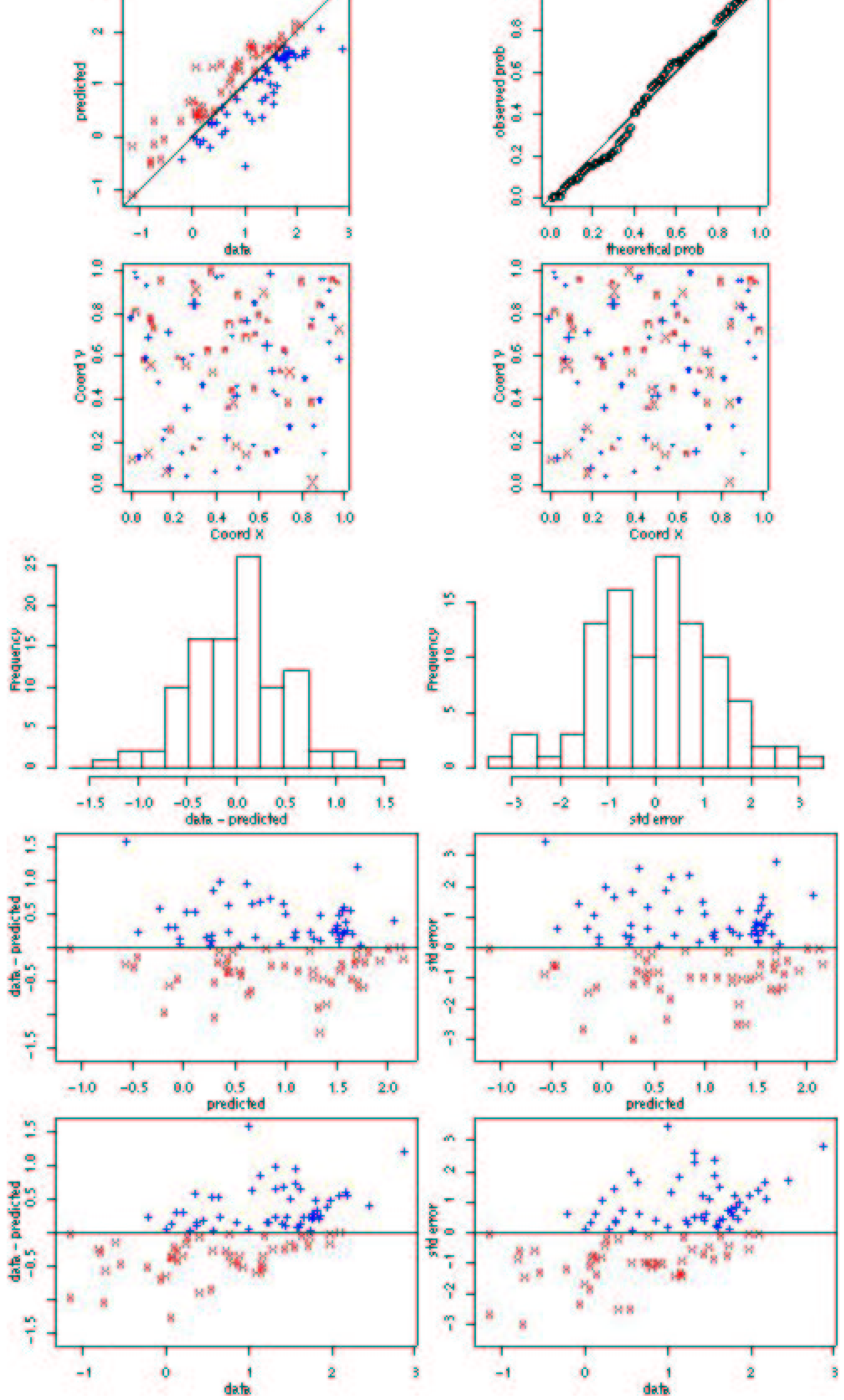
4. CROSS-VALIDATION

The function xvalid performs cross-validation either using the *leaving-one-out* strategy or on a different det of locations proviced by the user. For the first data points are removed one by one and predicted by kriging using the remaining data. The commands belows illustrates cross-validation for the models fitted by maximum likelihood and weighted least squares. In the first two calls the model parameters remains the same for the prediction at each location. In the next two calls the model parameters are re-estimated each time a point is removed from the data-set. Graphical results are shown for one of the cross-validation results.

```
xv.ml <- xvalid(s100, model=ml)
xv.wls <- xvalid(s100, model=wls)
```

