Ordinary kriging using \texttt{geoR} and \texttt{gstat}

In this document we will discuss kriging using the R packages \texttt{geoR} and \texttt{gstat}. We will use the numerical example from last lecture. Here it is:

**A simple example:**

Consider the following data

<table>
<thead>
<tr>
<th>$s_i$</th>
<th>$x$</th>
<th>$y$</th>
<th>$z(s_i)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$s_1$</td>
<td>61</td>
<td>139</td>
<td>477</td>
</tr>
<tr>
<td>$s_2$</td>
<td>63</td>
<td>140</td>
<td>696</td>
</tr>
<tr>
<td>$s_3$</td>
<td>64</td>
<td>129</td>
<td>227</td>
</tr>
<tr>
<td>$s_4$</td>
<td>68</td>
<td>128</td>
<td>646</td>
</tr>
<tr>
<td>$s_5$</td>
<td>71</td>
<td>140</td>
<td>606</td>
</tr>
<tr>
<td>$s_6$</td>
<td>73</td>
<td>141</td>
<td>791</td>
</tr>
<tr>
<td>$s_7$</td>
<td>75</td>
<td>128</td>
<td>783</td>
</tr>
<tr>
<td>$s_0$</td>
<td>65</td>
<td>137</td>
<td>??</td>
</tr>
</tbody>
</table>

Our goal is to estimate the unknown value at location $s_0$. Here is the $x - y$ plot:
For these data, let’s assume that we use the exponential semivariogram model with parameters $c_0 = 0, c_1 = 10, \alpha = 3.33$.

$$\gamma(h) = c_0 + c_1 (1 - e^{-\frac{h}{\alpha}}) = 10 (1 - e^{-\frac{h}{3.33}}).$$

which is equivalent to the covariance function

$$C(h) = \begin{cases} c_0 + c_1, & h = 0 \\ c_1 e^{-\frac{h}{\alpha}}, & h > 0 \end{cases} \Rightarrow C(h) = \begin{cases} 10, & h = 0 \\ 10 e^{-\frac{h}{3.33}}, & h > 0 \end{cases}$$

The predicted value at location $s_0$ is equal to:

$$\hat{z}(s_0) = \sum_{i=1}^{n} w_i z(s_i) = 0.174(477) + \cdots + 0.086(783) = 592.59.$$ 

And the variance:

$$\sigma^2_e = \sum_{i=1}^{n} w_i \gamma(s_i - s_0) + \lambda = 0.174(7.384) + \cdots + 0.086(9.823) + 0.906 = 8.96.$$ 

**Kriging using geoR:**

We will use now the geoR package to find the same result. First we read our data as a geodata object:

```r
> a <- read.table("http://www.stat.ucla.edu/~nchristo/statistics_c173_c273/kriging_11.txt", header=TRUE)
> b <- as.geodata(a)
```

To predict the unknown value at location $(x = 65, y = 137)$ we use the following:

```r
> prediction <- ksline(b, cov.model="exp", cov.pars=c(10,3.33), nugget=0, locations=c(65,137))
```

where,

- `b` The geodata
- `cov.model` The model we are using
- `cov.pars` The parameters of the model (partial sill and range)
- `nugget` The value of the nugget effect
- `locations` The coordinates $(x, y)$ of the points to be predicted

The object “prediction” contains among other things the predicted value at location $x = 65, y = 137$ and its variance. We can obtain them as follows:

```r
> prediction$predict
[1] 592.7587
> prediction$krige.var
[1] 8.960294
```
Suppose now we want to predict the value at many locations. The following commands will produce a grid whose points will be estimated using kriging:

```r
> x <- seq(61, 75, by=1)
> y <- seq(128,141, by=1)
> xv <- rep(x,14)
> yv <- rep(y, each=15)
> in_mat <- as.matrix(cbind(xv,yv))
```

Of course the matrix can be constructed also as follows:

```r
> x.range <- as.integer(range(a[,1]))
> y.range <- as.integer(range(a[,2]))
> x=seq(from=x.range[1], to=x.range[2], by=1)
> y=seq(from=y.range[1], to=y.range[2], by=1)
> length(x)
> length(y)
> xv <- rep(x,length(y))
> yv <- rep(y, each=length(x))
> in_mat <- as.matrix(cbind(xv,yv))
> plot(in_mat)
```

