

Overview of geostatistics

- Let $Z(s)$ and $Z(s+h)$ two random variables at locations s and $s+h$. Intrinsic stationarity is defined as follows:

$$E(Z(s+h) - Z(s)) = 0$$

and

$$Var(Z(s+h) - Z(s)) = 2\gamma(h)$$

The quantity $2\gamma(h)$ is known as the variogram and is very crucial in geostatistics. The variogram says that differences of variables lagged h -apart vary in a way that depends only on h . This is called an isotropic variogram. If the variogram depends not only on the length h but also the direction, it is called an anisotropic variogram. Assuming a constant mean (no trend) we have $E(Z(s)) = \mu$ and we can write

$$\text{Var}(Z(s+h) - Z(s)) = E(Z(s+h) - Z(s))^2$$

Therefore we can use the method of moments estimator for the variogram (also called the classical estimator):

$$2\hat{\gamma}(h) = \frac{1}{N(h)} \sum_{N(h)} (Z(s_i) - Z(s_j))^2,$$

where the sum is over $N(h)$ such that $s_i - s_j = h$.

Robust estimator:

Cressie and Hawkins (1980) proposed the following estimator for the variogram which is robust to outliers compared to the classical estimator:

$$2\bar{\gamma}(h) = \frac{\left\{ \frac{1}{N(h)} \sum_{N(h)} |Z(s_i) - Z(s_j)|^{\frac{1}{2}} \right\}^4}{0.457 + \frac{0.494}{N(h)}}$$

where the sum is over $N(h)$ such that $s_i - s_j = h$.

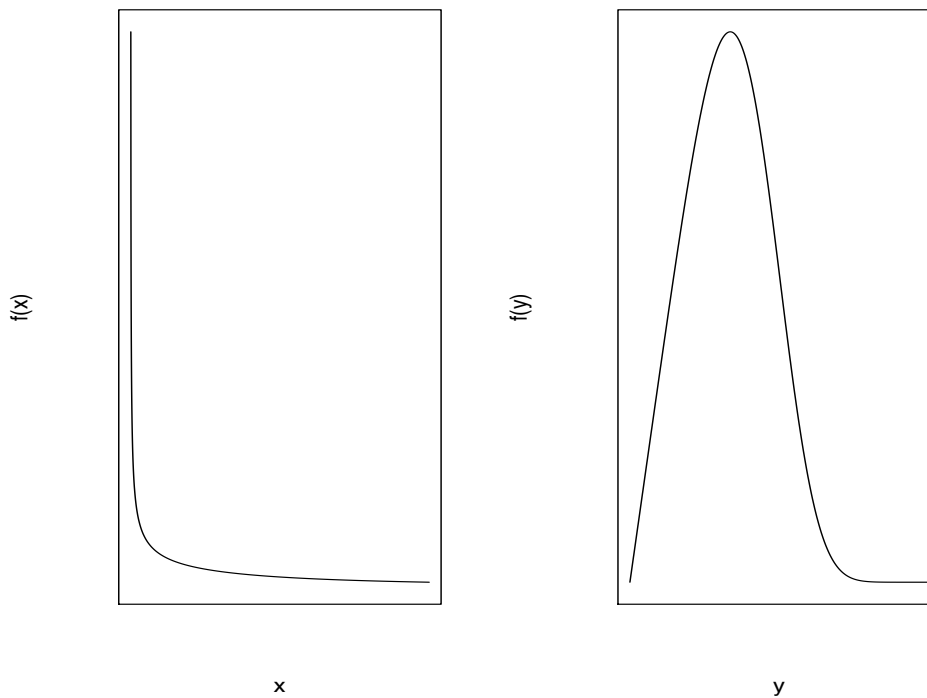
The idea behind the robust estimator is described below: If the process $Z(s)$ follows the normal distribution then

$$Z(s+h) - Z(s) \sim N\left(0, \sqrt{2\gamma(h)}\right)$$

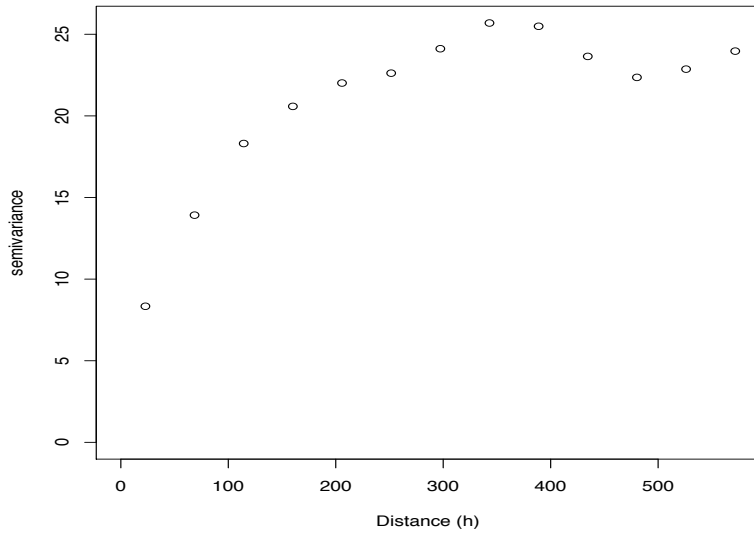
Therefore:

$$\left(\frac{Z(s+h) - Z(s)}{\sqrt{2\gamma(h)}}\right)^2 \sim \chi_1^2 \quad (\chi^2 \text{ distribution with 1 degree of freedom}).$$