WARNING: RUNNING THE NEXT COMMAND CAN BE TIME-CONSUMING

```
xvR.ml <- xvalid(s100, model=ml, reest=TRUE)
xvR.wls <- xvalid(s100, model=wls, reest=TRUE, variog.obj=bin1)

par(mfcol = c(5,2), mar=c(3,3,.5,.5), mgp=c(1.5,.7,0))
plot(xv.wls)
par(par.ori)
```



5. SPATIAL INTERPOLATION

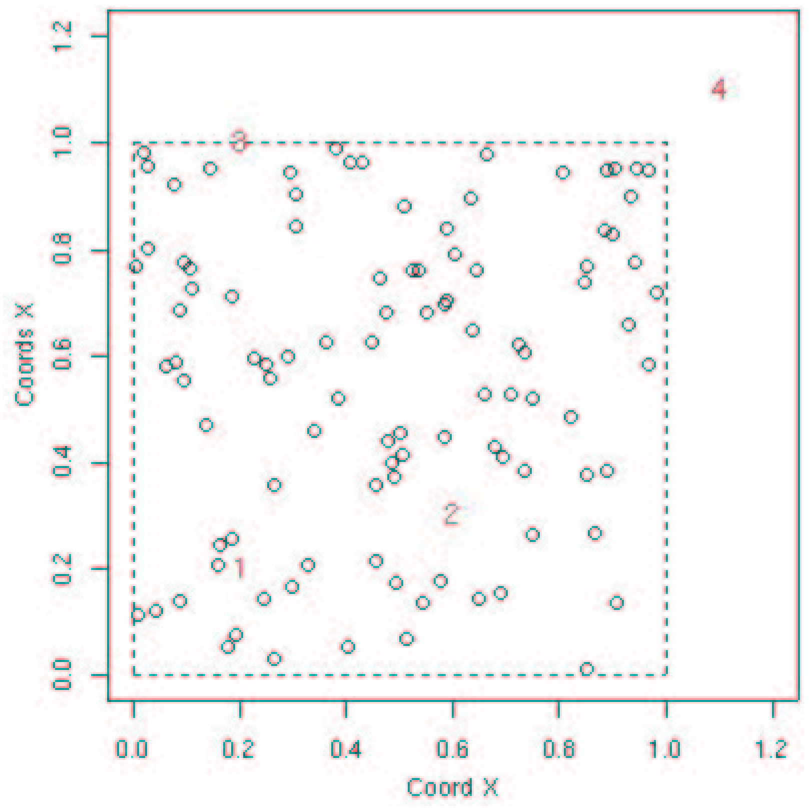
Conventional geostatistical spatial interpolation (*kriging*) can be performed with options for:

- *Simple kriging*
- *Ordinary kriging*
- *Trend (universal) kriging*

There are additional options for Box-Cox transformation (and back transformation of the results) and anisotropic models. Simulations can be drawn from the resulting predictive distributions if requested.

As a first example consider the prediction at four locations labeled *1, 2, 3, 4* and indicated in the figure below.

```
plot(s100$coords, xlim=c(0,1.2), ylim=c(0,1.2))
loci <- matrix(c(0.2, 0.6, 0.2, 1.1, 0.2, 0.3, 1.0, 1.1), ncol=2)
text(loci, as.character(1:4), col="red")
polygon(x=c(0,1,1,0), y=c(0,0,1,1), lty=2)
```



