# 5

# First steps (meuse)

## 5.1 Introduction

This exercise introduces geostatistical tools that can be used to analyze various types of environmental data. It is not intended as a complete analysis of the example data set. Indeed some of the steps here can be questioned, expanded, compared, and improved. The emphasis is on seeing what R and some of its add-in packages can do in combination with an open source GIS such as SAGA GIS. The last section demonstrates how to export produced maps to Google Earth. This whole chapter is, in a way, a prerequisite to other exercises in the book.

We will use the meuse data set, which is a classical geostatistical data set used frequently by the creator of the gstat package to demonstrate various geostatistical analysis steps (Bivand et al., 2008, §8). The data set is documented in detail by Rikken and Van Rijn (1993), and Burrough and McDonnell (1998). It consists of 155 samples of top soil heavy metal concentrations (ppm), along with a number of soil and landscape variables. The samples were collected in a flood plain of the river Meuse, near the village Stein (Lat. 50° 58' 16", Long. 5° 44' 39"). Historic metal mining has caused the widespread dispersal of lead, zinc, copper and cadmium in the alluvial soil. The pollutants may constrain the land use in these areas, so detailed maps are required that identify zones with high concentrations. Our specific objective will be to generate a map of a heavy metal (zinc) in soil, and a map of soil liming requirement (binary variable) using point observations, and a range of auxiliary maps.

Upon completion of this exercise, you will be able to plot and fit variograms, examine correlation between various variables, run spatial predictions using the combination of continuous and categorical predictors and visualize results in external GIS packages/browsers (SAGA GIS, Google Earth). If you are new to R syntax, you should consider first studying some of the introductory books (listed in the section 3.4.2).

## 5.2 Data import and exploration

Download the attached meuse.R script from the book's homepage and open it in Tinn-R. First, open a new R session and change the working directory to where all your data sets will be located (C:/meuse/). This directory will be empty at the beginning, but you will soon be able to see data sets that you will load, generate and/or export. Now you can run the script line by line. Feel free to experiment with the code and extend it as needed. Make notes if you experience any problems or if you are not able to perform some operation.

Before you start processing the data, you will need to load the following packages:

```
> library(maptools)
> library(gstat)
> library(rgdal)
> library(lattice)
> library(RSAGA)
> library(geoR)
> library(spatstat)
```

You can get a list of methods in each package with the `help` method, e.g.:

```
> help(package="maptools")
```

The `meuse` data set is in fact available in the installation directory of the `gstat` package. You can load the field observations by typing:

```
> data(meuse)
> str(meuse)

  'data.frame':        155 obs. of  14 variables:
   $ x      : num  181072 181025 181165 181298 181307 ...
   $ y      : num  333611 333558 333537 333484 333330 ...
   $ cadmium: num  11.7 8.6 6.5 2.6 2.8 3 3.2 2.8 2.4 1.6 ...
   $ copper : num  85 81 68 81 48 61 31 29 37 24 ...
   $ lead   : num  299 277 199 116 117 137 132 150 133 80 ...
   $ zinc   : num  1022 1141  640  257  269 ...
   $ elev   : num  7.91 6.98 7.80 7.66 7.48 ...
   $ dist   : num  0.00136 0.01222 0.10303 0.19009 0.27709 ...
   $ om     : num  13.6 14 13 8 8.7 7.8 9.2 9.5 10.6 6.3 ...
   $ ffreq  : Factor w/ 3 levels "1","2","3": 1 1 1 1 1 1 1 1 1 1 ...
   $ soil   : Factor w/ 3 levels "1","2","3": 1 1 1 2 2 2 2 1 1 2 ...
   $ lime   : Factor w/ 2 levels "0","1": 2 2 2 1 1 1 1 1 1 1 ...
   $ landuse: Factor w/ 15 levels "Aa","Ab","Ag",..: 4 4 4 11 4 11 4 2 2 15 ...
   $ dist.m : num  50 30 150 270 380 470 240 120 240 420 ...
```

which shows a table with 155 observations of 14 variables. To get a complete description of this data set, type:

```
> ?meuse

  Help for 'meuse' is shown in the browser
```

which will open your default web-browser and show the Html help page for this data set. Here you can also find what the abbreviated names for the variables mean. We will focus on mapping the following two variables: `zinc` — topsoil zinc concentration in ppm; and `lime` — the logical variable indicating whether the soil needs liming or not.

Now we can start to visually explore the data set. For example, we can visualize the target variable with a histogram:

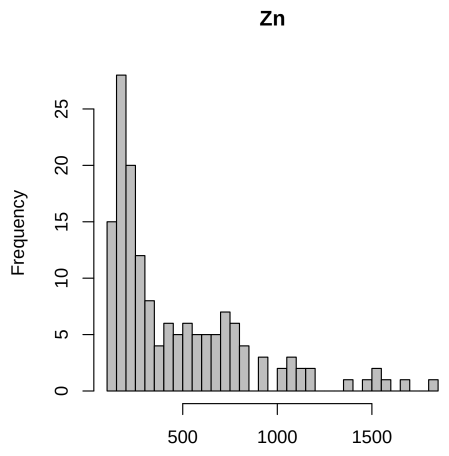


Fig. 5.1: Histogram plot for zinc (meuse data set).

```
> hist(meuse$zinc, breaks=25, col="grey")
```

which shows that the target variable is skewed towards lower values (Fig. 5.1), and it needs to be transformed before we can run any linear interpolation.

To be able to use spatial operations in R e.g. from the `gstat` package, we must convert the imported table into a `SpatialPointDataFrame`, a point map (with attributes), using the `coordinates` method:

```
# 'attach coordinates' - convert table to a point map:
> coordinates(meuse) <- ~ x+y
> str(meuse)

  Formal class 'SpatialPointsDataFrame' [package "sp"] with 5 slots
    ..@ data       :'data.frame':        155 obs. of  12 variables:
    .. ..$ cadmium: num [1:155] 11.7 8.6 6.5 2.6 2.8 3 3.2 2.8 2.4 1.6 ...
    .. ..$ copper : num [1:155] 85 81 68 81 48 61 31 29 37 24 ...
  .. ..$ lead   : num [1:155] 299 277 199 116 117 137 132 150 133 80 ...
  .. ..$ zinc   : num [1:155] 1022 1141  640  257  269 ...
  .. ..$ elev   : num [1:155] 7.91 6.98 7.80 7.66 7.48 ...
  .. ..$ dist   : num [1:155] 0.00136 0.01222 0.10303 0.19009 0.27709 ...
  .. ..$ om     : num [1:155] 13.6 14 13 8 8.7 7.8 9.2 9.5 10.6 6.3 ...
  .. ..$ ffreq  : Factor w/ 3 levels "1","2","3": 1 1 1 1 1 1 1 1 1 1 ...
  .. ..$ soil   : Factor w/ 3 levels "1","2","3": 1 1 1 2 2 2 2 1 1 2 ...
  .. ..$ lime   : Factor w/ 2 levels "0","1": 2 2 2 1 1 1 1 1 1 1 ...
  .. ..$ landuse: Factor w/ 15 levels "Aa","Ab","Ag",..: 4 4 4 11 4 11 4 2 2 15 ...
  .. ..$ dist.m : num [1:155] 50 30 150 270 380 470 240 120 240 420 ...
  ..@ coords.nrs : int [1:2] 1 2
  ..@ coords     : num [1:155, 1:2] 181072 181025 181165 181298 181307 ...
  .. ..- attr(*, "dimnames")=List of 2
  .. .. ..$ : NULL
  .. .. ..$ : chr [1:2] "x" "y"
  ..@ bbox       : num [1:2, 1:2] 178605 329714 181390 333611
  .. ..- attr(*, "dimnames")=List of 2
  .. .. ..$ : chr [1:2] "x" "y"
  .. .. ..$ : chr [1:2] "min" "max"
  ..@ proj4string:Formal class 'CRS' [package "sp"] with 1 slots
  .. .. ..@ projargs: chr NA
```

Note that the structure is now more complicated, with a nested structure and 5 '*slots*'[1] (Bivand et al., 2008, §2):

(1.) `@data` contains the actual data in a table format (a copy of the original dataframe minus the coordinates);

(2.) `@coords.nrs` has the coordinate dimensions;

(3.) `@coords` contains coordinates of each element (point);

(4.) `@bbox` stands for '*bounding box*' — this was automatically estimated by `sp`;

(5.) `@proj4string` contains the definition of projection system following the proj4[2] format.

The projection and coordinate system are at first unknown (listed as `NA` meaning 'not applicable'). Coordinates are just numbers as far as it is concerned. We know from the data set producers that this map is in the so-called *"Rijksdriehoek"* or RDH (Dutch triangulation), which is extensively documented[3]. This is a:

- stereographic projection (parameter `+proj`);
- on the Bessel ellipsoid (parameter `+ellps`);
- with a fixed origin (parameters `+lat_0` and `+lon_0`);
- scale factor at the tangency point (parameter `+k`);
- the coordinate system has a false origin (parameters `+x_0` and `+y_0`);
- the center of the ellipsoid is displaced with respect to the standard WGS84 ellipsoid (parameter `+towgs84`, with three distances, three angles, and one scale factor)[4];

It is possible to specify all this information with the `CRS` method; however, it can be done more simply if the datum is included in the European Petroleum Survey Group (EPSG) database[5], now maintained by the International Association of Oil & Gas producers (OGP). This database is included as text file (`epsg`) in the `rgdal` package, in the subdirectory `library/rgdal/proj` in the R installation folder. Referring to the EPSG registry[6], we find the following entry:

[1]This is the S4 objects vocabulary. *Slots* are components of more complex objects.
[2]`http://trac.osgeo.org/proj/`
[3]`http://www.rdnap.nl`
[4]The so-called seven datum transformation parameters (translation + rotation + scaling); also known as the *Bursa Wolf* method.
[5]`http://www.epsg-registry.org/`
[6]`http://spatialreference.org/ref/epsg/28992/`

```
# Amersfoort / RD New <28992> +proj=sterea +lat_0=52.15616055555555
+lon_0=5.38763888888889 +k=0.999908 +x_0=155000 +y_0=463000 +ellps=bessel
+towgs84=565.237,50.0087,465.658,-0.406857,0.350733,-1.87035,4.0812
+units=m +no_defs <>
```

This shows that the `Amersfoort / RD New` system is EPSG reference 28992. Note that some older installations of GDAL do not carry the seven-transformation parameters that define the geodetic datum! Hence, you will need to add these parameters manually to your `library/rgdal/proj/epsg` file. Once you have set the correct parameters in the system, you can add the projection information to this data set using the `CRS` method:

```
> proj4string(meuse) <- CRS("+init=epsg:28992")
> meuse@proj4string

 CRS arguments:
  +init=epsg:28992 +proj=sterea +lat_0=52.15616055555555
  +lon_0=5.38763888888889 +k=0.9999079 +x_0=155000 +y_0=463000 +ellps=bessel
  +towgs84=565.237,50.0087,465.658,-0.406857,0.350733,-1.87035,4.0812
  +units=m +no_defs
```

so now the correct projection information is included in the `proj4string` slot and we will be able to transform this spatial layer to geographic coordinates, and then export and visualize further in Google Earth.

Once we have converted the table to a point map we can proceed with spatial exploration data analysis, e.g. we can simply plot the target variable in relation to sampling locations. A common plotting scheme used to display the distribution of values is the `bubble` method. In addition, we can import also a map of the river, and then display it together with the values of zinc (Bivand et al., 2008):

```
# load river (lines):
> data(meuse.riv)
# convert to a polygon map:
> tmp <- list(Polygons(list(Polygon(meuse.riv)), "meuse.riv"))
> meuse.riv <- SpatialPolygons(tmp)
> class(meuse.riv)

 [1] "SpatialPolygons"
 attr(,"package")
 [1] "sp"


> proj4string(meuse.riv) <- CRS("+init=epsg:28992")
# plot together points and river:
> bubble(meuse, "zinc", scales=list(draw=T), col="black", pch=1, maxsize=1.5,
+   sp.layout=list("sp.polygons", meuse.riv, col="grey"))
```

which will produce the plot shown in Fig. 5.2, left[7]. Alternatively, you can also export the meuse data set to ESRI Shapefile format:

```
> writeOGR(meuse, ".", "meuse", "ESRI Shapefile")
```

which will generate four files in your working directory: `meuse.shp` (geometry), `meuse.shx` (auxiliary file), `meuse.dbf` (table with attributes), and `meuse.prj` (coordinate system). This shapefile you can now open in SAGA GIS and display using the same principle as with the `bubble` method (Fig. 5.2, right). Next, we import the gridded maps (40 m resolution). We will load them from the web repository[8]:

```
# download the gridded maps:
> setInternet2(use=TRUE)  # you need to login on the book's homepage first!
> download.file("http://spatial-analyst.net/book/system/files/meuse.zip",
+      destfile=paste(getwd(), "meuse.zip", sep="/"))
> grid.list <- c("ahn.asc", "dist.asc", "ffreq.asc", "soil.asc")
```

[7]See also **http://r-spatial.sourceforge.net/gallery/** for a gallery of plots using meuse data set.
[8]This has some extra layers compared to the existing meusegrid data set that comes with the sp package.