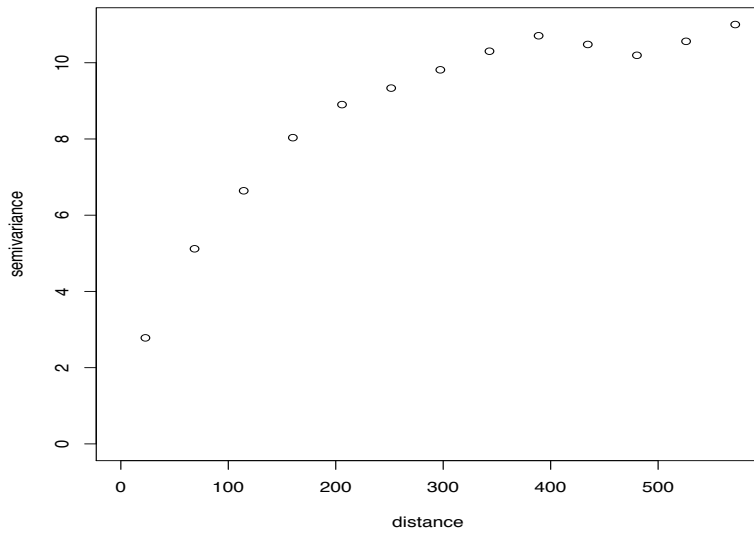
This is a highly skewed distribution. However if $X \sim \chi_1^2$ then $Y = X^{\frac{1}{4}}$ has an approximately symmetric distribution (see figure below). We would expect that the quantity $(Z(s+h) - Z(s))^{\frac{1}{2}}$ will behave much better than $(Z(s+h) - Z(s))^2$.



A typical semivariogram plot (classical estimator):



The semivariogram plot (robust estimator):



- **Modeling the sample variogram**

Once the sample variogram is computed, a function is fit to it. In other words, we try to come up with what the variogram graph would look like if we had the entire population of all possible pairs. Popular variogram models that are used are the linear, spherical, and exponential (also see graphs on next pages).

Linear model:

This is the simplest model for the semivariogram graph. It depends on one parameter, the slope b .

$$\gamma(h; \theta) = \begin{cases} 0, & h = 0 \\ c_0 + bh, & h \neq 0 \end{cases}$$

$$\theta = (c_0, b)', \text{ where } c_0 \geq 0 \text{ and } b \geq 0.$$

Spherical model:

This is the model proposed by Matheron. It has two parameters: The range of influence and the sill (or plateau) which the graph reaches at distances h larger than the range. Generally, the range of influence is the distance beyond which pairs are unrelated.

$$\gamma(h; \theta) = \begin{cases} 0, & h = 0 \\ c_0 + c_1 \left(\frac{3}{2} \left(\frac{h}{\alpha} \right) - \frac{1}{2} \left(\frac{h}{\alpha} \right)^3 \right), & 0 < h \leq \alpha \\ c_0 + c_1, & h \geq \alpha \end{cases}$$

$$\theta = (c_0, c_1, \alpha)', \text{ where } c_0 \geq 0, c_1 \geq 0, \text{ and } \alpha \geq 0.$$

Exponential model:

This model represents an exponential decay of influence between two sample (larger distance between two samples means larger decay). It depends on two parameters, the range and the sill (plateau).

$$\gamma(h; \theta) = \begin{cases} 0, & h = 0 \\ c_0 + c_1 \left(1 - \exp\left(-\frac{h}{\alpha}\right) \right), & h \neq 0 \end{cases}$$

$$\theta = (c_0, c_1, \alpha)', \text{ where } c_0 \geq 0, c_1 \geq 0, \text{ and } \alpha \geq 0.$$

Other models:

There are other models, such as, the Gaussian model, the hole effect model, the Paddington mix model, the circular model, cubic model, Matérn function, etc.

Variogram calculations and fitting

```
#Example using stat:
library(gstat)
#Access the data:
a <- read.table("http://www.stat.ucla.edu/~frederic/416/F19
wolfcamp.txt", header=T)

#Create a gstat object:
g <- gstat(id="level", formula = level~1, locations = ~x+y, data = a)

q <- variogram(g)
plot(q)

#Or
plot(variogram(g))

#There is a trend.
g_trend <- gstat(id="level", formula = level~x+y,
  locations = ~x+y, data = a)

#Plot new variogram:
q <- variogram(g_trend)
plot(q)

#Fit a noel variogram by eye:
fit_var <- vgm(30000,"Sph",70,10000)

plot(q, fit_var)

#Variogram fitting using OLS, GLS, etc.
v.fit <- fit.variogram(q, vgm(30000,"Sph",60,10000))

v.fit1 <- fit.variogram(variogram(g_trend), vgm(30000,"Sph",60,10000), fit.method=1)
v.fit2 <- fit.variogram(variogram(g_trend), vgm(30000,"Sph",60,10000), fit.method=2)
v.fit6 <- fit.variogram(variogram(g_trend), vgm(30000,"Sph",60,10000), fit.method=6)
v.fit7 <- fit.variogram(variogram(g_trend), vgm(30000,"Sph",60,10000), fit.method=7)

plot(q, v.fit1)
plot(q, v.fit2)
plot(q, v.fit6)
plot(q, v.fit7)
```

Ordinary kriging

Kriging (Matheron 1963) owes its name to D. G. Krige a South African mining engineer and it was first applied in mining data. Kriging assumes a random field expressed through a variogram or covariance function. It is a very popular method to solve the spatial prediction problem. Let $\mathbf{Z} = (Z(s_1), Z(s_2), \dots, Z(s_n))'$ be the vector of the observed data at known spatial locations $s_1, s_2, \dots, s_n$. The objective is to estimate the unobserved value $Z(s_0)$ at location s_0 .

The model:

The model assumption is:

$$Z(s) = \mu + \delta(s)$$

where $\delta(s)$ is a zero mean stochastic term with variogram $2\gamma(\cdot)$.

The Kriging System

The predictor assumption is

$$\hat{Z}(s_0) = \sum_{i=1}^n w_i Z(s_i)$$

i.e. it is a weighted average of the sample values, and $\sum_{i=1}^n w_i = 1$ to ensure unbiasedness. The w_i 's are the weights that will be estimated.