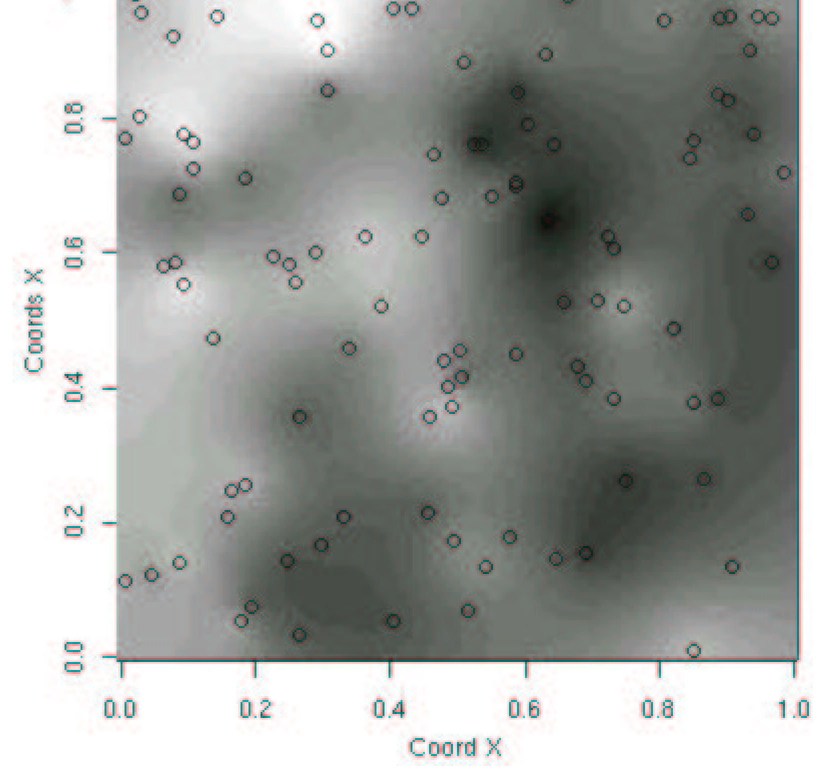
The command to perform *ordinary kriging* using the parameters estimated by weighted least squares with nugget fixed to zero would be:

```
kc4 <- krige.conv(s100, locations = loci, krige = krige.control(cov.pars = wls$cov.pars))
```

The output is a list including the predicted values (`kc4$predict`) and the kriging variances (`kc4$krige.var`).

Consider now a second example. The goal is to perform prediction on a grid covering the area and to display the results. Again, we use ordinary kriging. The commands are:

```
# defining the grid
pred.grid <- expand.grid(seq(0,1, l=51), seq(0,1, l=51))
# kriging calculations
kc <- krige.conv(s100, locations = pred.grid, krige = krige.control(cov.pars = ml$cov.pars))
# displaying predicted values
image(kc, loc = pred.grid, coords = s100$coords, col=gray(seq(1,0.1,l=30)))
```



6. BAYESIAN ANALYSIS

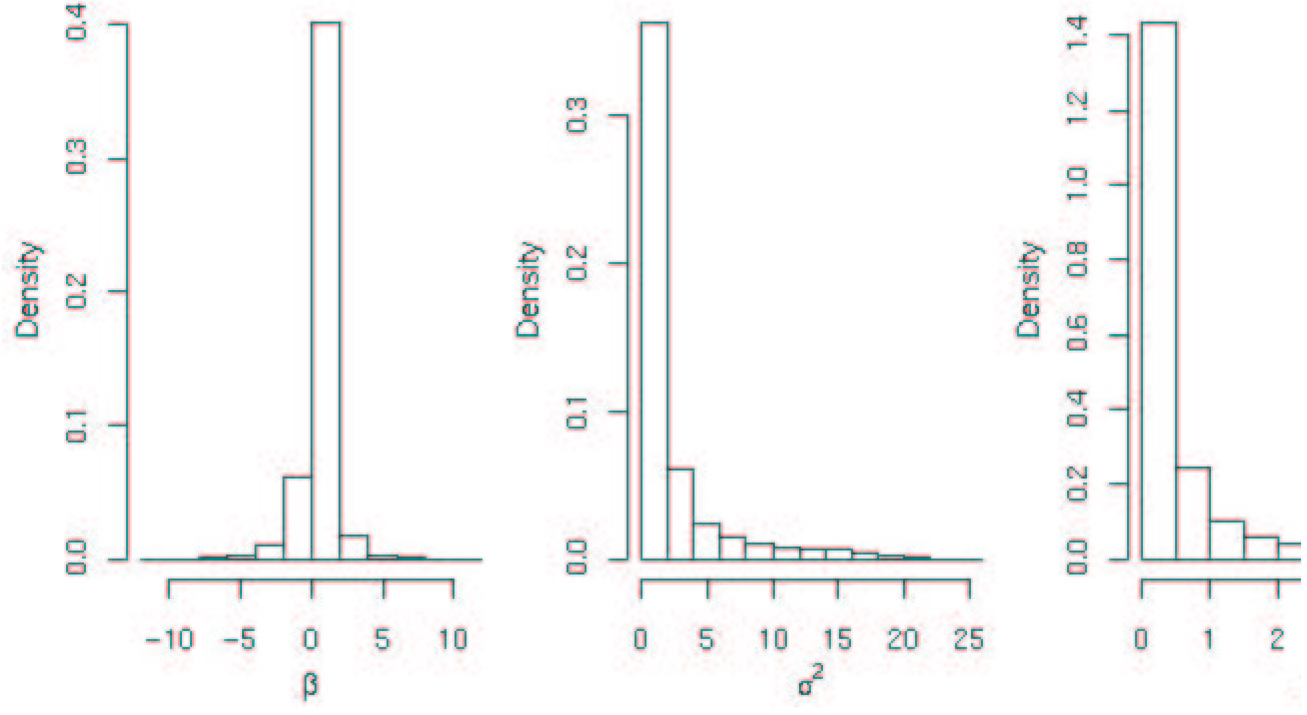
Bayesian analysis for Gaussian models is implemented by the function `krige.bayes`. It can be performed for different "degrees of uncertainty", meaning that model parameters can be treated as fixed or random.