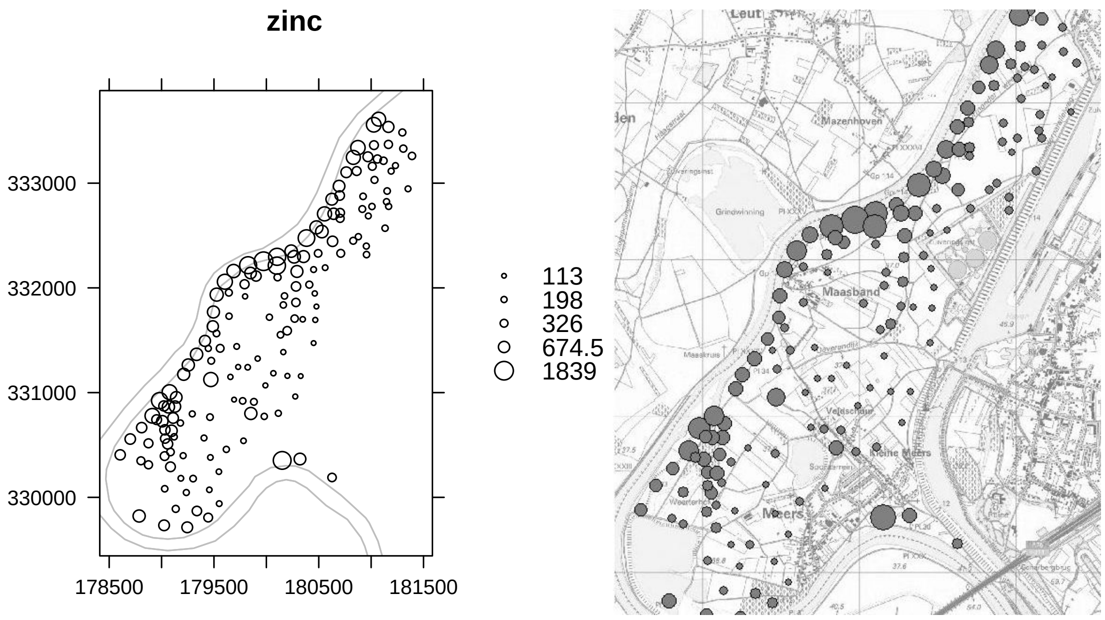


Fig. 5.2: Meuse data set and values of zinc (ppm): visualized in R (left), and in SAGA GIS (right).

```
# unzip the maps in a loop:
> for(j in grid.list){
>   fname <- zip.file.extract(file=j, zipname="meuse.zip")
>   file.copy(fname, paste("./", j, sep=""), overwrite=TRUE)
> }
```

These are the explanatory variables that we will use to improve spatial prediction of the two target variables:

(1.) `ahn` — digital elevation model (in cm) obtained from the LiDAR survey of the Netherlands[9];

(2.) `dist` — distance to river Meuse (in metres).

(3.) `ffreq` — flooding frequency classes: (1) high flooding frequency, (2) medium flooding frequency, (3) no flooding;

(4.) `soil` — map showing distribution of soil types, following the Dutch classification system: (1) Rd10A, (2) Rd90C-VIII, (3) Rd10C (de Fries et al., 2003);

In addition, we can also unzip the 2 m topomap that we can use as the background for displays (Fig. 5.2, right):

```
# the 2 m topomap:
> fname <- zip.file.extract(file="topomap2m.tif", zipname="meuse.zip")
> file.copy(fname, "./topomap2m.tif", overwrite=TRUE)
```

We can load the grids to R, also by using a loop operation:

```
> meuse.grid <- readGDAL(grid.list[1])

  ahn.asc has GDAL driver AAIGrid
  and has 104 rows and 78 columns
```

[9] `http://www.ahn.nl`

```
# fix the layer name:
> names(meuse.grid)[1] <- sub(".asc", "", grid.list[1])
> for(i in grid.list[-1]) {
>   meuse.grid@data[sub(".asc", "", i[1])] <- readGDAL(paste(i))$band1
> }
```

```
dist.asc has GDAL driver AAIGrid
and has 104 rows and 78 columns
ffreq.asc has GDAL driver AAIGrid
and has 104 rows and 78 columns
soil.asc has GDAL driver AAIGrid
and has 104 rows and 78 columns
```

```
# set the correct coordinate system:
> proj4string(meuse.grid) <- CRS("+init=epsg:28992")
```

1 Note that two of the four predictors imported (ffreq and soil) are categorical variables. However they
2 are coded in the ArcInfo ASCII file as integer numbers, which R does not recognize automatically. We need to
3 tell R that these are categories:

```
> meuse.grid$ffreq <- as.factor(meuse.grid$ffreq)
> table(meuse.grid$ffreq)
```

```
   1    2    3
 779 1335  989
```

```
> meuse.grid$soil <- as.factor(meuse.grid$soil)
> table(meuse.grid$soil)
```

```
   1    2    3
1665 1084  354
```

4 If you examine at the structure of the meuse.grid object, you will notice that it basically has a similar
5 structure to a SpatialPointsDataFrame, except this is an object with a grid topology:

```
Formal class 'SpatialGridDataFrame' [package "sp"] with 6 slots
  ..@ data       :'data.frame': 8112 obs. of  4 variables:
  .. ..$ ahn  : int [1:8112] NA NA NA NA NA NA NA NA NA NA ...
  .. ..$ dist : num [1:8112] NA NA NA NA NA NA NA NA NA NA ...
  .. ..$ ffreq: Factor w/ 3 levels "1","2","3": NA NA NA NA NA NA NA NA NA NA ...
  .. ..$ soil : Factor w/ 3 levels "1","2","3": NA NA NA NA NA NA NA NA NA NA ...
  ..@ grid       :Formal class 'GridTopology' [package "sp"] with 3 slots
  .. .. ..@ cellcentre.offset: Named num [1:2] 178460 329620
  .. .. .. ..- attr(*, "names")= chr [1:2] "x" "y"
  .. .. ..@ cellsize         : num [1:2] 40 40
  .. .. ..@ cells.dim        : int [1:2] 78 104
  ..@ grid.index : int(0)
  ..@ coords     : num [1:2, 1:2] 178460 181540 329620 333740
  .. ..- attr(*, "dimnames")=List of 2
  .. .. ..$ : NULL
  .. .. ..$ : chr [1:2] "x" "y"
  ..@ bbox       : num [1:2, 1:2] 178440 329600 181560 333760
  .. ..- attr(*, "dimnames")=List of 2
  .. .. ..$ : chr [1:2] "x" "y"
  .. .. ..$ : chr [1:2] "min" "max"
  ..@ proj4string:Formal class 'CRS' [package "sp"] with 1 slots
  .. .. ..@ projargs: chr " +init=epsg:28992 +proj=sterea +lat_0=52.15616055
  +lon_0=5.38763888888889 +k=0.999908 +x_0=155000 +y_0=463000 +ellps=bess"|
   __truncated__
```

6 Many of the grid nodes are unavailable (NA sign), so that it seems that the layers carry no information. To
7 check that everything is ok, we can plot the four gridded maps together (Fig. 5.3):

```
ffreq.plt <- spplot(meuse.grid["ffreq"],
+    col.regions=grey(runif(length(levels(meuse.grid$ffreq)))),
+    main="Flooding frequency classes")
dist.plt <- spplot(meuse.grid["dist"],
+    col.regions=grey(rev(seq(0,1,0.025))),
+    main="Distance to river")
soil.plt <- spplot(meuse.grid["soil"],
+    col.regions=grey(runif(length(levels(meuse.grid$ffreq)))),
+    main="Soil type classes")
ahn.plt <- spplot(meuse.grid["ahn"],
+    col.regions=grey(rev(seq(0,1,0.025))),
+    main="Elevation (cm)")
> print(ffreq.plt, split=c(1, 1, 4, 1), more=TRUE)
> print(dist.plt, split=c(2, 1, 4, 1), more=TRUE)
> print(ahn.plt, split=c(3, 1, 4, 1), more=TRUE)
> print(soil.plt, split=c(4, 1, 4, 1), more=TRUE)
```

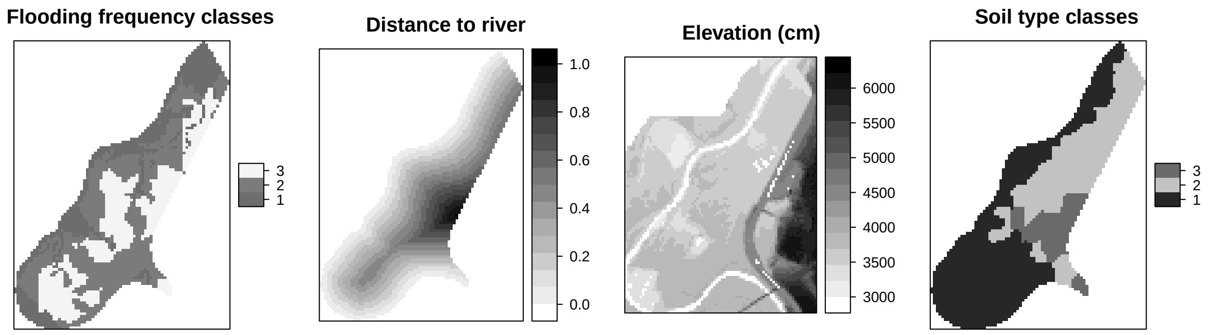


Fig. 5.3: Meuse auxiliary predictors.

### 5.2.1 Exploratory data analysis: sampling design

As noted in the preface, no geostatistician can promise high quality products without quality input point samples. To assess how representative and consistent the input data are, we can run some basic exploratory analysis to look at the point geometry and how well the environmental features are represented. We can start with point pattern analysis as implemented in the spatstat package, e.g. to determine the average spacing between the points (Baddeley, 2008):

```
# coerce to a ppp object:
> mg_owin <- as.owin(meuse.grid["dist"])
> meuse.ppp <- ppp(x=coordinates(meuse)[,1], y=coordinates(meuse)[,2],
+       marks=meuse$zinc, window=mg_owin)
# plot(meuse.ppp)
> summary(dist.points)

     Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
    43.93   77.88  107.40  111.70  137.70  353.00
```

which shows that the means shortest distance is 111 m. The following two questions are relevant for further analysis: (1) are the sampling locations distributed independently and uniformly over the area of interest (i.e. is there a significant clustering of locations)? (2) is the environmental feature space well represented? To answer the first question we can test the sampling design for *Complete Spatial Randomness* (CSR). CRS assumes that there are no regions in the study area where events are more likely to occur, and that the presence of a given event does not modify the probability of other events appearing nearby (Bivand et al., 2008).

The compatibility of a sampling design with CSR can be assessed by plotting the empirical function against the theoretical expectation (Bivand et al., 2008, p.160–163):

```
> env.meuse <- envelope(meuse.ppp, fun=Gest)

  Generating 99 simulations of CSR ...
  1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15,
  ... 91, 92, 93, 94, 95, 96, 97, 98, 99.


> plot(env.meuse, lwd=list(3,1,1,1), main="CSR test (meuse)")
```

which will run 100 simulations using the given point pattern and derive confidence bands for a CSR using the so called *G* function — this measures the distribution of the distances from an arbitrary event to its nearest event (Diggle, 2003). The plot of distributions, actual versus expected CSR (Fig. 5.4), shows that the sampling design is somewhat clustered at shorter distances up to 75 m. Although the line of the observed distribution is in >80% of distance range outside the confidence bands (*envelopes*), we can say that the sampling plan is, in general, representative relative to geographical space.

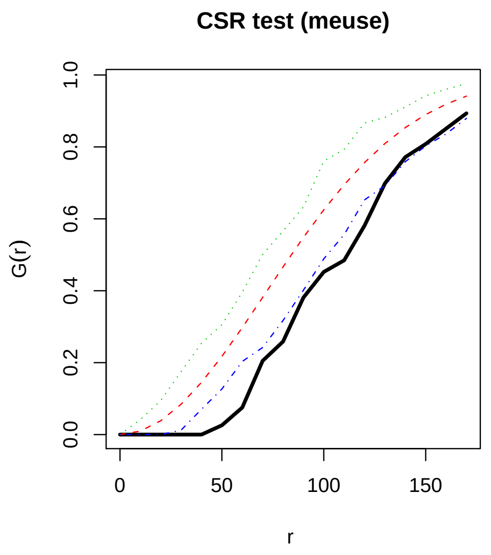


Fig. 5.4: Comparison of the confidence bands for the *G* function (Complete Spatial Randomness) and the actual observed distribution (bold line). Derived using the `envelope` method in spatstat.