Kriging minimizes the mean squared error of prediction

$$\min \sigma_e^2 = E[Z(s_0) - \hat{Z}(s_0)]^2$$

or

$$\min \sigma_e^2 = E \left[Z(s_0) - \sum_{i=1}^n w_i Z(s_i) \right]^2$$

For intrinsically stationary process the last equation can be written as:

$$\sigma_e^2 = 2 \sum_{i=1}^n w_i \gamma(s_0 - s_i) - \sum_{i=1}^n \sum_{j=1}^n w_i w_j \gamma(s_i - s_j) \quad (1)$$

See next page for the proof:

Let's examine $(Z(s_0) - \sum_{i=1}^n w_i Z(s_i))^2$:

$$\begin{aligned}
& \left(z(s_0) - \sum_{i=1}^n w_i z(s_i) \right)^2 = \\
& z^2(s_0) - 2z(s_0) \sum_{i=1}^n w_i z(s_i) + \sum_{i=1}^n \sum_{j=1}^n w_i w_j z(s_i) z(s_j) = \\
& \sum_{i=1}^n w_i z^2(s_0) - 2 \sum_{i=1}^n w_i z(s_0) z(s_i) + \sum_{i=1}^n \sum_{j=1}^n w_i w_j z(s_i) z(s_j) \\
& - \frac{1}{2} \sum_{i=1}^n w_i z^2(s_i) - \frac{1}{2} \sum_{j=1}^n w_j z^2(s_j) + \sum_{i=1}^n w_i z^2(s_i) = \\
& - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n w_i w_j [z(s_i) - z(s_j)]^2 + \sum_{i=1}^n w_i [z(s_0) - z(s_i)]^2
\end{aligned}$$

If we take expectations on the last expression we have

$$\begin{aligned}
& - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n w_i w_j E[z(s_i) - z(s_j)]^2 + \sum_{i=1}^n w_i E[z(s_0) - z(s_i)]^2 = \\
& - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n w_i w_j \text{var}[z(s_i) - z(s_j)] + \sum_{i=1}^n w_i \text{var}[z(s_0) - z(s_i)]
\end{aligned}$$

But $\text{var}[z(s_i) - z(s_j)] = 2\gamma(\cdot)$ is the definition of the variogram, and therefore the previous expression is written as: $2 \sum_{i=1}^n w_i \gamma(s_0 - s_i) - \sum_{i=1}^n \sum_{j=1}^n w_i w_j \gamma(s_i - s_j)$

Therefore kriging minimizes

$$\begin{aligned}
\sigma_e^2 &= E[(Z(s_0) - \sum_{i=1}^n w_i Z(s_i))^2] = \\
& 2 \sum_{i=1}^n w_i \gamma(s_0 - s_i) - \sum_{i=1}^n \sum_{j=1}^n w_i w_j \gamma(s_i - s_j) \\
& \text{subject to} \\
& \sum_{i=1}^n w_i = 1
\end{aligned}$$

The minimization is carried out over $(w_1, w_2, \dots, w_n)$, subject to the constraint $\sum_{i=1}^n w_i = 1$. Therefore the minimization problem can be written as:

$$\min 2 \sum_{i=1}^n w_i \gamma(s_0 - s_i) - \sum_{i=1}^n \sum_{j=1}^n w_i w_j \gamma(s_i - s_j) - 2\lambda \left(\sum_{i=1}^n w_i - 1 \right) \quad (2)$$

where λ is the Lagrange multiplier. After differentiating (2) with respect to $w_1, w_2, \dots, w_n$, and λ and set the derivatives equal to zero we find that

$$- \sum_{j=1}^n w_j \gamma(s_i - s_j) + \gamma(s_0 - s_i) - \lambda = 0, \quad i = 1, \dots, n$$

and

$$\sum_{i=1}^n w_i = 1$$

Using matrix notation the previous system of equations can be written as

$$\mathbf{\Gamma}\mathbf{W} = \gamma$$

Therefore the weights $w_1, w_2, \dots, w_n$ and the Lagrange multiplier λ can be obtained by

$$\mathbf{W} = \mathbf{\Gamma}^{-1}\gamma$$

where

$$\mathbf{W} = (w_1, w_2, \dots, w_n, \lambda)$$

$$\gamma = (\gamma(s_0 - s_1), \gamma(s_0 - s_2), \dots, \gamma(s_0 - s_n), 1)'$$

$$\mathbf{\Gamma} = \begin{cases} \gamma(s_i - s_j), & i = 1, 2, \dots, n, \quad j = 1, 2, \dots, n, \\ 1, & i = n + 1, \quad j = 1, \dots, n, \\ 1, & j = n + 1, \quad i = 1, \dots, n, \\ 0, & i = n + 1, \quad j = n + 1. \end{cases}$$

The variance of the estimator:

So far, we found the weights and therefore we can compute the estimator: $\hat{Z}(s_0) = \sum_{i=1}^n w_i Z(s_i)$. How about the variance of the estimator, namely σ_e^2 ?

We multiply

$$-\sum_{j=1}^n w_j \gamma(s_i - s_j) + \gamma(s_0 - s_i) - \lambda = 0$$

by w_i and we sum over all $i = 1, \dots, n$ to get:

$$-\sum_{i=1}^n w_i \sum_{j=1}^n w_j \gamma(s_i - s_j) + \sum_{i=1}^n w_i \gamma(s_0 - s_i) - \sum_{i=1}^n w_i \lambda = 0$$

Or

$$-\sum_{i=1}^n \sum_{j=1}^n w_i w_j \gamma(s_i - s_j) + \sum_{i=1}^n w_i \gamma(s_0 - s_i) - \sum_{i=1}^n w_i \lambda = 0$$

Therefore,

$$\sum_{i=1}^n \sum_{j=1}^n w_i w_j \gamma(s_i - s_j) = \sum_{i=1}^n w_i \gamma(s_0 - s_i) - \sum_{i=1}^n w_i \lambda$$