As an example consider a model without nugget and including uncertainty in the mean, sill and range parameters. Prediction at the four locations indicated above is performed by typing a command like:

WARNING: RUNNING THE NEXT COMMAND CAN BE TIME-CONSUMING
```
bsp4 <- krige.bayes(s100, loc = loci, prior = prior.control(phi.discrete = seq(0,5,l=101), phi.prior="rec"),
output=output.control(n.post=5000))
```

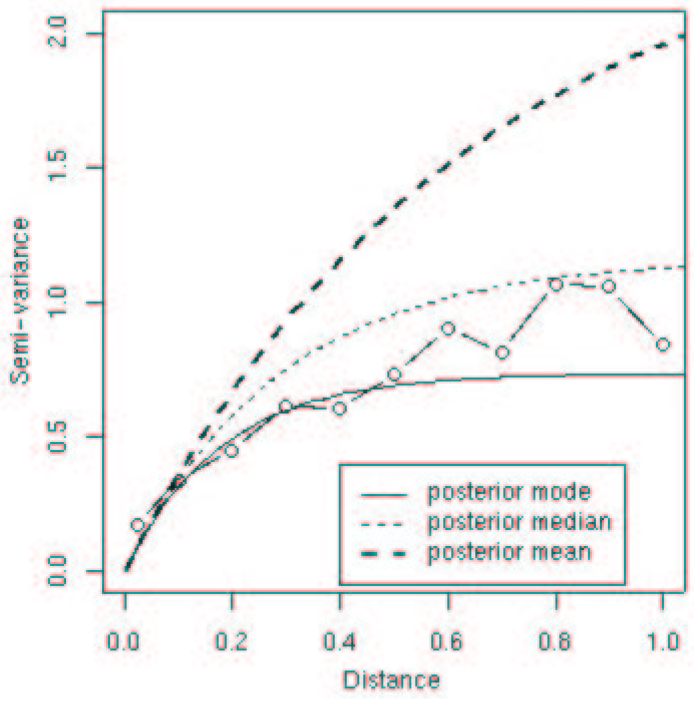
Histograms showing posterior distribution for the model parameters can be plotted by typing:

```
par(mfrow=c(1,3), mar=c(3,3,.5,.5), mgp=c(2,1,0))
hist(bsp4$posterior$sample$beta, main="", xlab=expression(beta), prob=T)
hist(bsp4$posterior$sample$sigmasq, main="", xlab=expression(sigma^2), prob=T)
hist(bsp4$posterior$sample$phi, main="", xlab=expression(phi), prob=T)
par(par.ori)
```



Using summaries of these posterior distributions (means, medians or modes) we can check the "estimated Bayesian variograms" against the empirical variogram, as shown in the next figure. Notice that it is also possible to compare these estimates with other fitted variograms such as the ones computed in Section 3.