This grid consists of $15 \times 14 = 210$ points stored in the matrix `in_mat`. The command that predicts the value at each one of these points is the following:

```r
> q <- ksline(b, cov.model="exp", cov.pars=c(10,3.33), nugget=0, locations=in_mat)
```

Kriging performed using global neighbourhood

We can access the predicted values and their variances using `q$predict` and `q$krige.var`. Here are the first 5 predicted values with their variances:

```r
> cbind(q$predict[1:5], q$krige.var[1:5])
   [,1]        [,2]
[1,] 458.4491  9.245493
[2,] 413.2103  7.850838
[3,] 362.4674  5.927999
[4,] 338.9828  4.516906
[5,] 393.3933  5.280417
```
To construct the raster map we type:

\[ \text{image}(q, \text{val}=q\text{'predict}) \]

Or simply:

\[ \text{image}(q) \]

Here is the plot:

And here is the plot with the data points:

\[ \text{points}(a) \]
We can construct a raster map of the variances:

```r
> image(q, val=q$krige.var)
```

Here is the plot:

![Raster map of variances](image)

And also we can construct a raster map of the standard errors:

```r
> image(q, val=sqrt(q$krige.var))
```

Here is the plot:

![Raster map of standard errors](image)
The following command will construct a perspective plot of the predicted values:

```r
> persp(x,y,matrix(q$predict,15,14), xlab="x coordinate",
   ylab="y coordinate", zlab="Predicted values of z",
   main="Perspective plot of the predicted values")
```

And here is the perspective plot of the standard errors:

```r
> persp(x,y,matrix(sqrt(q$krige.var),15,14), xlab="x coordinate",
   ylab="y coordinate", zlab="Predicted values of z",
   main="Perspective plot of the standard errors")
```
Commnets:
The argument locations for the function ksline can be a matrix or a data frame. So far we use a matrix (in_mat). We can also use a data frame as follows:

```r
> x.range <- as.integer(range(a[,1]))
> y.range <- as.integer(range(a[,2]))
> grd <- expand.grid(x=seq(from=x.range[1], to=x.range[2], by=1),
                    y=seq(from=y.range[1], to=y.range[2], by=1))
> q <- ksline(b, cov.model="exp", cov.pars=c(10, 3.33), nugget=0,
              locations=grd)
```

Another function in geoR that performs kriging is the `krige.conv` function. It can be used as follows:

```r
> kc <- krige.conv(b, loc=in_mat,
                   krige=krige.control(cov.pars=c(10, 3.33), nugget=0))
krige.conv: model with constant mean
krige.conv: Kriging performed using global neighbourhood
```

Or using a data frame argument for locations:

```r
> kc <- krige.conv(b, loc=grd,
                   krige=krige.control(cov.pars=c(10, 3.33), nugget=0))
krige.conv: model with constant mean
krige.conv: Kriging performed using global neighbourhood
```

In case you have a variofit output you can use it as an input of the argument krig as follows (this is only an example):

```r
var1 <- variog(b, max.dist=1000)
fit1 <- variofit(var1, cov.model="exp", ini.cov.pars=c(1000, 100),
                fix.nugget=FALSE, nugget=250)

qq <- krige.conv(b, locations=grd, krige=krige.control(obj.model=fit1))
```
**Kriging using gstat:**
We will use now the `gstat` package to find the same result. First we read our data and create the grid for prediction as follows:

```r
> a <- read.table("http://www.stat.ucla.edu/~nchristo/statistics_c173_c273/ kriging_11.txt", header=TRUE)
> x.range <- as.integer(range(a[,1]))
> y.range <- as.integer(range(a[,2]))
> grd <- expand.grid(x=seq(from=x.range[1], to=x.range[2], by=1),
  y=seq(from=y.range[1], to=y.range[2], by=1))
```

We now define the model. Normally the model must be estimated from the sample variogram, but for this simple example we assume that it is given as below:

```r
> library(gstat)
> m <- vgm(10, "Exp", 3.33, 0)
```

There are two ways to perform ordinary kriging with `gstat`. The data and the grid are used as data frames, with the extra argument `locations` as shown below:

```r
> q1 <- krige(id="z", formula=z~1, data=a, newdata=grd, model = m,
  locations=~x+y)
```