If we substitute this result into equation (1) we finally get:

$$\sigma_e^2 = \sum_{i=1}^n w_i \gamma(s_i - s_0) + \lambda \tag{3}$$

The Kriging System

$$\begin{pmatrix} \gamma(s_1 - s_1) & \gamma(s_1 - s_2) & \gamma(s_1 - s_3) & \dots & \gamma(s_1 - s_n) & 1 \\ \gamma(s_2 - s_1) & \gamma(s_2 - s_2) & \gamma(s_2 - s_3) & \dots & \gamma(s_2 - s_n) & 1 \\ \dots & \dots & \ddots & \dots & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \dots & 1 \\ \gamma(s_n - s_1) & \gamma(s_n - s_2) & \gamma(s_n - s_3) & \dots & \gamma(s_n - s_n) & 1 \\ 1 & 1 & \dots & \dots & 1 & 0 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ \vdots \\ w_n \\ \lambda \end{pmatrix} = \begin{pmatrix} \gamma(s_0 - s_1) \\ \gamma(s_0 - s_2) \\ \vdots \\ \vdots \\ \gamma(s_0 - s_n) \\ 1 \end{pmatrix}$$

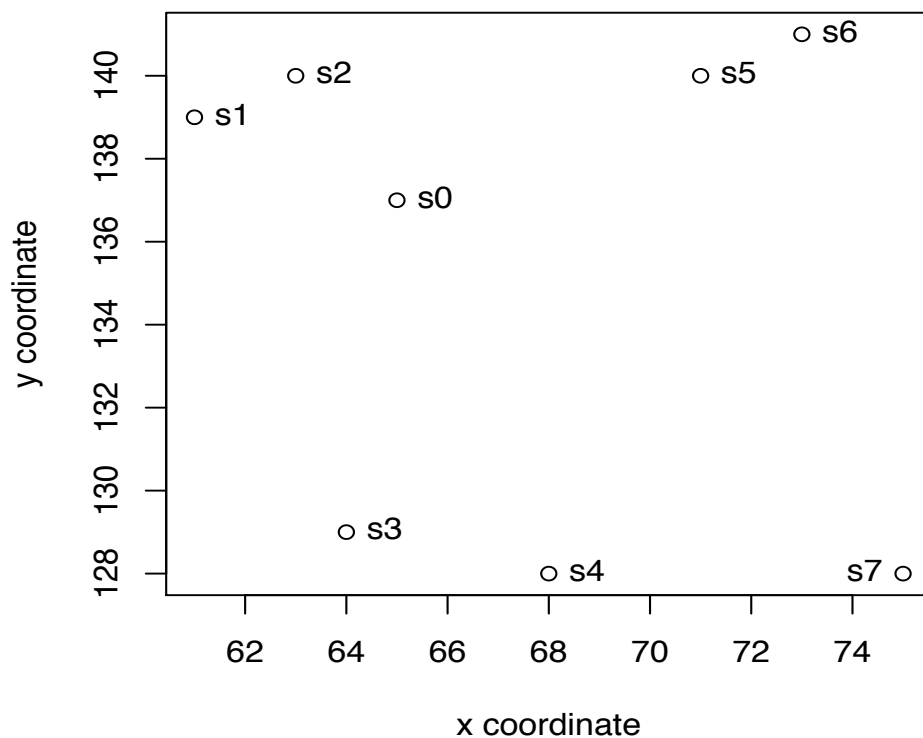
We understand now why the sample variogram cannot be used directly in the kriging system, and instead a theoretical variogram is used. First, the γ vector may call for variogram values for distances that are not available from sample data. There are situations where the distance from the point being estimated to a particular sample is smaller than the distance between pairs of available samples. Since the sample data set cannot provide any pairs for these small distances, we must rely on a function that provides variogram values for all distances. Second, the use of the sample variogram does not guarantee the existence and uniqueness of the solution to the kriging system. In other words the sample variogram version of $\mathbf{\Gamma}$ might not be positive definite. To be guaranteed of having one and only one solution, we must ensure that our system has the property of positive definiteness. This is ensured by the choice of one of the model variograms mentioned earlier.

A simple example:

Consider the following data

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

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 $c_0 = 0, c_1 = 10, \alpha = 3.33$.

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

We need to construct the matrix $\mathbf{\Gamma}$ and the vector γ . First we calculate the distance matrix as shown below:

$$\text{Distance matrix} = \begin{pmatrix} & s_0 & s_1 & s_2 & s_3 & s_4 & s_5 & s_6 & s_7 \\ s_0 & 0.00 & 4.47 & 3.61 & 8.06 & 9.49 & 6.71 & 8.94 & 13.45 \\ s_1 & 4.47 & 0.00 & 2.24 & 10.44 & 13.04 & 10.05 & 12.17 & 17.80 \\ s_2 & 3.61 & 2.24 & 0.00 & 11.05 & 13.00 & 8.00 & 10.05 & 16.97 \\ s_3 & 8.06 & 10.44 & 11.05 & 0.00 & 4.12 & 13.04 & 15.00 & 11.05 \\ s_4 & 9.49 & 13.04 & 13.00 & 4.12 & 0.00 & 12.37 & 13.93 & 7.00 \\ s_5 & 6.71 & 10.05 & 8.00 & 13.04 & 12.37 & 0.00 & 2.24 & 12.65 \\ s_6 & 8.94 & 12.17 & 10.05 & 15.00 & 13.93 & 2.24 & 0.00 & 13.15 \\ s_7 & 13.45 & 17.80 & 16.90 & 11.05 & 7.00 & 2.65 & 13.15 & 0.00 \end{pmatrix}$$