Next we look at the feature space coverage. For example, we can check whether there is a significant difference in the distribution of values at sampling locations and in the whole area of interest. To run this type of analysis we need to overlay sampling points and predictors to create an object[10] with just the sample points, values of the target variable and of the feature-space predictors. We use the `overlay` method of the sp package to extract the values from the grid maps:

```
> meuse.ov <- overlay(meuse.grid, meuse)
> meuse.ov@data <- cbind(meuse.ov@data, meuse[c("zinc", "lime")]@data)
> str(meuse.ov@data)

  'data.frame':   155 obs. of  6 variables:
   $ ahn  : int  3214 3402 3277 3563 3406 3355 3428 3476 3522 3525 ...
   $ dist : num  0.00136 0.01222 0.10303 0.19009 0.27709 ...
   $ ffreq: Factor w/ 3 levels "1","2","3": 1 1 1 1 1 1 1 1 1 1 ...
   $ soil : Factor w/ 3 levels "1","2","3": 1 1 1 2 2 2 2 1 1 2 ...
   $ zinc : num  1022 1141 640 257 269 ...
   $ lime : Factor w/ 2 levels "0","1": 2 2 2 1 1 1 1 1 1 1 ...
```

Now we can run some explanatory analyzes that focus on the feature space. First, we can visually compare the histograms of the maps with the histograms of values at point locations, e.g. by using a back to back histogram[11]:

```
> library(Hmisc)
> options(digits=1)
> dist.histbb <- histbackback(meuse.ov$dist, meuse.grid$dist, prob=TRUE,
+      xlab=c("sample","map"), main="Distance (m)")
> barplot(-dist.histbb$left, col="dark grey" , horiz=TRUE, space=0, add=TRUE,
+      axes=FALSE)
> barplot(dist.histbb$right, col="grey", horiz=TRUE, space=0, add=TRUE, axes=FALSE)
> ahn.histbb <- histbackback(meuse.ov$ahn, meuse.grid$ahn, prob=TRUE,
+      xlab=c("sample","map"), main="AHN (cm)")
```

[10] Often refer to as the "*regression matrix*".
[11] This requires installation of the package Hmisc.

```
> barplot(-ahn.histbb$left, col="dark grey" , horiz=TRUE, space=0, add=TRUE,
+      axes=FALSE)
> barplot(ahn.histbb$right, col="grey", horiz=TRUE, space=0, add=TRUE, axes=FALSE)
> par(mfrow=c(1,2))
> print(dist.histbb, add=TRUE)
> print(ahn.histbb, add=FALSE)
> dev.off()
> options(digits=3)
```

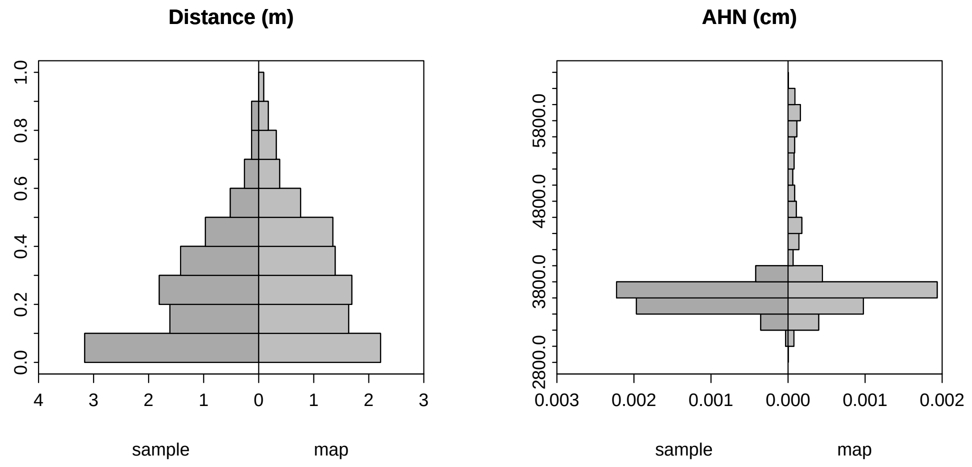


Fig. 5.5: Histogram for sampled values of `dist` and `ahn` (155 locations) versus the histogram of the raster map (all raster nodes). Produced using the `histbackback` method.

This will produce two histograms next to each other so that we can visually compare how well the samples 1
represent the original feature space of the raster maps (Fig. 5.5). In the case of the `points` data set, we can 2
see that the samples are misrepresenting higher elevations, but distances from the river are well represented. 3
We can actually test if the histograms of sampled variables are significantly different from the histograms of 4
original raster maps e.g. by using a non-parametric test such as the Kolmogorov-Smirnov test: 5

```
> ks.test(dist.histbb$left, dist.histbb$right)

        Two-sample Kolmogorov-Smirnov test

 data:  dist.histbb$left and dist.histbb$right
 D = 0.2, p-value = 0.9945
 alternative hypothesis: two-sided

> ks.test(ahn.histbb$left, ahn.histbb$right)

        Two-sample Kolmogorov-Smirnov test

 data:  ahn.histbb$left and ahn.histbb$right
 D = 0.7, p-value = 0.0001673
 alternative hypothesis: two-sided

 Warning message:
 In ks.test(ahn.histbb$left, ahn.histbb$right) :
   cannot compute correct p-values with ties
```

which shows that the first two histograms (`dist`) do not differ much, but the second two (`ahn`) have signif- 6
icantly different distributions ($D$=0.7, $p$-value=0.0001673). Another test that you might do to compare the 7
histograms is to run the correlation test[12]: 8

[12]Also known as the test of no correlation because it computes t-value for correlation coefficient being equal to zero.

```
> cor.test(ahn.histbb$left, ahn.histbb$right)
```

In the step of geographic analysis of the sampling design we will assess whether the sampling density within different soil mapping units (`soil`) is consistent. First, we look at how many points fall into each zone:

```
> summary(meuse.ov$soil)

  1  2  3
 97 46 12
```

then we need to derive the observed inspection density using:

```
# observed:
> inspdens.obs <- summary(meuse.ov$soil)[1:length(levels(meuse.ov$soil))]/
+      (summary(meuse.grid$soil)[1:length(levels(meuse.grid$soil))]
+      *meuse.grid@grid@cellsize[[1]]^2)
# expected:
> inspdens.exp <- rep(length(meuse.ov$soil)/
+      (length(meuse.grid$soil[!is.na(meuse.grid$soil)])
+      *meuse.grid@grid@cellsize[[1]]^2), length(levels(meuse.ov$soil)))
# inspection density in no./ha:
> inspdens.obs*10000

     1     2     3
 0.364 0.265 0.212


> inspdens.exp*10000

 [1] 0.312 0.312 0.312
```

which can also be compared by using the Kolmogorov-Smirnov test:

```
> ks.test(inspdens.obs, inspdens.exp)


        Two-sample Kolmogorov-Smirnov test

 data:  inspdens.obs and inspdens.exp
 D = 0.667, p-value = 0.5176
 alternative hypothesis: two-sided

 Warning message:
 In ks.test(inspdens.obs, inspdens.exp) :
   cannot compute correct p-values with ties
```

In this case, we see that inspection density is also significantly inconsistent considering the map of `soil`, which is not by chance (*p*-value=0.5176). We could also run a similar analysis for land cover types or any other factor-type predictors.

So in summary, we can conclude for the `meuse` sampling design that:

- the average distance to the nearest neighbor is 111 m and the size of the area is 496 ha;
- the sampling intensity is 3 points per 10 ha, which corresponds to a grid cell size of about 15 m (Hengl, 2006);
- the sampling density varies in geographical space — sampling is significantly clustered for smaller distance (<75 m);
- the sampling is unrepresentative considering the maps of `ahn` and `soil` — higher elevations and soil class 3 are significantly under-sampled;

These results do not mean that this data set is unsuitable for generating maps, but they do indicate that it has some limitations considering representativeness, independency and consistency requirements.

## 5.3 Zinc concentrations

### 5.3.1 Regression modeling

The main objective of regression-kriging analysis is to build a regression model by using the explanatory gridded maps. We have previously estimated values of explanatory maps and target variables in the same table (overlay operation), so we can start by visually exploring the relation between the target variable and the *continuous* predictors e.g. by using a smoothed `scatterplot` (Fig. 5.6):

```
> par(mfrow = c(1, 2))
> scatter.smooth(meuse.ov$dist, meuse.ov$zinc, span=18/19,
+     col="grey", xlab="Distance to river (log)", ylab="Zinc (ppm)")
> scatter.smooth(meuse.ov$ahn, meuse.ov$zinc, span=18/19,
+     col="grey", xlab="Elevation (cm)", ylab="Zinc (ppm)")
```

which shows that the values of zinc decrease as the distance from (water) streams and elevation increases. This supports our knowledge about the area — the majority of heavy metals has been originated from fresh water deposition. The relation seems to be particulary clear, but it appears to be non-linear as the fitted lines are curved.

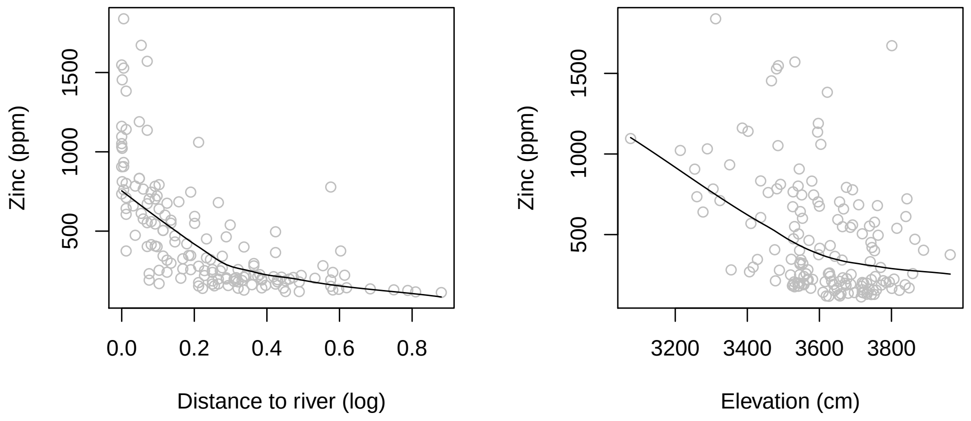


Fig. 5.6: Scatterplots showing the relation between zinc and distance from river, and elevation.

Another useful analysis relevant for the success of regression modeling is to look at the multicolinearity of predictors. Some predictors show the same feature, i.e. they are not independent. For example, `dist.asc` and `ahn.asc` maps are correlated:

```
> pairs(zinc ~ ahn+dist, meuse.ov)
> cor(meuse.grid$ahn, meuse.grid$dist, use="complete.obs")

  [1] 0.294
```

To visualize the relationship between the target variable and the *classified* predictors we used a grouped `boxplot`; this also allows us to count the samples in each class (Fig. 5.7):

```
> par(mfrow=c(1,2))
> boxplot(log1p(meuse.ov$zinc) ~ meuse.ov$soil,
+      col=grey(runif(length(levels(meuse.ov$soil)))),
+      xlab="Soil type classes", ylab="Zinc (ppm)")
> boxplot(log1p(meuse.ov$zinc) ~ meuse.ov$ffreq,
+      col=grey(runif(length(levels(meuse.ov$soil)))),
+      xlab="Flooding frequency classes", ylab="Zinc (ppm)")
> dev.off()
> boxplot(log1p(meuse.ov$zinc) ~ meuse.ov$soil, plot=FALSE)$n
```

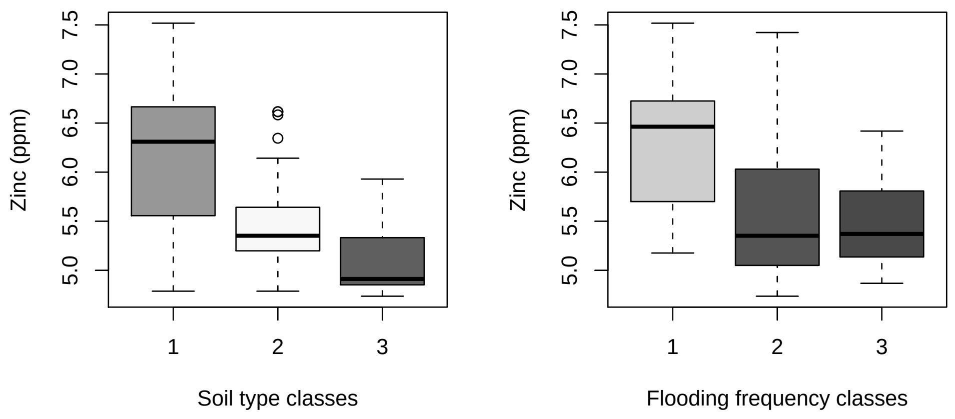


Fig. 5.7: Boxplots showing differences in zinc values (log-scale) between various soil and flooding frequency mapping units.

```
  [1] 97 46 12
```

```
> boxplot(log1p(meuse.ov$zinc) ~ meuse.ov$ffreq, plot=FALSE)$n
```

```
  [1] 73 53 29
```

which indicates that soil class "1" carries significantly higher zinc content than the remaining two classes. Note that there are only 12 field samples in the soil class "3", but still enough[13] to fit a regression model.

Now that we have some idea of the qualitative relation between the predictors and target variable, we proceed with fitting a regression model. We will first try to explain variation in the target variable by using all possible physical predictors — continuous and categorical. Because the target variable is heavily skewed towards lower values, we will use its transform to fit a linear model:

```
> lm.zinc <- lm(log1p(zinc) ~ ahn+dist+ffreq+soil, meuse.ov)
> summary(lm.zinc)
```

```
  Call:
  lm(formula = log1p(zinc) ~ ahn + dist + ffreq + soil, data = meuse.ov)

  Residuals:
      Min      1Q  Median      3Q     Max 
  -0.8421 -0.2794  0.0036  0.2469  1.3669 

  Coefficients:
               Estimate Std. Error t value Pr(>|t|)    
  (Intercept)  8.114955   1.121854    7.23  2.3e-11 ***
  ahn         -0.000402   0.000320   -1.26  0.21069    
  dist        -1.796855   0.257795   -6.97  9.7e-11 ***
  ffreq2      -0.434477   0.092897   -4.68  6.5e-06 ***
  ffreq3      -0.415166   0.121071   -3.43  0.00078 ***
  soil2       -0.368315   0.094768   -3.89  0.00015 ***
  soil3       -0.097237   0.163533   -0.59  0.55302    
  ---
  Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 

  Residual standard error: 0.43 on 148 degrees of freedom
  Multiple R-squared: 0.658,      Adjusted R-squared: 0.644 
  F-statistic: 47.4 on 6 and 148 DF,  p-value: <2e-16
```

[13]By a rule of thumb, we should have at least 5 observations per mapping unit to be able to fit a reliable model.