The other way is to convert the data and the grid as spatial data points data frame:

```r
> coordinates(a) <- ~x+y
> coordinates(grd) <- ~x+y
> q2 <- krige(id="z", formula=z~1, a, newdata=grd, model = m)
```

Important note: If we use the second way the argument `data=` is not allowed. We simply use the name of the data, here just `a`. Also, `q1` is a data frame, while `q2` is spatial data points data frame. Using `q1` we can create a 3D plot with the libraries `scatterplot3d` and `rgl` as follows:

```r
> library(scatterplot3d)
> library(rgl)
> scatterplot3d(q1$x, q1$y, q1$z.pred, xlab="x", ylab="y",
  zlab="Predicted values")
> plot3d(q1$x, q1$y, q1$z.pred, size=3)
```
Here are the plots:
(a). Using the `scatterplot3d` command.

(b). Using the `plot3d` command.
A complete example on kriging using \texttt{gstat}:

We will use again the soil data from the \textit{Maas} river. Here is some background.

The actual data set contains many variables but here we will use the $x, y$ coordinates and the concentration of lead and zinc in ppm at each data point. The motivation for this study is to predict the concentration of heavy metals around the banks of the Maas river in the area west of the town Stein in the Netherlands. These heavy metals were accumulated over the years because of river pollution. Here is the area of study:
You can access the data at

```r
> a <- read.table("http://www.stat.ucla.edu/~nchristo/statistics_c173_c273/soil.txt", header=TRUE)
# Save the original image function:
> image.orig <- image
```

To load the `gstat` package type

```r
> library(gstat)
```

First, we will compute the descriptive statistics of the data set, construct the stem-and-leaf plots, histograms, and boxplots:

```r
> stem(a$lead)
> boxplot(a$lead)
> hist(a$lead)
> stem(a$zinc)
> boxplot(a$zinc)
> hist(a$zinc)
> summary(a)
```

Transform the data (logarithm transformation):

```r
> log_lead <- log10(a$lead)
> log_zinc <- log10(a$zinc)
> stem(log_lead)
> boxplot(log_lead)
> hist(log_lead)
> stem(log_zinc)
> boxplot(log_zinc)
> hist(log_zinc)
```

#Create a gstat object;
```r
> g <- gstat(id="log_lead", formula = log(lead)^1, locations = ~x+y,
data = a)
```

#Plot the variogram:
```r
> plot(variogram(g), main="Semivariogram of the log_lead")
```

#Fit a model variogram to the sample variogram:
```r
> v.fit <- fit.variogram(variogram(g), vgm(0.5,"Sph",1000,0.1))
> plot(variogram(g),v.fit)
```

#Note: The values above were the initial values for the partial sill, range, and nugget. Then the function fit.variogram uses a minimization procedure to fit a model variogram to the sample variogram. Type v.fit
#to get the estimates of the model parameters.

```r
> v.fit
    model   psill   range
 1  Nug 0.05156252 0.0000
 2  Sph 0.51530678 965.1506
```

#There are different weights you can use in the minimization procedure. The default (the one used above) is $N_h/h^2$ where $N_h$ is the number of pairs and $h$ the separation distance. You can chose the type of weights by using the argument fit.method=integer, where integer is a number from the table below:

<table>
<thead>
<tr>
<th>fit.method</th>
<th>weights</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$N_h$</td>
</tr>
<tr>
<td>2</td>
<td>$N_h/\gamma(h;\theta)^2$ (Cressie’s weights)</td>
</tr>
<tr>
<td>6</td>
<td>OLS (no weights)</td>
</tr>
<tr>
<td>7</td>
<td>$N_h/h^2$ (default)</td>
</tr>
</tbody>
</table>

#Use kriging to estimate the value of log(lead) at the grid values. First we create the grid.
```r
> x.range <- as.integer(range(a[,1]))
> x.range
> y.range <- as.integer(range(a[,2]))
> y.range
> grd <- expand.grid(x=seq(from=x.range[1], to=x.range[2], by=50),
y=seq(from=y.range[1], to=y.range[2], by=50))
```

#We want now to use kriging to predict log(lead) at each point on the grid:
```r
> pr.ok <- krige(id="log_lead",log(lead)~1, locations=~x+y,
model=v.fit,
data=a, newdata=grd)
```