The ij_{th} entry in the matrix above was computed as follows:

$$d_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$$

Now, we can find the entries of the matrix $\mathbf{\Gamma}$ and the vector $\boldsymbol{\gamma}$. Each entry will be computed using the exponential semivariogram $\gamma(h) = 10(1 - e^{-\frac{h}{3.33}})$. Here they are:

$$\mathbf{\Gamma} = \begin{pmatrix} 0 & 4.893 & 9.564 & 9.800 & 9.510 & 9.740 & 9.952 & 1 \\ 4.893 & 0 & 9.637 & 9.798 & 9.093 & 9.510 & 9.938 & 1 \\ 9.564 & 9.637 & 0 & 7.095 & 9.800 & 9.889 & 9.637 & 1 \\ 9.800 & 9.798 & 7.095 & 0 & 9.755 & 9.847 & 8.775 & 1 \\ 9.510 & 9.093 & 9.800 & 9.755 & 0 & 4.893 & 9.775 & 1 \\ 9.740 & 9.510 & 9.889 & 9.847 & 4.893 & 0 & 9.806 & 1 \\ 9.952 & 9.938 & 9.637 & 8.775 & 9.775 & 9.806 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

$$\boldsymbol{\gamma} = \begin{pmatrix} 7.384 \\ 6.614 \\ 9.109 \\ 9.420 \\ 8.664 \\ 9.316 \\ 9.823 \\ 1 \end{pmatrix}$$

The weights and the Lagrange multiplier can be obtained as follows:

$$\mathbf{W} = \mathbf{\Gamma}^{-1}\boldsymbol{\gamma} = \begin{pmatrix} 0 & 4.893 & 9.564 & 9.800 & 9.510 & 9.740 & 9.952 & 1 \\ 4.893 & 0 & 9.637 & 9.798 & 9.093 & 9.510 & 9.938 & 1 \\ 9.564 & 9.637 & 0 & 7.095 & 9.800 & 9.889 & 9.637 & 1 \\ 9.800 & 9.798 & 7.095 & 0 & 9.755 & 9.847 & 8.775 & 1 \\ 9.510 & 9.093 & 9.800 & 9.755 & 0 & 4.893 & 9.775 & 1 \\ 9.740 & 9.510 & 9.889 & 9.847 & 4.893 & 0 & 9.806 & 1 \\ 9.952 & 9.938 & 9.637 & 8.775 & 9.775 & 9.806 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}^{-1} \begin{pmatrix} 7.384 \\ 6.614 \\ 9.109 \\ 9.420 \\ 8.664 \\ 9.316 \\ 9.823 \\ 1 \end{pmatrix}.$$

The answer is:

$$\mathbf{W} = \begin{pmatrix} 0.174 \\ 0.317 \\ 0.129 \\ 0.086 \\ 0.151 \\ 0.057 \\ 0.086 \\ 0.906 \end{pmatrix}.$$

The last element of the $\mathbf{W}$ vector is the Lagrange multiplier, $\lambda = 0.906$. We can verify that the sum of the elements 1 through 7 is equal to 1, as it should be.

The predicted value at location s_0 is equal to:

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

And the variance:

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

Under the assumption that $Z(s)$ is Gaussian a 95% confidence interval can be computed as follows:

$$592.59 \pm 1.96\sqrt{8.96}$$

Or

$$577.09 \leq Z(s_0) \leq 588.83$$

Ordinary kriging using `geoR` and `gstat`

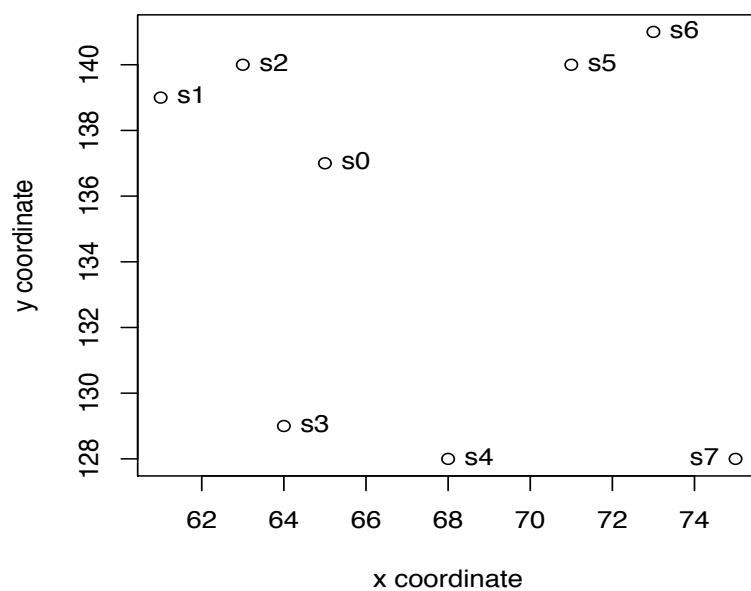
We discuss next kriging using the R packages `geoR` and `gstat`. We will use the numerical example from last lecture. Here it is:

A simple example:

Consider the following data

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

Our goal is to predict 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

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

The predicted value at location s_0 is equal to:

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

And the variance:

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

Kriging using geor:

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

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

~frederic/416/F19/

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

```
> 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:

```
> 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 predicted using kriging:

```
> 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 <- kslsline(b, cov.model="exp", cov.pars=c(10,3.33), nugget=0,
  locations=grd)
```

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

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

q <- krige.conv(b, locations=grd, krige=krige.control(obj.model=fit1))
```

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:

```
> 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
```

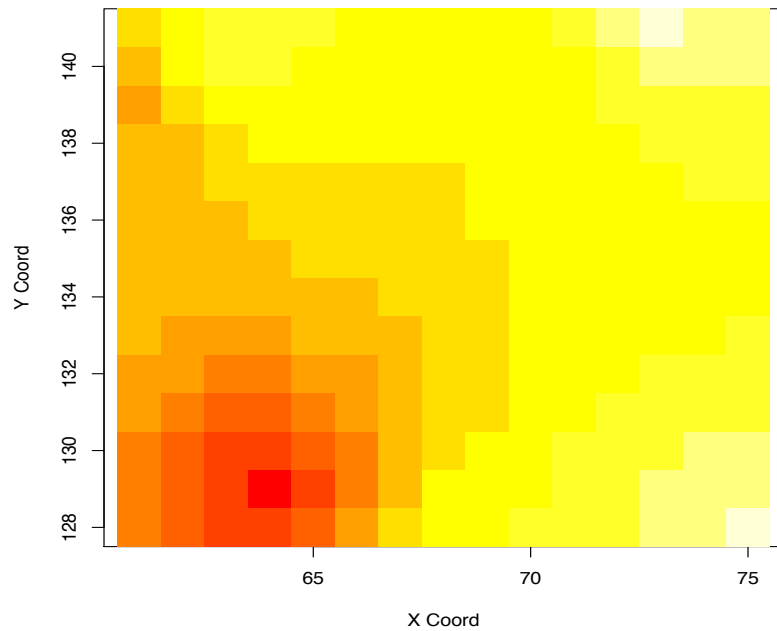
To construct the raster map we type:

```
image(q, val=q$predict)
```

Or simply:

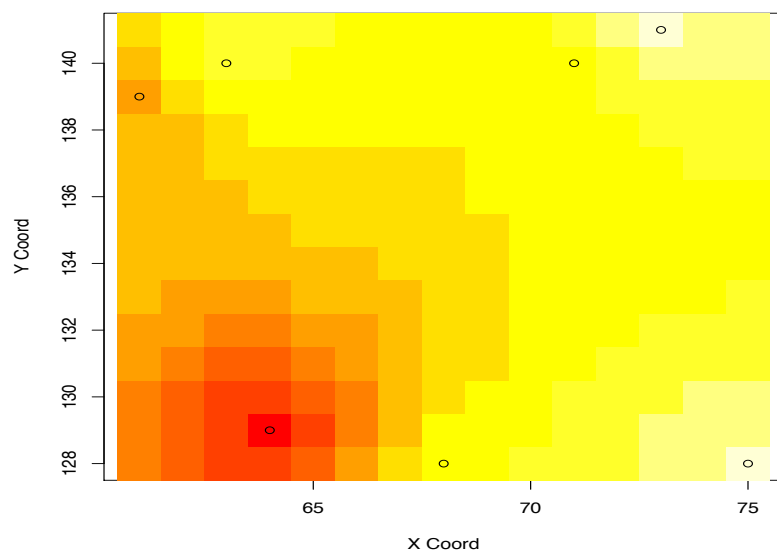
```
image(q)
```

Here is the plot:



And here is the plot with the data points:

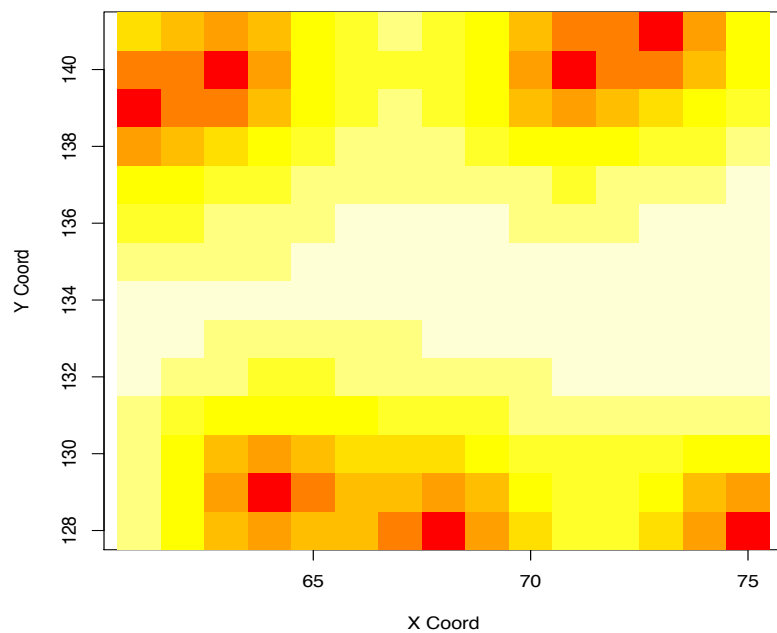
```
points(a)
```



We can construct a raster map of the variances:

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

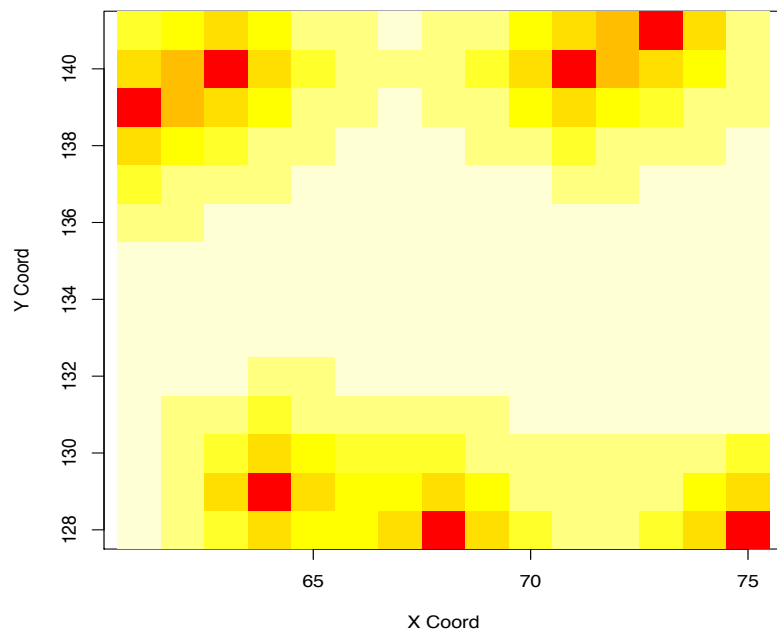
Here is the plot:



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

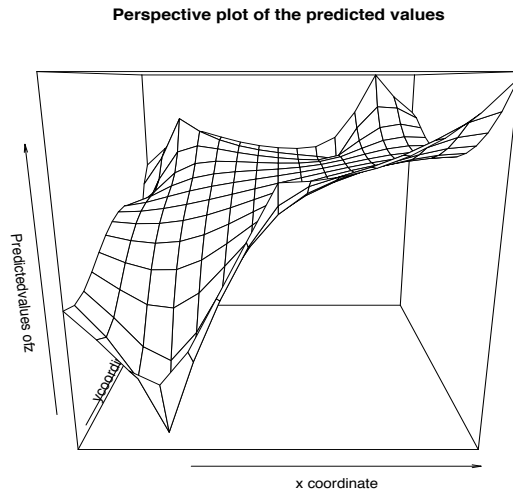
```
> image(q, val=sqrt(q$krige.var))
```

Here is the plot:



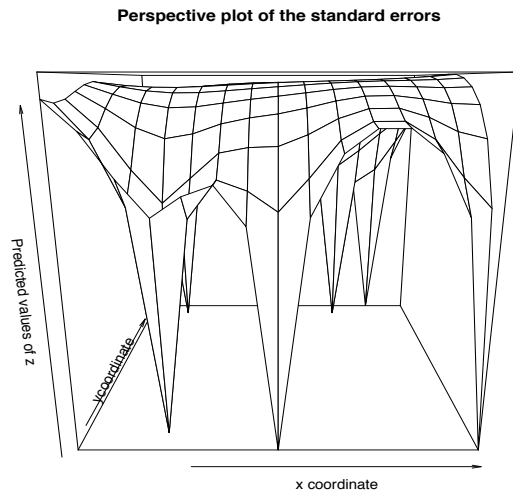
The following command will construct a perspective plot of the predicted values:

```
> 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:

```
> 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")
```



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:

```
> a <- read.table("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:

```
> 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:

```
> 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:

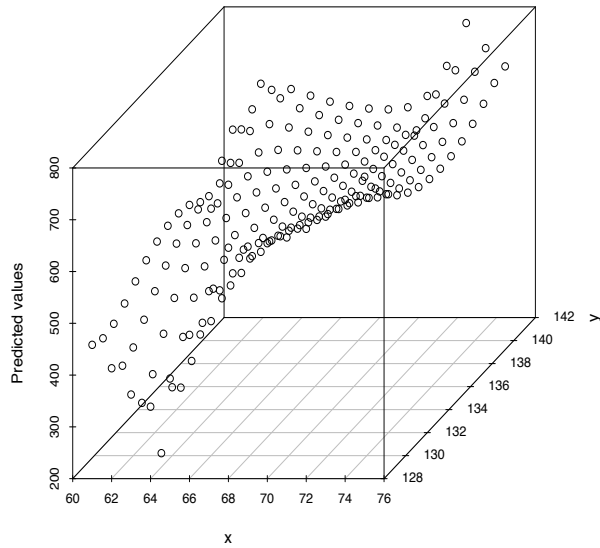
```
> coordinates(a) <- ~x+y
> coordinates(grd) <- ~x+y
> q2 <- krige(id="z", formula=z~1, a, newdata=grd, model = m)
```

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:

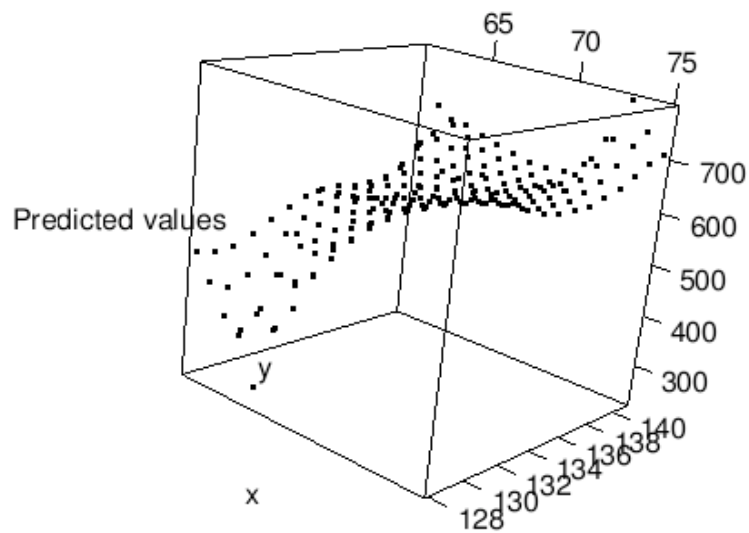
```
> library(scatterplot3d)
> library(rgl)
> scatterplot3d(q1$x, q1$y, q1$z.pred, xlab="x", ylab="y",
  zlab="Predicted values")
> plot3d(q1$x, q1$y, q1$z.pred, size=3)
```

Here are the plots:

(a). Using the `scatterplot3d` command.



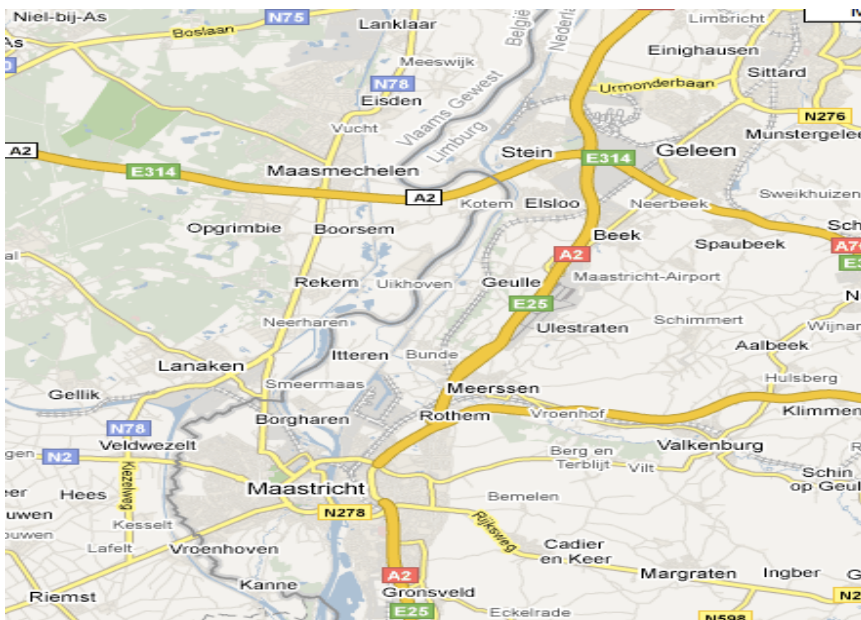
(b). Using the `plot3d` command.



A complete example on kriging using gstat:

We will use again the soil data from the *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

~frederic/222/S19/

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

To load the gstat package type