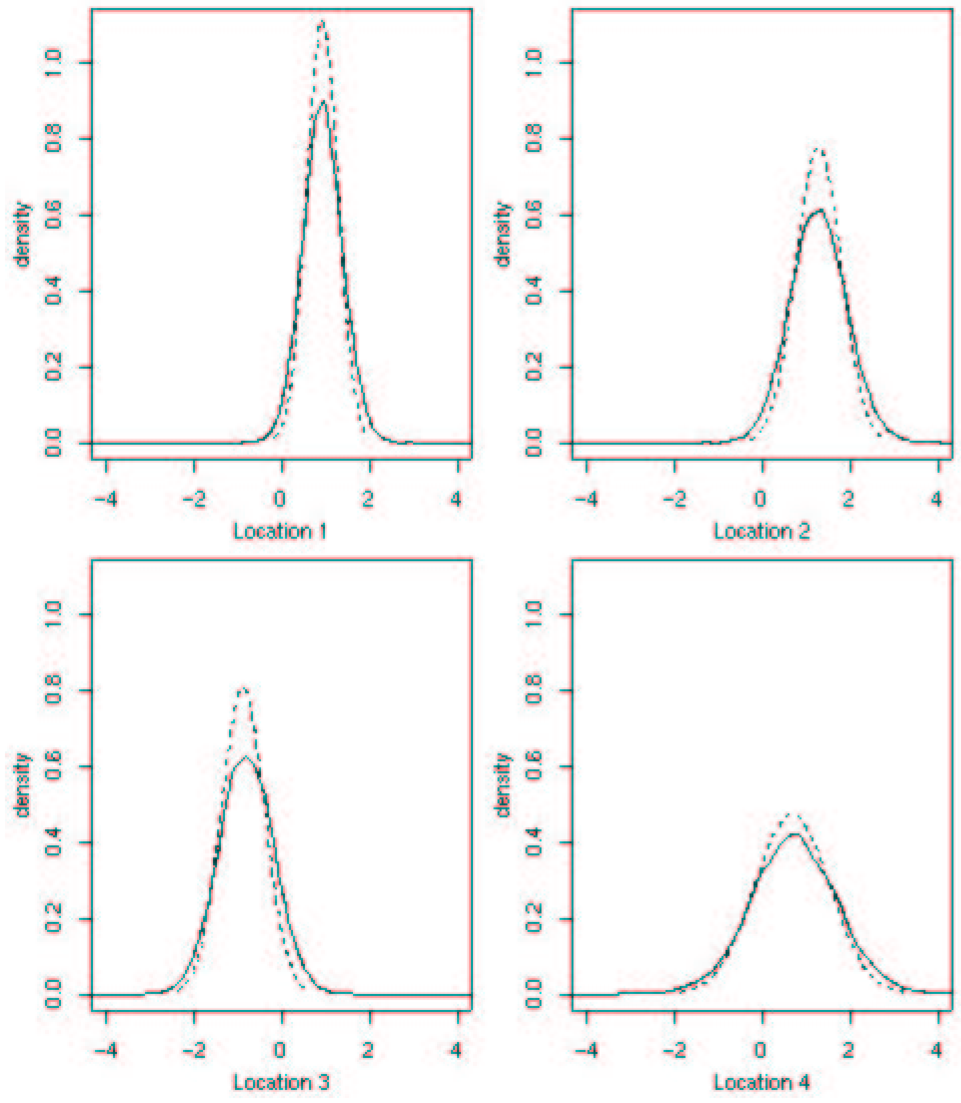
```
plot(bin1, ylim = c(0,2))
lines(bsp4, max.dist = 1.2)
lines(bsp4, max.dist = 1.2, summ = "median", lty = 2)
lines(bsp4, max.dist = 1.2, summ = "mean", lwd = 2, lty = 2)
legend(0.5, 0.3, legend = c("posterior mode", "posterior median", "posterior mean"), lty = c(1,2,2), lwd = c(1,1,2))
```



The next figure shows predictive distributions at the four selected locations.
Dashed lines show Gaussian distributions with mean and variance given by results of ordinary kriging obtained in Section 4.