#To find what the object pr.ok contains type:
```r
> names(pr.ok)
[1] "x"       "y"       "log_lead.pred" "log_lead.var"
```

#To see the predicted values you type:
```r
> pr.ok$log_lead.pred
```

#And the kriging variances:
```r
> pr.ok$log_lead.var
```
The plot of the sample variogram:

```r
> plot(variogram(g), main="Semivariogram of the log_lead")
```

![Semivariogram of the log_lead](image)

The fitted spherical variogram to the sample variogram:

```r
> plot(variogram(g), v.fit)
```

![Fitted spherical semivariogram](image)
Here is the grid for the kriging predictions:

> plot(grd)

![Grid for the kriging predictions](image)

Load the library `scatterplot3d`:

> library(scatterplot3d)
> scatterplot3d(pr_ok$x, pr_ok$y, pr_ok$log_lead.pred, main="Predicted values")

![Predicted values](image)
Load the library `lattice` to use the `levelplot` function:

```r
> library(lattice)
> levelplot(pr_ok$log_lead.pred~x+y,pr_ok, aspect ="iso",
            main="Ordinary kriging predictions")
```

```
Ordinary kriging predictions
```

```r
> levelplot(pr_ok$log_lead.var~x+y,pr_ok, aspect ="iso",
            main="Ordinary kriging variances")
```

```
Ordinary kriging variances
```
Use the `image` function:
We will use now the function `image.orig` that was saved at the beginning (before we loaded the `gstat` library) to construct similar graphs.

```r
# Function to convert a vector to a matrix:
vec.2.Mx <- function( xvec, nrow, ncol ) {
  Mx.out <- matrix(0, nrow, ncol )
  for(j in 1:ncol) {
    for(i in 1:nrow) {
      Mx.out[i, j] <- xvec[ (j-1)*nrow + i ]
    }
  }
  return( Mx.out )
}
```

> levelplot(sqrt(pr_ok$log_lead.var)~x+y,pr_ok, aspect ="iso", main="Ordinary kriging standard errors")
Now we can use the function to create a matrix (\textit{qqq} below):

\begin{verbatim}
> qqq <- vec.2.Mx( pr_ok$log_lead.pred,
    length(seq(from=x.range[1], to=x.range[2], by=50)),
    length(seq(from=y.range[1], to=y.range[2], by=50))
)
\end{verbatim}

Much easier the vector of the predicted values can be collapsed into a matrix with the \texttt{matrix} function:

\begin{verbatim}
#Collapse the predicted values into a matrix:
qqq <- matrix(pr_ok$log_lead.pred,
    length(seq(from=x.range[1], to=x.range[2], by=50)),
    length(seq(from=y.range[1], to=y.range[2], by=50)))
\end{verbatim}

And we can use the original image function to create the raster map of the predicted values:

\begin{verbatim}
> image.orig(seq(from=x.range[1], to=x.range[2], by=50),
    seq(from=y.range[1], to=y.range[2], by=50), qqq,
    xlab="West to East", ylab="South to North", main="Predicted values")
\end{verbatim}

\begin{verbatim}
> points(a) #The data points can be plotted on the raster map.
\end{verbatim}
We can also create the raster map of the kriging variances:

```r
> qqq <- vec.2.Mx( pr_ok$log_lead.var,
    length(seq(from=x.range[1], to=x.range[2], by=50)),
    length(seq(from=y.range[1], to=y.range[2], by=50)) )

> image.orig(seq(from=x.range[1], to=x.range[2], by=50),
    seq(from=y.range[1], to=y.range[2], by=50), qqq,
    xlab="West to East", ylab="South to North", main="Kriging variances")
```

![Kriging variances](image)
And finally the raster map of the kriging standard errors:

```r
> qqq <- vec.2.Mx( sqrt(pr.ok$log_lead.var),
    length(seq(from=x.range[1], to=x.range[2], by=50)),
    length(seq(from=y.range[1], to=y.range[2], by=50)) )

> image.orig(seq(from=x.range[1], to=x.range[2], by=50),
    seq(from=y.range[1], to=y.range[2], by=50), qqq,
    xlab="West to East", ylab="South to North", main="Kriging standard errors")
```

**Kriging standard errors**

**Exercise:**
Repeat for \( \log(\text{zinc}) \).