```
> library(gstat)
```

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

```
> 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):

```
> 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;

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

#Plot the variogram:

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

#Fit a model variogram to the sample variogram:

```
> 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.

```
> 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:

fit.method	weights
1	N_h
2	$N_h/\gamma(h;\theta)^2$ (Cressie's weights)
6	OLS (no weights)
7	N_h/h^2 (default)

```
#Use kriging to estimate the value of log(lead) at the grid values.
#First we create the grid.
> 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:
> pr_ok <- krige(id="log_lead",log(lead)~1, locations=~x+y,
model=v.fit,
data=a, newdata=grd)
```

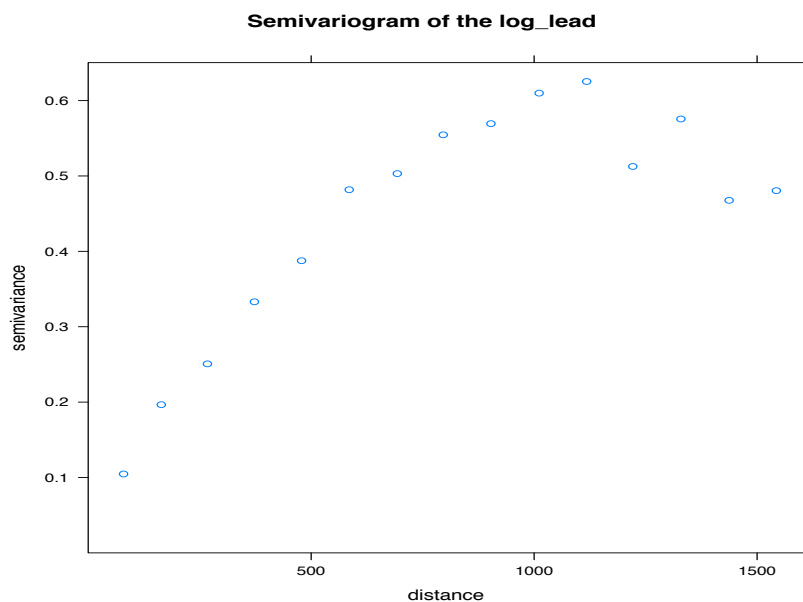
```
#To find what the object pr_ok contains type:
> names(pr_ok)
[1] "x" "y" "log_lead.pred" "log_lead.var"
```

```
#To see the predicted values you type:
> pr_ok$log_lead.pred
```

```
#And the kriging variances:
> pr_ok$log_lead.var
```

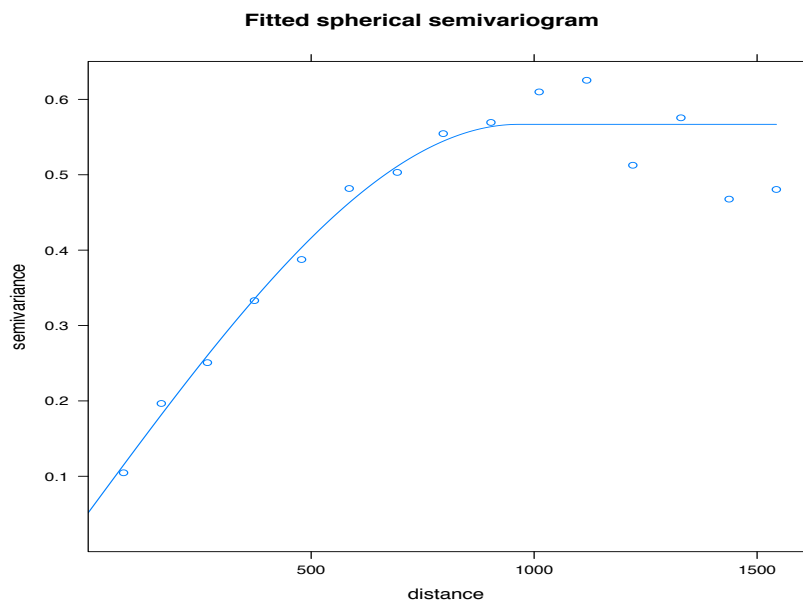
The plot of the sample variogram:

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



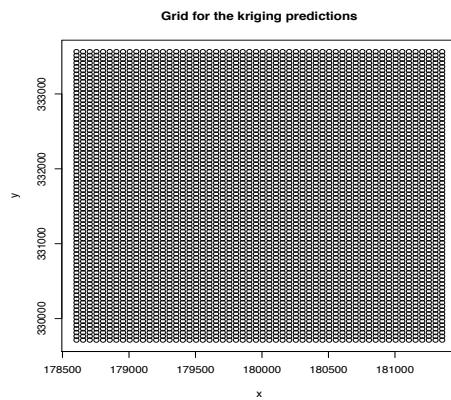
The fitted spherical variogram to the sample variogram:

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



Here is the grid for the kriging predictions:

```
> plot(grd)
```



The vector of the predicted values must be collapsed into a matrix with the `matrix` function:

```
#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)))
```

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

```
> image(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")

> points(a) #The data points can be plotted on the raster map.
```