The `lm` method has automatically converted factor-variables into indicator (*dummy*) variables. The summary statistics show that our predictors are significant in explaining the variation in `log1p(zinc)`. However, not all of them are equally significant; some could probably be left out. We have previously demonstrated that some predictors are cross-correlated (e.g. `dist` and `ahn`). To account for these problems, we will do the following: first, we will generate indicator maps to represent all classes of interest:

```
> meuse.grid$soil1 <- ifelse(meuse.grid$soil=="1", 1, 0)
> meuse.grid$soil2 <- ifelse(meuse.grid$soil=="2", 1, 0)
> meuse.grid$soil3 <- ifelse(meuse.grid$soil=="3", 1, 0)
> meuse.grid$ffreq1 <- ifelse(meuse.grid$ffreq=="1", 1, 0)
> meuse.grid$ffreq2 <- ifelse(meuse.grid$ffreq=="2", 1, 0)
> meuse.grid$ffreq3 <- ifelse(meuse.grid$ffreq=="3", 1, 0)
```

so that we can convert all grids to principal components to reduce their multi-dimensionality[14]:

```
> pc.predmaps <- prcomp( ~ ahn+dist+soil1+soil2+soil3+ffreq1+ffreq2+ffreq3,
+     scale=TRUE, meuse.grid)
> biplot(pc.predmaps, xlabs=rep(".", length(pc.predmaps$x[,1])), arrow.len=0.1,
+     xlab="First component", ylab="Second component")
```

After the principal component analysis, we need to convert the derived PCs (10) to grids, since they have lost their spatial reference. This will take few steps:

```
> pc.comps <- as.data.frame(pc.predmaps$x)
# insert grid index:
> meuse.grid$nrs <- seq(1, length(meuse.grid@data[[1]]))
> meuse.grid.pnt <- as(meuse.grid["nrs"], "SpatialPointsDataFrame")
# mask NA grid nodes:
> maskpoints <- as.numeric(attr(pc.predmaps$x, "dimnames")[[1]])
# attach coordinates:
> pc.comps$X <- meuse.grid.pnt@coords[maskpoints, 1]
> pc.comps$Y <- meuse.grid.pnt@coords[maskpoints, 2]
> coordinates(pc.comps) <- ~ X + Y
# convert to a grid:
> gridded(pc.comps) <- TRUE
> pc.comps <- as(pc.comps, "SpatialGridDataFrame")
> proj4string(pc.comps) <- meuse.grid@proj4string
> names(pc.comps)

 [1] "PC1" "PC2" "PC3" "PC4" "PC5" "PC6" "PC7" "PC8"
```

overlay the points and PCs again, and re-fit a regression model:

```
> meuse.ov2 <- overlay(pc.comps, meuse)
> meuse.ov@data <- cbind(meuse.ov@data, meuse.ov2@data)
```

Because all predictors should now be independent, we can reduce their number by using step-wise regression:

```
> lm.zinc <- lm(log1p(zinc) ~ PC1+PC2+PC3+PC4+PC5+PC6+PC7+PC8, meuse.ov)
> step.zinc <- step(lm.zinc)
> summary(step.zinc)

 Call:
 lm(formula = log1p(zinc) ~ PC1 + PC2 + PC3 + PC4 + PC6, data=meuse.ov)

 Residuals:
       Min        1Q    Median        3Q       Max
 -0.833465 -0.282418  0.000112  0.261798  1.415499
```

[14]An important assumption of linear regression is that the predictors are mutually independent (Kutner et al., 2004).

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   5.6398     0.0384  146.94  < 2e-16 ***
PC1          -0.3535     0.0242  -14.59  < 2e-16 ***
PC2          -0.0645     0.0269   -2.40  0.01756 *
PC3          -0.0830     0.0312   -2.66  0.00869 **
PC4           0.0582     0.0387    1.50  0.13499
PC6          -0.2407     0.0617   -3.90  0.00014 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.426 on 149 degrees of freedom
Multiple R-squared: 0.661,        Adjusted R-squared: 0.65
F-statistic: 58.2 on 5 and 149 DF,  p-value: <2e-16
```

The resulting models shows that there are only two predictors that are highly significant, and four that are marginally significant, while four predictors can be removed from the list. You should also check the diagnostic plots for this regression model to see if the assumptions[15] of linear regression are met.

### 5.3.2 Variogram modeling

We proceed with modeling of the variogram, which will be later used to make predictions using universal kriging in gstat. Let us first compute the sample (experimental) variogram with the variogram method of the gstat package:

```
> zinc.svar <- variogram(log1p(zinc) ~ 1, meuse)
> plot(zinc.svar)
```

This shows that the semivariance reaches a definite sill at a distance of about 1000 m (Fig. 5.8, left). We can use the automatic fitting method[16] in gstat to fit a suitable variogram model. This method requires some initial parameters. We can set them using the following rule of thumb:

- Nugget is zero;
- Sill is the total (nonspatial) variance of the data set;
- Range is one-quarter of the diagonal of the bounding box.

In R, we can code this by using:

```
> zinc.vgm <- fit.variogram(zinc.svar, model=zinc.ivgm)
> zinc.vgm

   model psill range
 1   Nug 0.000     0
 2   Exp 0.714   449


> zinc.vgm.plt <- plot(zinc.svar, zinc.vgm, pch="+", pl=TRUE,
+     col="black", main="log1p(zinc)")
```

The idea behind using default values for initial variogram is that the process can be automated, without need to visually examine each variogram; although, for some variograms the automated fit may not converge to a reasonable solution (if at all). In this example, the fitting runs without a problem and you should get something like Fig. 5.8.

In order to fit the regression-kriging model, we actually need to fit the variogram for the residuals:

[15]Normally distributed, symmetric residuals around the regression line; no heteroscedascity, outliers or similar unwanted effects.
[16]The fit.variogram method uses weighted least-squares.

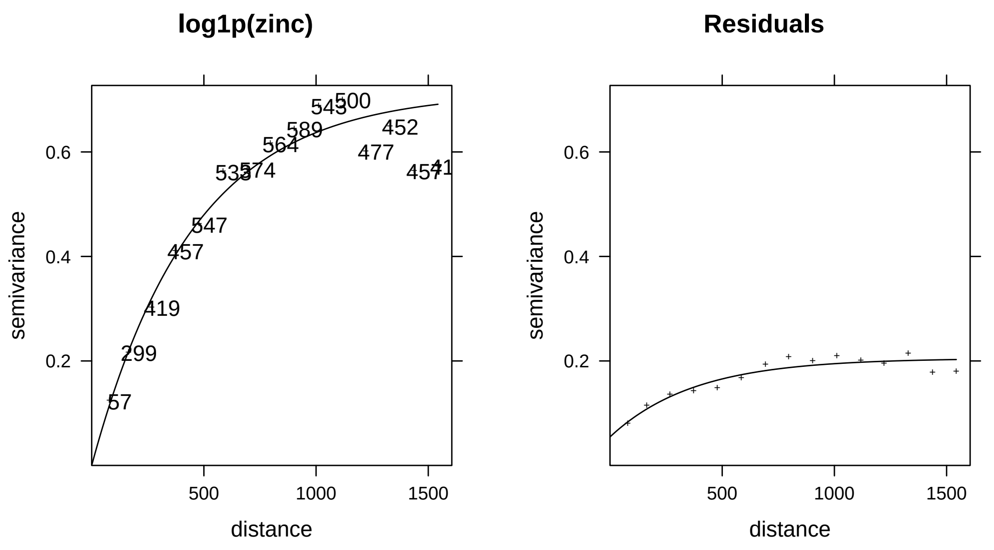


Fig. 5.8: Variogram for original variable, and regression residuals.

```
> zinc.rsvar <- variogram(residuals(step.zinc) ~ 1, meuse.ov)
> zinc.ivgm <- vgm(nugget=0, model="Exp",
+     range=sqrt(diff(meuse@bbox["x",])^2 + diff(meuse@bbox["y",])^2)/4,
+     psill=var(residuals(step.zinc)))
> zinc.rvgm <- fit.variogram(zinc.rsvar, model=zinc.ivgm)
> zinc.rvgm

   model  psill range
 1   Nug 0.0546     0
 2   Exp 0.1505   374
```

```
> zinc.rvgm.plt <- plot(zinc.rsvar, zinc.rvgm, pc="+", pl=FALSE,
+    col="black", main="Residuals")
# synchronize the two plots:
> zinc.rvgm.plt$x.limits <- zinc.vgm.plt$x.limits
> zinc.rvgm.plt$y.limits <- zinc.vgm.plt$y.limits
> print(zinc.vgm.plt, split=c(1,1,2,1), more=TRUE)
> print(zinc.rvgm.plt, split=c(2,1,2,1), more=FALSE)
```

which shows a somewhat different picture than in the case of the original variable (`zinc.vgm`): the sill parameter is now much smaller, as you can notice from the plot (Fig. 5.8, right). This is expected because that the regression model (§5.3.1) has already explained 65% of the variation in the target variable. 1 2 3

### 5.3.3 Spatial prediction of Zinc 4

Once we have fitted both the regression model (deterministic part of variation) and the variogram for residuals (stochastic, spatially-autocorrelated part of variation), we can proceed with regression-kriging. This method is implemented in the gstat's generic spatial prediction method called `krige`: 5 6 7

```
> zinc.rk <- krige(step.zinc$call$formula, meuse.ov, pc.comps, zinc.rvgm)

 [using universal kriging]
```

```
# back-transform the values:
> zinc.rk$var1.rk <- expm1(zinc.rk$var1.pred)
```

where `step.zinc$call$formula` is the regression model estimated in the previous section:

```
> step.zinc$call$formula

  log1p(zinc) ~ PC1 + PC2 + PC3 + PC4 + PC6
```

where `zinc.rvgm` is the fitted residual variogram, and `expm1` is back-transformation function. For a comparison, we can make predictions at all locations of interest also using ordinary kriging:

```
> zinc.ok <- krige(log1p(zinc) ~ 1, meuse, meuse.grid["soil"], zinc.vgm)

  [using ordinary kriging]


> zinc.ok$var1.rk <- expm1(zinc.ok$var1.pred)
```

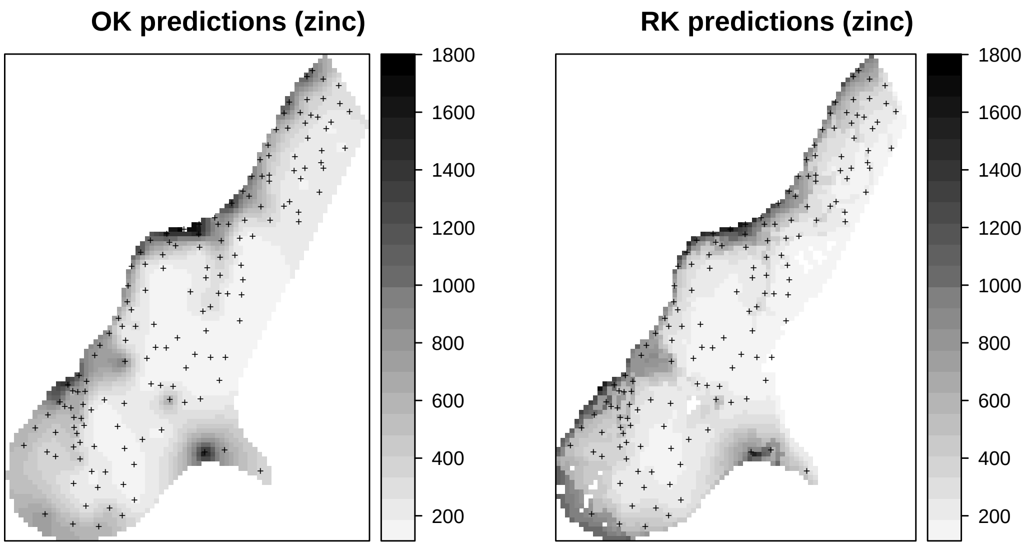


Fig. 5.9: Ordinary kriging vs regression-kriging: spatial prediction of zinc.

and compare the two maps side-by-side:

```
# display limits:
> at.zinc <- seq(min(meuse$zinc),max(meuse$zinc),sd(meuse$zinc)/5)
> zinc.ok.plt <- spplot(zinc.ok["var1.rk"],
+    col.regions=grey(rev(seq(0,0.97,1/length(at.zinc)))), at=at.zinc,
+    main="OK predictions (zinc)", sp.layout=list("sp.points",pch="+",
+    col="black", meuse))
> zinc.rk.plt <- spplot(zinc.rk["var1.rk"],
+    col.regions=grey(rev(seq(0,0.97,1/length(at.zinc)))), at=at.zinc,
+    main="RK predictions (zinc)", sp.layout=list("sp.points", pch="+",
+    col="black", meuse))
> print(zinc.ok.plt, split=c(1,1,2,1), more=T)
> print(zinc.rk.plt, split=c(2,1,2,1), more=F)
```

Visually, there are some clear differences between the two maps. The regression-kriging map shows much more local detail (the maps showing distance from river and soil and flooding frequency classes are reflected in the output map); the locations of hot-spots on both maps are, on the other hand, very similar. But visual comparison is not enough. Hence, we also would like to see which technique is more accurate. To achieve this, we use use the *leave-one-out cross validation method*, as implemented in the `krige.cv` method of `gstat` package (Pebesma, 2004). To run cross-validations, we simply use the built-in `krive.cv` method:

```
> cross.zinc.ok <- krige.cv(log1p(zinc) ~ 1, meuse.ov,
+     zinc.vgm, verbose=FALSE) # show no output
> cross.zinc.rk <- krige.cv(step.zinc$call$formula, meuse.ov,
+     zinc.rvgm, verbose=FALSE)
```

You will notice that the kriging system is solved once for each input data point. To evaluate the cross-validation, we can compare RMSE summaries (§1.4), and in particular the standard deviations of the errors (field `residual` of the cross-validation object). To estimate how much of variation has been explained by the two models, we can run:

```
# amount of variation explained by the models:
> 1-var(cross.zinc.ok$residual, na.rm=T)/var(log1p(meuse$zinc))

  [1] 0.701

> 1-var(cross.zinc.rk$residual, na.rm=T)/var(log1p(meuse$zinc))

  [1] 0.773
```

which shows that OK is not much worse than RK — RK is a *better* predictor, but the difference is only 7%. This is possibly because variables `dist` and `soil` are also spatially continuous, and because the samples are equally spread in geographic space. Indeed, if you look at Fig. 5.9 again, you will notice that the two maps do not differ much. Note also that amount of variation explained by RK geostatistical model is about 80%, which is satisfactory.

## 5.4 Liming requirements

### 5.4.1 Fitting a GLM

In the second part of this exercise, we will try to interpolate a categorical variable using the same regression-kriging model. This variable is not as simple as zinc, since it ranges from 0 to 1 i.e. it is a binomial variable. We need to respect that property of the data, and try to fit it using a GLM (Kutner et al., 2004):

$$\mathbb{E}(\mathbf{P_c}) = \mu = g^{-1}(\mathbf{q}\cdot\beta) \tag{5.4.1}$$

where E($\mathbf{P}$) is the expected probability of class $c$ ($P_c \in [0,1]$), $\mathbf{q}\cdot\beta$ is the linear regression model, and $g$ is the link function. Because the target variable is a binomial variable, we need to use the *logit* link function:

$$g(\mu) = \mu^{+} = \ln\left(\frac{\mu}{1-\mu}\right) \tag{5.4.2}$$

so the Eq.(5.4.1) becomes logistic regression (Kutner et al., 2004). How does this works in R? Instead of fitting a simple linear model (`lm`), we can use a more generic `glm` method with the `logit` link function (Fig. 5.10, left):

```
> glm.lime <- glm(lime ~ PC1+PC2+PC3+PC4+PC5+PC6+PC7+PC8, meuse.ov,
+      family=binomial(link="logit"))
> step.lime <- step(glm.lime)
# check if the predictions are within 0-1 range:
> summary(round(step.lime$fitted.values, 2))

     Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
    0.000   0.010   0.090   0.284   0.555   0.920
```

What you do not see from your R session is that the GLM model is fitted iteratively, i.e. using a more sophisticated approach than if we would simply fit a `lm` (e.g. using ordinary least square — no iterations). To learn more about the GLMs and how are they fitted and how to interpret the results see Kutner et al. (2004).

Next, we can predict the values[17] at all grid nodes using this model:

[17] Important: note that we focus on values in the transformed scale, i.e. logits.

```
> p.glm <- predict(glm.lime, newdata=pc.comps, type="link", se.fit=T)
> str(p.glm)

 List of 3
  $ fit           : Named num [1:3024] 2.85 2.30 2.25 1.83 2.77 ...
   ..- attr(*, "names")= chr [1:3024] "68" "144" "145" "146" ...
  $ se.fit        : Named num [1:3024] 1.071 0.813 0.834 0.729 1.028 ...
   ..- attr(*, "names")= chr [1:3024] "68" "144" "145" "146" ...
  $ residual.scale: num 1
```

which shows that the spatial structure of the object was lost. Obviously, we will not be able to display the results as a map until we convert it to a gridded data frame. This takes few steps:

```
# convert to a gridded layer:
> lime.glm <- as(pc.comps, "SpatialPointsDataFrame")
> lime.glm$lime <- p.glm$fit
> gridded(lime.glm) <- TRUE
> lime.glm <- as(lime.glm, "SpatialGridDataFrame")
> proj4string(lime.glm) <- meuse.grid@proj4string
```

### 5.4.2 Variogram fitting and final predictions

The remaining residuals we can interpolate using ordinary kriging. This is assuming that the residuals follow an approximately normal distribution. If the GLM we use is appropriate, this should indeed be the case. First, we estimate the variogram model:

```
> hist(residuals(step.lime), breaks=25, col="grey")
# residuals are normal;
> lime.ivgm <- vgm(nugget=0, model="Exp",
+    range=sqrt(diff(meuse@bbox["x",])^2 + diff(meuse@bbox["y", ])^2)/4,
+    psill=var(residuals(step.lime)))
> lime.rvgm <- fit.variogram(variogram(residuals(step.lime) ~ 1, meuse.ov),
+    model=lime.ivgm)
```

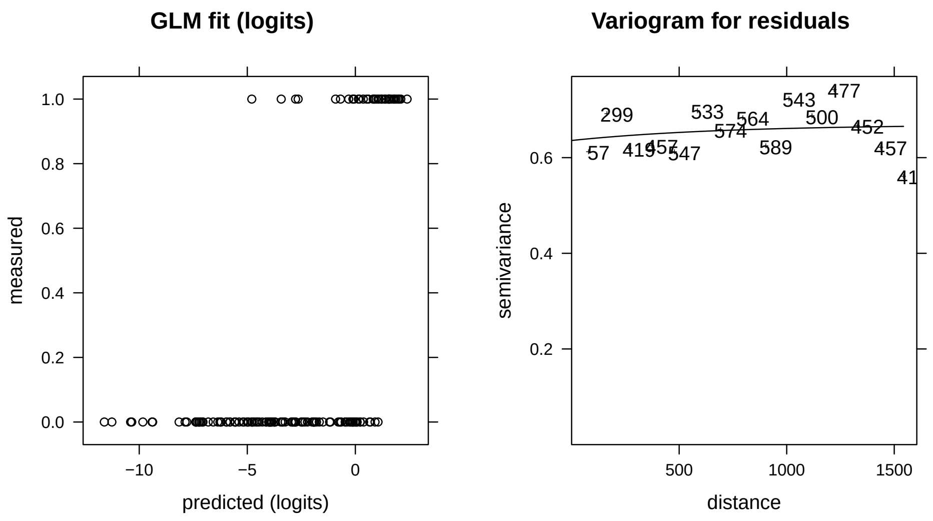
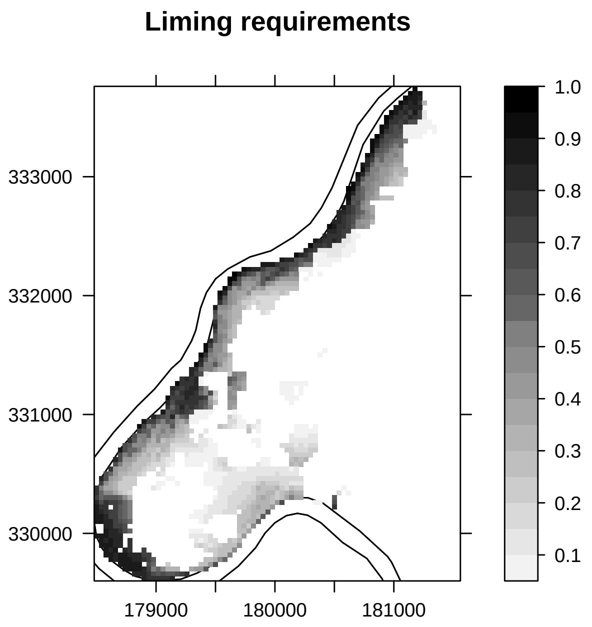


Fig. 5.10: Measured and predicted (GLM with binomial function) values for lime variable (left); variogram for the GLM residuals (right).



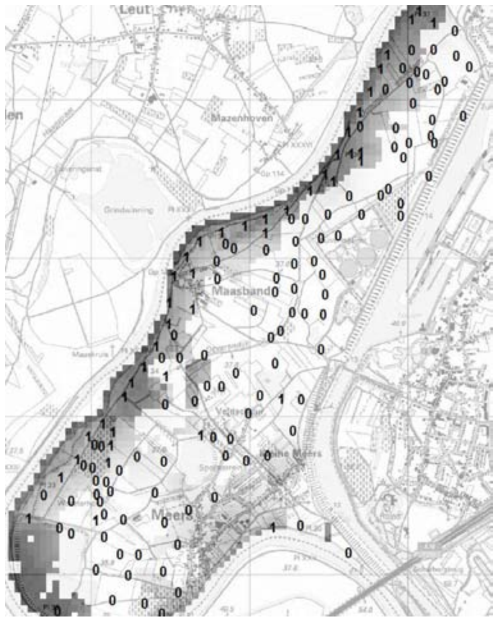


Fig. 5.11: Liming requirements predicted using regression-kriging; as shown in R (left) and in SAGA GIS (right).

which shows that the variogram is close to pure nugget effect (Fig. 5.10, right)[18]. We can still interpolate the residuals using ordinary kriging: 1 2

```
> lime.rk <- krige(residuals(step.lime) ~ 1, meuse.ov, pc.comps, lime.rvgm)

  [using ordinary kriging]
```

and then add back to the predicted regression part of the model: 3

```
> lime.rk$var1.rk <- lime.glm$lime + lime.rk$var1.pred
> lime.rk$var1.rko <- exp(lime.rk$var1.rk)/(1 + exp(lime.rk$var1.rk))
# write to a GIS format:
> write.asciigrid(lime.rk["var1.rko"], "lime_rk.asc", na.value=-1)
> lime.plt <- spplot(lime.rk["var1.rko"], scales=list(draw=T),
+     at=seq(0.05, 1, 0.05), col.regions=grey(rev(seq(0, 0.95, 0.05))),
+     main="Liming requirements", sp.layout=list("sp.polygons",
+     col="black", meuse.riv))
```

After you export the resulting map to SAGA GIS, a first step is to visually explore the maps to see how well the predicted values match the field observations (Fig. 5.11). Note that the map has problems predicting the right class at several isolated locations. To estimate the accuracy of predicting the right class, we can use: 4 5 6

```
> lime.ov <- overlay(lime.rk, meuse)
> lime.ov@data <- cbind(lime.ov@data, meuse["lime"]@data)
> library(mda)
> library(vcd) # kappa statistics
> Kappa(confusion(lime.ov$lime, as.factor(round(lime.ov$var1.rko, 0))))

             value    ASE
  Unweighted 0.678 0.0671
  Weighted   0.678 0.0840
```

which shows that in 68% of cases the predicted liming requirement class matches the field records. 7

[18]The higher the nugget, the more the algorithm will smooth the residuals. In the case of pure nugget effect, it does not make any difference if we use only results of regression, or if we add interpolated residuals to the regression predictions.

## 5.5 Advanced exercises

### 5.5.1 Geostatistical simulations

A problem with kriging is that it over-smooths reality; especially processes that exhibits a nugget effect in the variogram model. The kriging predictor is the "best linear unbiased predictor" (BLUP) at each point, but the resulting field is commonly smoother than in reality (recall Fig. 1.4). This causes problems when running distributed models, e.g. erosion and runoff, and also gives a distorted view of nature to the decision-maker.

A more realistic visualization of reality is achieved by the use of *conditional geostatistical simulations*: the sample points are taken as known, but the interpolated points reproduce the variogram model including the local noise introduced by the nugget effect. The same `krige` method in `gstat` can be used to generate simulations, by specifying the optional `nsim` ("*number of simulations*") argument. It's interesting to create several 'alternate realities', each of which is equally-probable. We can re-set R's random number generator with the `set.seed` method to ensure that the simulations will be generated with the same random number seed[19], and then generate four realizations:

```
> set.seed(25)
> zinc.rksim <- krige(step.zinc$call$formula, meuse.ov, pc.comps,
+     zinc.rvgm, nsim=4, nmax=100)
```

```
  drawing 4 GLS realisations of beta...
  [using conditional Gaussian simulation]
```

Now back-transform the predicted values, and plot all four simulations together:

```
# back-transform the values:
> for(i in 1:length(zinc.rksim@data)){
>   zinc.rksim@data[,i] <- expm1(zinc.rksim@data[,i])
> }
> spplot(zinc.rksim, col.regions=grey(c(rev(seq(0,0.97,1/length(at.zinc))),0)),
+       at=at.zinc, main="RK simulations of log(zinc)")
```

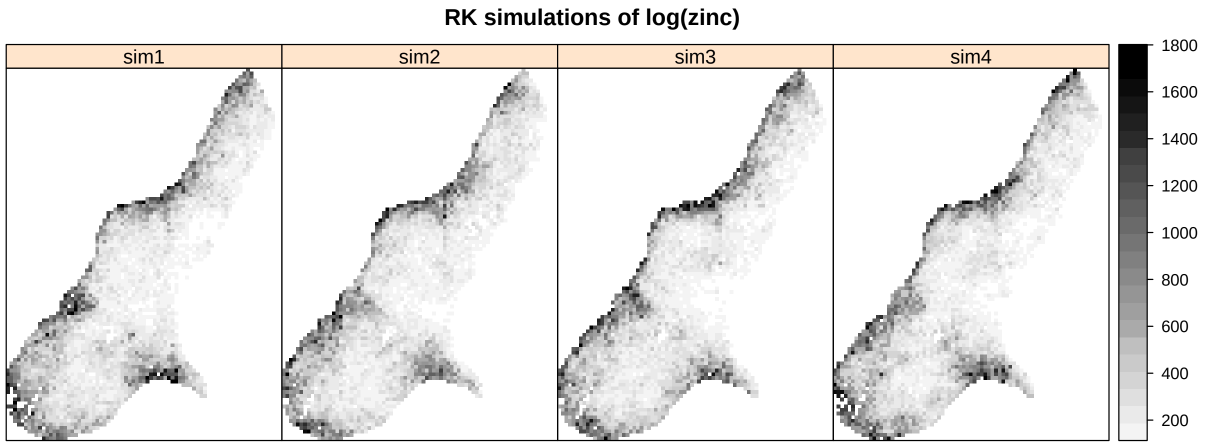


Fig. 5.12: Four simulations of zinc using the fitted regression kriging model. Back-transformed to original scale (ppm). Compare with Fig. 5.9.

which shows that the general pattern of the zinc distribution repeats in each simulation (Fig. 5.12). However, we can also notice that some small features are not as clear as they look in Fig. 5.9. For example, it is relatively hard to notice the borders of the soil units, which in this case change from simulation to simulation. This confirms that the best predictor of zinc is the distance to the river (`dist.asc` map).

To produce simulations of liming requirements, we can run (Bivand et al., 2008, p.230):

[19] Hence differences between the simulated realizations are due only to the different values of the model parameters.

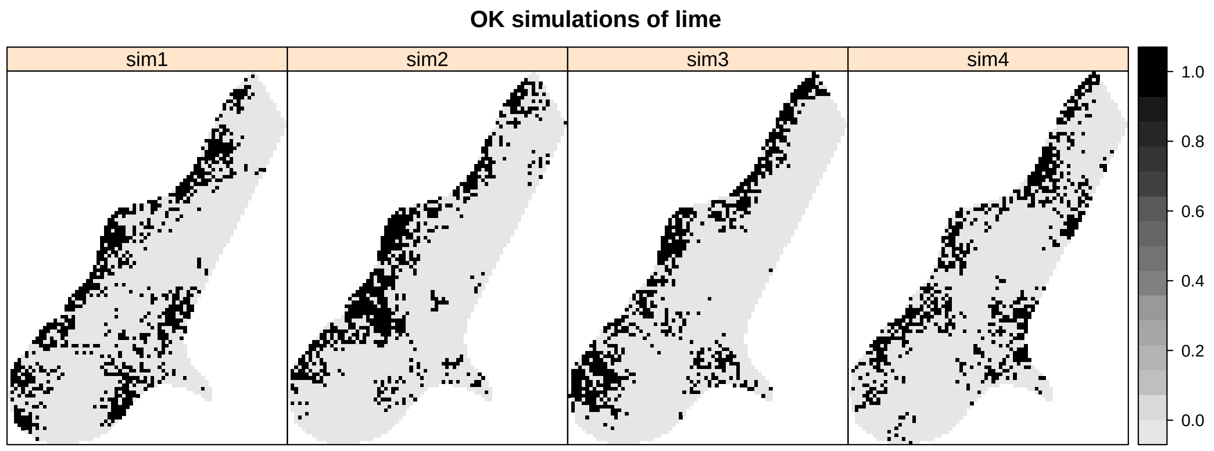


Fig. 5.13: Four simulations of liming requirements (indicator variable) using ordinary kriging. Compare with Fig. 5.11.

```
# fit a variogram:
> lime.ovgm <- fit.variogram(variogram(I(lime == 1) ~ 1, meuse), vgm(1, "Sph", 800, 1))
> lime.sim <- krige(I(lime == 1) ~ 1, meuse, meuse.grid, lime.ovgm,
+          nsim=4, indicators=TRUE, nmax=40)

  drawing 4 GLS realisations of beta...
  [using conditional indicator simulation]

> spplot(lime.sim, col.regions=grey(c(rev(seq(0,0.9,0.05)), 0))
+         main="OK simulations of lime")
```

the result is shown in Fig. 5.13. Note that in the case of liming requirements, there is a distinct difference between the variogram of the original variable and of the residuals: most of spatially-correlated variation in the lime requirements can be explained with auxiliary predictors, so that the variogram of residuals shows pure nugget effect (Fig. 5.10, right).

### 5.5.2 Spatial prediction using SAGA GIS

Although SAGA has relatively limited geostatistical functionality, it contains a number of modules that are of interest for geostatistical mapping: multiple linear regression (points and grids), ordinary kriging, and regression-kriging. To start, we can examine if the algorithms implemented in gstat and SAGA are the same. We can use the same model parameters estimated in section 5.3 to produce predictions of `log1p(zinc)`. First, we need to prepare vector and gridded maps in SAGA format:

```
# export the point data (transformed!):
> meuse.ov$log1p_zinc <- log1p(meuse.ov$zinc)
> writeOGR(meuse.ov["log1p_zinc"], ".", "zinc", "ESRI Shapefile")
# export the grids to SAGA format:
> PCs.list <- names(step.zinc$model)[-1]
> for(i in PCs.list){
>   write.asciigrid(pc.comps[i], paste(i, ".asc", sep=""), na.value=-9999)
> }
> rsaga.esri.to.sgrd(in.grids=set.file.extension(PCs.list, ".asc"),
+     out.sgrds=set.file.extension(PCs.list, ".sgrd"), in.path=getwd())
```

and then make the predictions by using the Universal kriging module in SAGA (Fig. 5.14):

```
# regression-kriging using the same parameters fitted previously:
> gridcell <- pc.comps@grid@cellsize[1]
> rsaga.geoprocessor(lib="geostatistics_kriging", module=8,
+     param=list(GRID="zinc_rk_SAGA.sgrd", SHAPES="zinc.shp",
+     GRIDS=paste(set.file.extension(PCs.list, ".sgrd"), collapse=";", sep=""),
+     BVARIANCE=F, BLOCK=F, FIELD=1, BLOG=F, MODEL=1, TARGET=0,
+     USER_CELL_SIZE=gridcell, NUGGET=zinc.rvgm$psill[1], SILL=zinc.rvgm$psill[2],
+     RANGE=zinc.rvgm$range[2], INTERPOL=0,
+     USER_X_EXTENT_MIN=pc.comps@bbox[1,1]+gridcell/2,
+     USER_X_EXTENT_MAX=pc.comps@bbox[1,2]-gridcell/2,
+     USER_Y_EXTENT_MIN=pc.comps@bbox[2,1]+gridcell/2,
+     USER_Y_EXTENT_MAX=pc.comps@bbox[2,2]-gridcell/2))


  SAGA CMD 2.0.4
  library path:   C:/Progra~1/saga_vc/modules
  library name:   geostatistics_kriging
  module name :   Universal Kriging (Global)
  author      :   (c) 2003 by O.Conrad

  Load shapes: zinc.shp...
  ready

  Load grid: PC1.sgrd...
  ready

  ...

  Load grid: PC6.sgrd...
  ready

  Parameters

  Grid: [not set]
  Variance: [not set]
  Points: zinc.shp
  Attribute: log1p_zinc
  Create Variance Grid: no
  Target Grid: user defined
  Variogram Model: Exponential Model
  Block Kriging: no
  Block Size: 100.000000
  Logarithmic Transformation: no
  Nugget: 0.054588
  Sill: 0.150518
  Range: 374.198454
  Linear Regression: 1.000000
  Exponential Regression: 0.100000
  Power Function - A: 1.000000
  Power Function - B: 0.500000
  Grids: 5 objects (PC1.sgrd, PC2.sgrd, PC3.sgrd, PC4.sgrd, PC6.sgrd))
  Grid Interpolation: Nearest Neighbor

  Save grid: zinc_rk_SAGA.sgrd...
```

1 Visually (Fig. 5.14), the results look as if there is no difference between the two pieces of software. We can
2 then load back the predictions into R to compare if the results obtained with gstat and SAGA match exactly:

```
> rsaga.sgrd.to.esri(in.sgrds="zinc_rk_SAGA",
+     out.grids="zinc_rk_SAGA.asc", out.path=getwd())
> zinc.rk$SAGA <- readGDAL("zinc_rk_SAGA.asc")$band1
> plot(zinc.rk$SAGA, zinc.rk$var1.pred, pch=19, xlab="SAGA", ylab="gstat")
> lines(3:8, 3:8, col="grey", lwd=4)
```

which shows that both software programs implement the same algorithm, but there are some small differences between the predicted values that are possibly due to rounding effect.

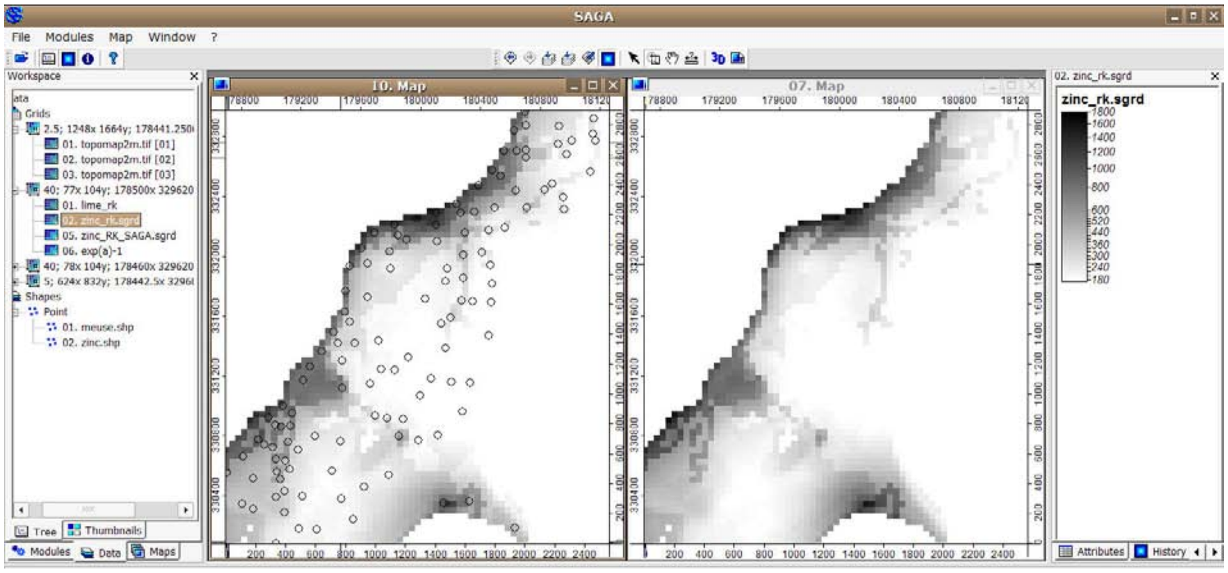


Fig. 5.14: Comparing results from SAGA (left map) and gstat (right map): regression-kriging using the same model parameters estimated in section 5.3.

Next, we want to compare the computational efficiency of gstat and SAGA, i.e. the processing time. To emphasize the difference in computation time, we will use a somewhat larger grid (2 m), and then re-run ordinary kriging in both software packages:

```
> meuse.grid2m <- readGDAL("topomap2m.tif")

  topomap2m.tif has GDAL driver GTiff
  and has 1664 rows and 1248 columns

> proj4string(meuse.grid2m) <- meuse.grid@proj4string
```

Processing speed can be measured from R by using the `system.time` method, which measures the elapsed seconds:

```
> system.time(krige(log1p(zinc) ~ 1, meuse, meuse.grid2m, zinc.vgm))

  [using ordinary kriging]
     user  system elapsed
   319.14    7.96  353.44
```

and now the same operation in SAGA:

```
> cellsize2 <- meuse.grid2m@grid@cellsize[1]
> system.time(rsaga.geoprocessor(lib="geostatistics_kriging", module=6,
+     param=list(GRID="zinc_ok_SAGA.sgrd", SHAPES="zinc.shp", BVARIANCE=F, BLOCK=F,
+     FIELD=1, BLOG=F, MODEL=1, TARGET=0, USER_CELL_SIZE=cellsize2,
+     NUGGET=zinc.vgm$psill[1], SILL=zinc.vgm$psill[2], RANGE=zinc.rvgm$range[2],
+     USER_X_EXTENT_MIN=meuse.grid2m@bbox[1,1]+cellsize2/2,
+     USER_X_EXTENT_MAX=meuse.grid2m@bbox[1,2]-cellsize2/2,
+     USER_Y_EXTENT_MIN=meuse.grid2m@bbox[2,1]+cellsize2/2,
+     USER_Y_EXTENT_MAX=meuse.grid2m@bbox[2,2]-cellsize2/2)))

     user  system elapsed
     0.03    0.71  125.69
```

We can see that SAGA will be faster for processing large data sets. This difference will become even larger if we would use large point data sets. Recall that the most '*expensive*' operation for any geostatistical mapping is the derivation of distances between points. Thus, by limiting the search radius one can always increase the processing speed. The problem is that a software needs to initially estimate which points fall within the search radius, hence it always has to take into account location of all points. Various *quadtree* and similar algorithms then exist to speed up the neighborhood search algorithm (partially available in gstat also), but their implementation can differ between various programming languages.

Note also that it is not really a smart idea to try to visualize large maps in R. R graphics plots grids as vectors; each grid cell is plotted as a separate polygon, which takes a huge amount of RAM for large grids, and can last up to few minutes. SAGA on other hand can handle and display grids ≫10 million pixels on a standard PC without any delays (Fig. 5.14). When you move to other exercises you will notice that we will typically use R to fit models, SAGA to run predictions and visualize results, and Google Earth to visualize and explore final products.

### 5.5.3 Geostatistical analysis in geoR

We start by testing the variogram fitting functionality of geoR. However, before we can do any analysis, we need to convert our point map (sp) to geoR geodata format:

```
> zinc.geo <- as.geodata(meuse.ov["zinc"])
> str(zinc.geo)
```

```
List of 2
 $ x , y    : num [1:155, 1:2] 181072 181025 181165 181298 181307 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:155] "300" "455" "459" "540" ...
  .. ..$ : chr [1:2] "x" "y"
 $ data       : num [1:155] 1022 1141 640 257 269 ...
 - attr(*, "class")= chr "geodata"
```

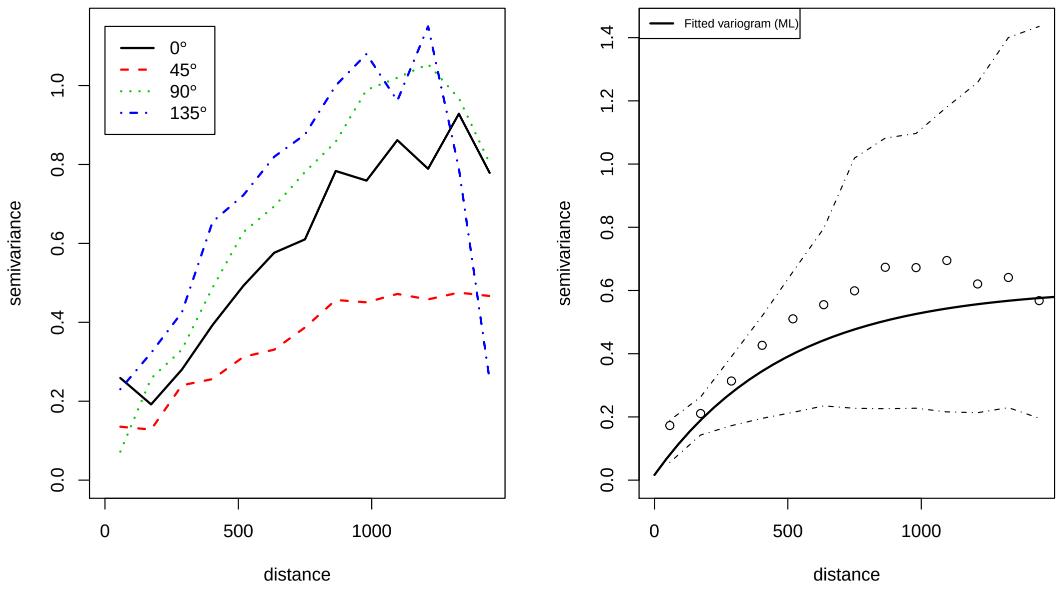


Fig. 5.15: Anisotropy (left) and variogram model fitted using the Maximum Likelihood (ML) method (right). The confidence bands (*envelopes*) show the variability of the sample variogram estimated using simulations from a given set of model parameters.

which shows much simpler structure than a `SpatialPointsDataFrame`. A `geodata`-type object contains only: a matrix with coordinates of sampling locations (`coords`), values of target variables (`data`), matrix with coordinates of the polygon defining the mask map (`borders`), vector or data frame with covariates (`covariate`). To produce the two standard variogram plots (Fig. 5.15), we will run:

```
> par(mfrow=c(1,2))
# anisotropy ("lambda=0" indicates log-transformation):
> plot(variog4(zinc.geo, lambda=0, max.dist=1500, messages=FALSE), lwd=2)
# fit variogram using likfit:
> zinc.svar2 <- variog(zinc.geo, lambda=0, max.dist=1500, messages=FALSE)
> zinc.vgm2 <- likfit(zinc.geo, lambda=0, messages=FALSE,
+       ini=c(var(log1p(zinc.geo$data)),500), cov.model="exponential")
> zinc.vgm2

  likfit: estimated model parameters:
        beta      tausq    sigmasq        phi
  "  6.1553" "  0.0164" "  0.5928" "500.0001"
  Practical Range with cor=0.05 for asymptotic range: 1498

  likfit: maximised log-likelihood = -1014


# generate confidence bands for the variogram:
> env.model <- variog.model.env(zinc.geo, obj.var=zinc.svar2, model=zinc.vgm2)

  variog.env: generating 99 simulations (with 155 points each) using grf
  variog.env: adding the mean or trend
  variog.env: computing the empirical variogram for the 99 simulations
  variog.env: computing the envelops


> plot(zinc.svar2, envelope=env.model); lines(zinc.vgm2, lwd=2);
> legend("topleft", legend=c("Fitted variogram (ML)"), lty=c(1), lwd=c(2), cex=0.7)
> dev.off()
```

where `variog4` is a method that generates semivariances in four directions, `lambda=0` is used to indicate the type of transformation[20], `likfit` is the generic variogram fitting method, `ini` is the given initial variogram, and `variog.model.env` calculates confidence limits for the fitted variogram model. Parameters `tausq` and `sigmasq` corresponds to nugget and sill parameters; `phi` is the range parameter.

In general, geoR offers much richer possibilities for variogram modeling than gstat. From Fig. 5.15(right) we can see that the variogram fitted using this method does not really go through all points (compare with Fig. 5.8). This is because the ML method discounts the potentially wayward influence of sample variogram at large inter-point distances (Diggle and Ribeiro Jr, 2007). Note also that the confidence bands (*envelopes*) also confirm that the variability of the empirical variogram increases with larger distances.

Now that we have fitted the variogram model, we can produce predictions using the ordinary kriging model. Because geoR does not work with sp objects, we need to prepare the prediction locations:

```
> locs <- pred_grid(c(pc.comps@bbox[1,1]+gridcell/2,
+     pc.comps@bbox[1,2]-gridcell/2), c(pc.comps@bbox[2,1]+gridcell/2,
+     pc.comps@bbox[2,2]-gridcell/2), by=gridcell)
# match the same grid as pc.comps;
```

and the mask map i.e. a polygon showing the borders of the area of interest:

```
> meuse.grid$mask <- ifelse(!is.na(meuse.grid$dist), 1, NA)
> write.asciigrid(meuse.grid["mask"], "mask.asc", na.value=-1)
# raster to polygon conversion;
> rsaga.esri.to.sgrd(in.grids="mask.asc", out.sgrd="mask.sgrd", in.path=getwd())
> rsaga.geoprocessor(lib="shapes_grid", module=6, param=list(GRID="mask.sgrd",
```

[20] geoR implements the Box–Cox transformation (Diggle and Ribeiro Jr, 2007, p.61), which is somewhat more generic than simple `log()` transformation.

```
+      SHAPES="mask.shp", CLASS_ALL=1))
> mask <- readShapePoly("mask.shp", proj4string=CRS("+init=epsg:28992"),
+      force_ring=T)
# coordinates of polygon defining the area of interest:
> mask.bor <- mask@polygons[[1]]@Polygons[[1]]@coords
> str(mask.bor)

 num [1:267, 1:2] 178880 178880 178760 178760 178720 ...
```

1 Ordinary kriging can be run by using the generic method for linear Gaussian models `krige.conv`[21]:

```
> zinc.ok2 <- krige.conv(zinc.geo, locations=locs,
+      krige=krige.control(obj.m=zinc.vgm2), borders=mask.bor)


krige.conv: results will be returned only for locations inside the borders
krige.conv: model with constant mean
krige.conv: performing the Box-Cox data transformation
krige.conv: back-transforming the predicted mean and variance
krige.conv: Kriging performed using global neighborhood


# Note: geoR will automatically back-transform the values!
> str(zinc.ok2)

List of 6
 $ predict     : num [1:3296] 789 773 756 740 727 ...
 $ krige.var   : num [1:3296] 219877 197718 176588 159553 148751 ...
 $ beta.est    : Named num 6.16
  ..- attr(*, "names")= chr "beta"
 $ distribution: chr "normal"
 $ message     : chr "krige.conv: Kriging performed using global neighbourhood"
 $ call        : language krige.conv(geodata = zinc.geo, locations = locs,
             borders = mask.bor,      krige = krige.control(obj.m = zinc.vgm2))
 - attr(*, "sp.dim")= chr "2d"
 - attr(*, "prediction.locations")= symbol locs
 - attr(*, "parent.env")=<environment: R_GlobalEnv>
 - attr(*, "data.locations")= language zinc.geo$coords
 - attr(*, "borders")= symbol mask.bor
 - attr(*, "class")= chr "kriging"
```

2 To produce plots shown in Fig. 5.16, we use:

```
> par(mfrow=c(1,2))
> image(zinc.ok2, loc=locs, col=gray(seq(1,0.1,l=30)), xlab="Coord X",
+     ylab="Coord Y")
> title(main="Ordinary kriging predictions")
> contour(zinc.ok2, add=TRUE, nlev=8)
> image(zinc.ok2, loc=locs, value=sqrt(zinc.ok2$krige.var),
+     col=gray(seq(1,0.1,l=30)), xlab="Coord X", ylab="Coord Y")
> title(main="Prediction error")
> krige.var.vals <- round(c(quantile(sqrt(zinc.ok2$krige.var),0.05),
+     sd(zinc.geo$data), quantile(sqrt(zinc.ok2$krige.var), 0.99)), 0)
> legend.krige(x.leg=c(178500,178800), y.leg=c(332500,333500),
+     values=sqrt(zinc.ok2$krige.var), vert=TRUE, col=gray(seq(1,0.1,l=30)),
+     scale.vals=krige.var.vals)
> points(zinc.geo[[1]], pch="+", cex=.7)
```

3 To run regression-kriging (in geoR "*external trend kriging*") we first need to add values of covariates to the
4 original `geodata` object:

[21] Meaning "*kriging conventional*" i.e. linear kriging.

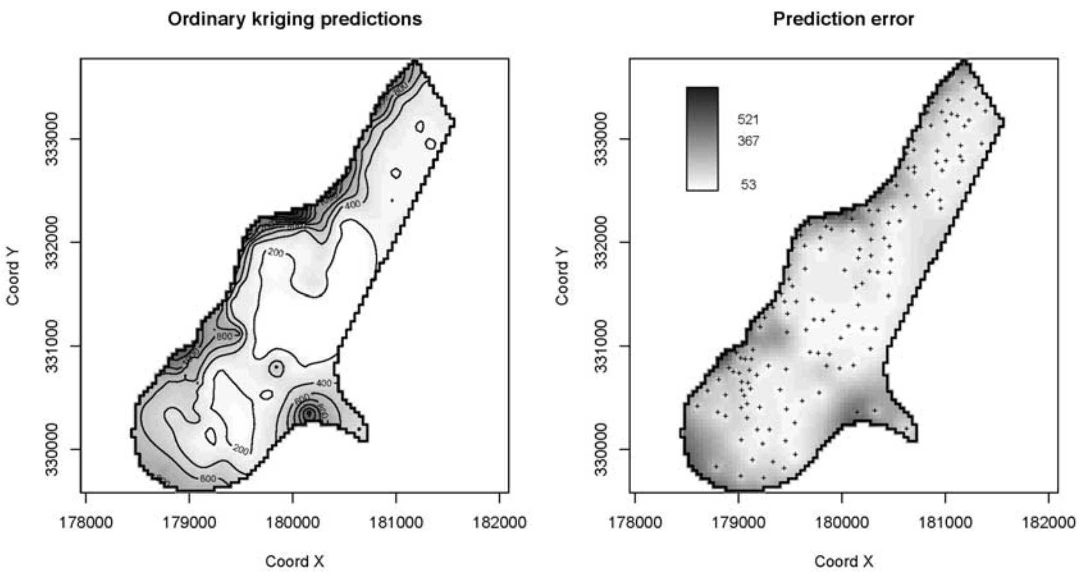


Fig. 5.16: Zinc predicted using ordinary kriging in geoR. The map on the left is considered to be below critical accuracy level in the areas where the prediction error (right map) exceeds the global variance (the middle value in legend). Compare with Fig. 5.9.