using samples from the predictive distributions.

```
par(mfrow=c(2,2), mar=c(3,3,.5,.5), mgp=c(1.5,.7,0))
for(i in 1:4){
kpx <- seq(kc4$pred[i] - 3*sqrt(kc4$krige.var[i]), kc4$pred[i] +3*sqrt(kc4$krige.var[i]), l=100)
kpy <- dnorm(kpx, mean=kc4$pred[i], sd=sqrt(kc4$krige.var[i]))
bp <- density(bsp4$predic$sim[i,])
rx <- range(c(kpx, bp$x))
ry <- range(c(kpy, bp$y))
plot(cbind(rx, ry), type="n", xlab=paste("Location", i), ylab="density", xlim=c(-4, 4), ylim=c(0,1.1))
lines(kpx, kpy, lty=2)
lines(bp)}
par(par.ori)
```



Consider now, under the same model assumptions, obtaining simulations from the predictive distributions on a grid of points covering the area. The commands to define the grid and perform Bayesian prediction are:

```
pred.grid <- expand.grid(seq(0,1, l=31), seq(0,1, l=31))
```
WARNING: RUNNING THE NEXT COMMAND CAN BE TIME-CONSUMING
```
bsp <- krige.bayes(s100, loc = pred.grid, prior = prior.control(phi.discrete = seq(0,5,l=51)), output=output.control(n.predictive=2))
```

Maps with the summaries and simulations of the predictive distribution can be plotted as follows.

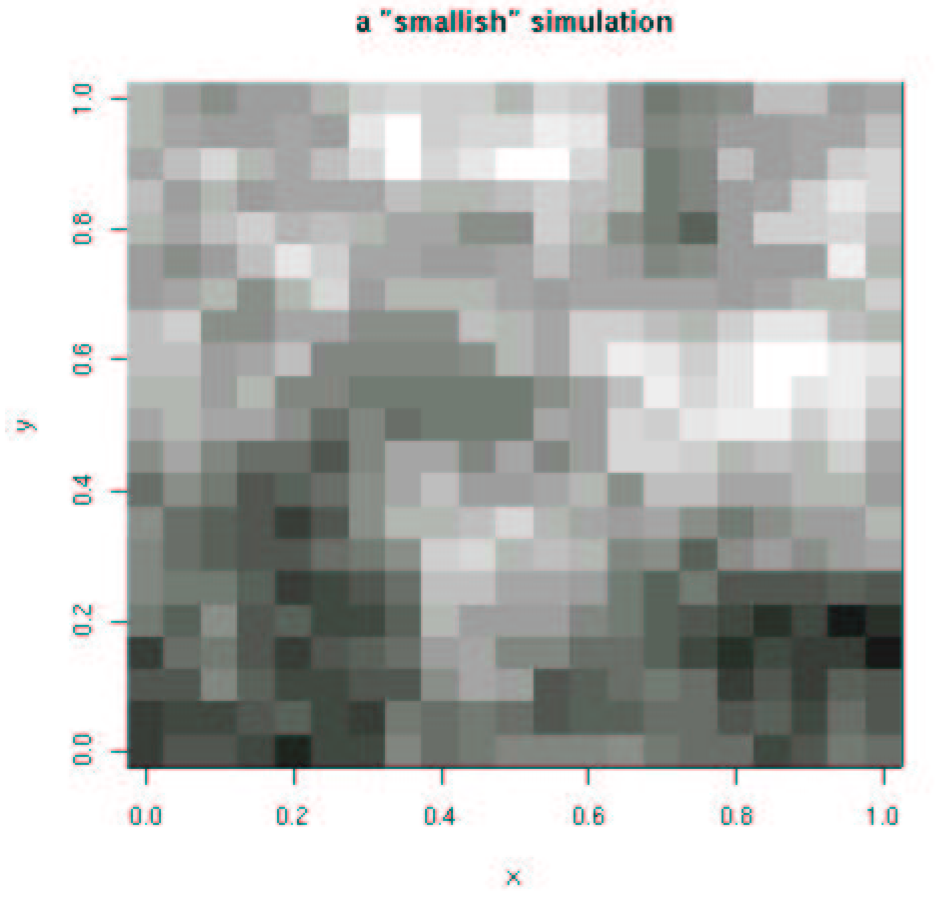
```
par(mfrow=c(2,2))
image(bsp, loc = pred.grid, main = "predicted", col=gray(seq(1,0.1,l=30)))
image(bsp, val ="variance", loc = pred.grid, main = "prediction variance", col=gray(seq(1,0.1,l=30)))
image(bsp, val = "simulation", number.col = 1, loc = pred.grid, main = "a simulation from\nthe predictive distribution",
col=gray(seq(1,0.1,l=30)))
image(bsp, val = "simulation", number.col = 2,loc = pred.grid, main = "another simulation from \n the predictive distribution",
col=gray(seq(1,0.1,l=30)))
```

7. Simulation of Gaussian Random Fields

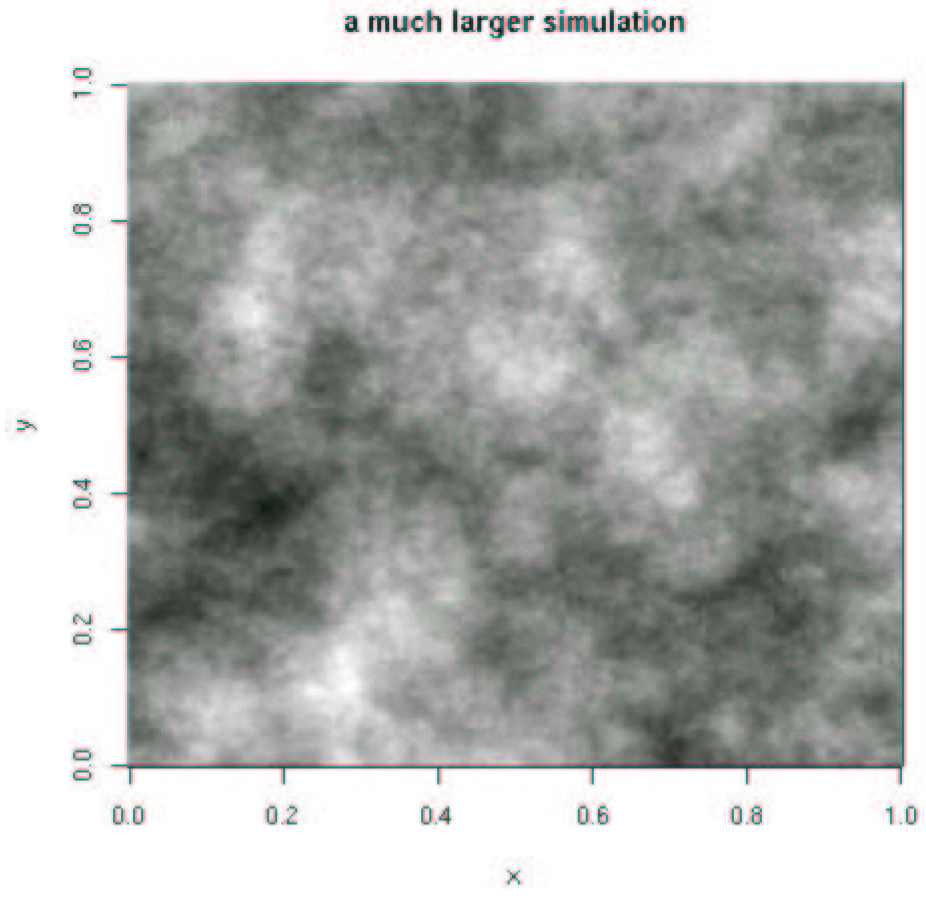
The function `grf` generates simulations of Gaussian random fields on regular or irregular sets of locations Some of its functionality is illustrated by the next commands.

```
sim1 <- grf(100, cov.pars=c(1, .25))
points.geodata(sim1, main="simulated locations and values")
plot(sim1, max.dist=1, main="true and empirical variograms")
```

```
sim2 <- grf(441, grid="reg", cov.pars=c(1, .25))
image(sim2, main="a small-ish simulation", col=gray(seq(1, .1, l=30)))
```



```
sim3 <- grf(40401, grid="reg", cov.pars=c(10, .2), met="circ")
image(sim3, main="simulation on a fine grid", col=gray(seq(1, .1, l=30)))
```



NOTE: see the package RandomFields for more on simulation of Gaussian Random Fields.

Site maintained by: Paulo J. Ribeiro Jr. (Paulo.Ribeiro@est.ufpr.br)