```
> zinc.geo$covariate <- meuse.ov@data[,PCs.list]
```

which now allows us to incorporate the `trend` argument in the variogram model: 1

```
# trend model:
> step.zinc$call$formula[c(1,3)]

  ~ PC1 + PC2 + PC3 + PC4 + PC6


> zinc.rvgm2 <- likfit(zinc.geo, lambda=0, trend=step.zinc$call$formula[c(1,3)],
+   messages=FALSE, ini=c(var(residuals(step.zinc)),500), cov.model="exponential")
> zinc.rvgm2

  likfit: estimated model parameters:
       beta0      beta1      beta2      beta3      beta4      beta5
  "  5.6919" " -0.4028" " -0.1203" " -0.0176" "  0.0090" " -0.3199"
       tausq    sigmasq        phi
  "  0.0526" "  0.1894" "499.9983"
  Practical Range with cor=0.05 for asymptotic range: 1498

  likfit: maximised log-likelihood = -975
```

Note that geoR reports also the regression coefficients for the five predictors (`beta0` is the intercept). In 2
the case of gstat this information will be hidden: gstat will typically fit a regression model only to derive the 3
residuals (regression coefficients can be printed by setting the debugging options). Neither gstat nor geoR 4
report on the goodness of fit and similar regression diagnostics. 5

Before we can make predictions, we also need to prepare the covariates at all locations. Unfortunately, 6
geoR is not compatible with sp grids, so we need to prepare the covariate values so they exactly match 7
prediction locations: 8

```
# get values of covariates at new locations:
> locs.sp <- locs
> coordinates(locs.sp) <- ~ Var1+Var2
> PCs.gr <- overlay(pc.comps, locs.sp)
# fix NAs:
> for(i in PCs.list){
>   PCs.gr@data[,i] <- ifelse(is.na(PCs.gr@data[,i]), 0, PCs.gr@data[,i])
> }
```

1 which allows us to run predictions using the same trend model as used in section 5.3.1:

```
# define the geostatistical model:
> KC <- krige.control(trend.d = step.zinc$call$formula[c(1,3)],
+     trend.l = ~ PCs.gr$PC1+PCs.gr$PC2+PCs.gr$PC3+PCs.gr$PC4+PCs.gr$PC6,
+     obj.m = zinc.rvgm2)
# run predictions (external trend kriging):
> zinc.rk2 <- krige.conv(zinc.geo, locations=locs, krige=KC, borders=mask.bor)
```

```
  krige.conv: results will be returned only for prediction inside the borders
  krige.conv: model with mean defined by covariates provided by the user
  krige.conv: performing the Box-Cox data transformation
  krige.conv: back-transforming the predicted mean and variance
  krige.conv: Kriging performed using global neighbourhood
```

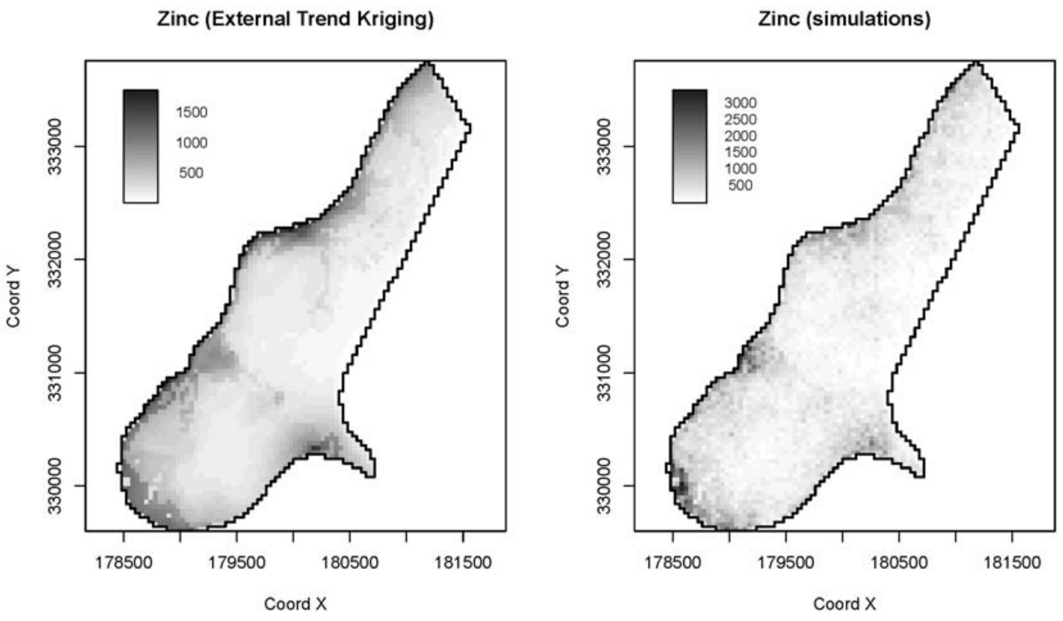


Fig. 5.17: Zinc predicted using external trend kriging in geoR (left); simulations using the same model (right). Compare with Figs. 5.9 and 5.12.

2 The result is shown in Fig. 5.17. geoR also allows generation of simulations using the same external trend
3 model by setting the `output.control` parameter (the resulting map shown in Fig. 5.17; right):

```
> zinc.rk2 <- krige.conv(zinc.geo, locations=locs, krige=KC, borders=mask.bor,
+     output=output.control(n.predictive=1))
```

```
  krige.conv: results will be returned only for prediction inside the borders
  krige.conv: model with mean defined by covariates provided by the user
  krige.conv: performing the Box-Cox data transformation
  krige.conv: sampling from the predictive distribution (conditional simulations)
  krige.conv: back-transforming the simulated values
  krige.conv: back-transforming the predicted mean and variance
  krige.conv: Kriging performed using global neighborhood
```

which shows a somewhat higher range of values than the simulation using a simple linear model (Fig. 5.12). In this case geoR seems to do better in accounting for the skewed distribution of values than gstat. However such simulations in geoR are extremely computationally intensive, and are not recommended for large data sets. In fact, many default methods implemented in geoR (Maximum Likelihood fitting for variograms, Bayesian methods and conditional simulations) are definitively not recommended with data sets with $\gg$1000 sampling points and/or over $\gg$100,000 new locations. Creators of geoR seem to have selected a path of running only global neighborhood analysis on the point data. Although the author of this guide supports that decision (see also section 2.2), some solution needs to be found to process larger point data sets because computing time exponentially increases with the size of the data set.

Finally, the results of predictions can be exported[22] to some GIS format by copying the values to an sp frame:

```
> mask.ov <- overlay(mask, locs.sp)
> mask.sel <- !is.na(mask.ov$MASK.SGRD)
> locs.geo <- data.frame(X=locs.sp@coords[mask.sel,1],
+    Y=locs.sp@coords[mask.sel,2], zinc.rk2=zinc.rk2[[1]],
+    zinc.rkvar2=zinc.rk2[[2]])
> coordinates(locs.geo) <- ~ X+Y
> gridded(locs.geo) <- TRUE
> write.asciigrid(locs.geo[1], "zinc_rk2.asc", na.value=-1)
```

## 5.6 Visualization of generated maps

### 5.6.1 Visualization of uncertainty

The following paragraphs explain how to visualize results of geostatistical mapping to explore uncertainty in maps. We will focus on the technique called **whitening**, which is a simple but efficient technique to visualize mapping error (Hengl and Toomanian, 2006). It is based on the Hue-Saturation-Intensity (HSI) color model (Fig. 5.18a) and calculations with colors using the color mixture (CM) concept. The HSI is a psychologically appealing color model — hue is used to visualize values or taxonomic space and whiteness (paleness) is used to visualize the uncertainty (Dooley and Lavin, 2007). For this purpose, a 2D legend was designed to accompany the visualizations. Unlike standard legends for continuous variables, this legend has two axis (Fig. 5.18b): (1) vertical axis (hues) is used to visualize the predicted values and (2) horizontal axis (whiteness) is used to visualize the prediction error. Fig. 5.19 shows an example of visualization using whitening for the meuse data set.

Visualization of uncertainty in maps using whitening can be achieved using one of the two software programs: ILWIS and R. In ILWIS, you can use the `VIS_error` script that can be obtained from the author's homepage. To visualize the uncertainty for your own case study using this technique, you should follow these steps (Hengl and Toomanian, 2006):

(1.) Download the ILWIS script (`VIS_error`[23]) for visualization of prediction error and unzip it to the default directory (`C:\Program Files\ILWIS\Scripts\`).

(2.) Derive the predictions and prediction variance for some target variable. Import both maps to ILWIS. The prediction variance needs to be then converted to normalized prediction variance by using Eq.(1.4.4), so you will also need to determine the global variance of your target variable.

(3.) Start ILWIS and run the script from the left menu (operations list) or from the main menu ↦ *Operations* ↦ *Scripts* ↦ `VIS_error`. Use the help button to find more information about the algorithm.

(4.) To prepare final layouts, you will need to use the `legend2D.tif` legend file[24].

A more interesting option is to visualize maps using whitening in R[25]. You will need to load the following additional package:

[22]Note that the results of prediction in geoR is simply a list of values without any spatial reference.

[23]`http://spatial-analyst.net/scripts/`

[24]`http://spatial-analyst.net/scripts/legend2D.tif`; This legend is a Hue-whitening legend: in the vertical direction only Hue values change, while in the horizontal direction amount of white color is linearly increased from 0.5 up to 1.0.

[25]`http://spatial-analyst.net/scripts/whitening.R`

```
> library(colorspace)
```

1 The example with the meuse data set:

```
# ordinary kriging:
> m <- vgm(.59, "Sph", 874, .04)
> vismaps <- krige(log(zinc) ~ 1, meuse, meuse.grid, model=m)
```

2 As a result of ordinary kriging, we have produced two maps: predictions and the prediction variance. Now,
3 we can visualize both maps together using whitening. We start by setting up threshold levels (lower and upper
4 limits), and stretching the values within that range:

```
> z1 <- min(log(meuse$zinc), na.rm=TRUE)
> z2 <- max(log(meuse$zinc), na.rm=TRUE)
> e1 <- 0.4
> e2 <- 0.7
> vismaps$er <- sqrt(vismaps$e)/sqrt(var(log(meuse$zinc)))
> vismaps$tmpz <- (vismaps$z-z1)/(z2-z1)
# Mask the values outside the 0-1 range:
> vismaps$tmpzc <- ifelse(vismaps$tmpz<=0, 0, ifelse(vismaps$tmpz>1, 1, vismaps$tmpz))
```

5 The Hue-Saturation-Value (HSV) bands we can generate using:

```
# The hues should lie between between 0 and 360, and the saturations
# and values should lie between 0 and 1.
> vismaps$tmpf1 <- -90-vismaps$tmpzc*300
> vismaps$tmpf2 <- ifelse(vismaps$tmpf1<=-360, vismaps$tmpf1+360, vismaps$tmpf1)
> vismaps$H <- ifelse(vismaps$tmpf2>=0, vismaps$tmpf2, (vismaps$tmpf2+360))
# Strech the error values (e) to the inspection range:
# Mask the values out of the 0-1 range:
> vismaps$tmpe <- (vismaps$er-e1)/(e2-e1)
> vismaps$tmpec <- ifelse(vismaps$tmpe<=0, 0, ifelse(vismaps$tmpe>1, 1, vismaps$tmpe))
# Derive the saturation and intensity images:
> vismaps$S <- 1-vismaps$tmpec
> vismaps$V <- 0.5*(1+vismaps$tmpec)
```

6 The HSV values can be converted to RGB bands using:

```
> RGBimg <- as(HSV(vismaps$H, vismaps$S, vismaps$V), "RGB")
> summary(RGBimg@coords)
> vismaps$red <- as.integer(ifelse(is.na(vismaps@data[1]), 255, RGBimg@coords[,1]*255))
> vismaps$green <- as.integer(ifelse(is.na(vismaps@data[1]), 255, RGBimg@coords[,2]*255))
> vismaps$blue <- as.integer(ifelse(is.na(vismaps@data[1]), 255, RGBimg@coords[,3]*255))
> summary(vismaps[c("red", "green", "blue")])
```

```
Object of class SpatialGridDataFrame
Coordinates:
     min    max
x 178440 181560
y 329600 333760
Is projected: NA
proj4string : [NA]
Number of points: 2
Grid attributes:
  cellcentre.offset cellsize cells.dim
x            178460       40        78
y            329620       40       104
Data attributes:
      red              green              blue
 Min.   :  0.0   Min.   :  0.0   Min.   :  0.0
 1st Qu.:153.0   1st Qu.:183.0   1st Qu.:194.0
 Median :255.0   Median :255.0   Median :255.0
 Mean   :206.2   Mean   :220.5   Mean   :219.2
 3rd Qu.:255.0   3rd Qu.:255.0   3rd Qu.:255.0
 Max.   :255.0   Max.   :255.0   Max.   :255.0
```

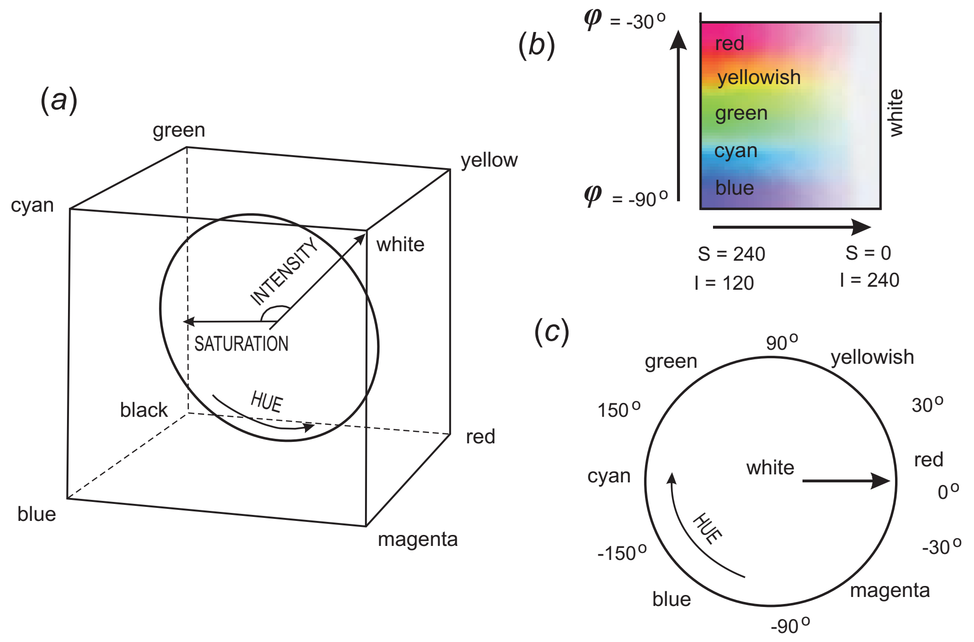


Fig. 5.18: Design of the special 2D legend used to visualize the prediction variance using whitening: (a) the HSI color model, (b) the 2D legend and (c) the common types of Hues. After Hengl et al. (2004a).

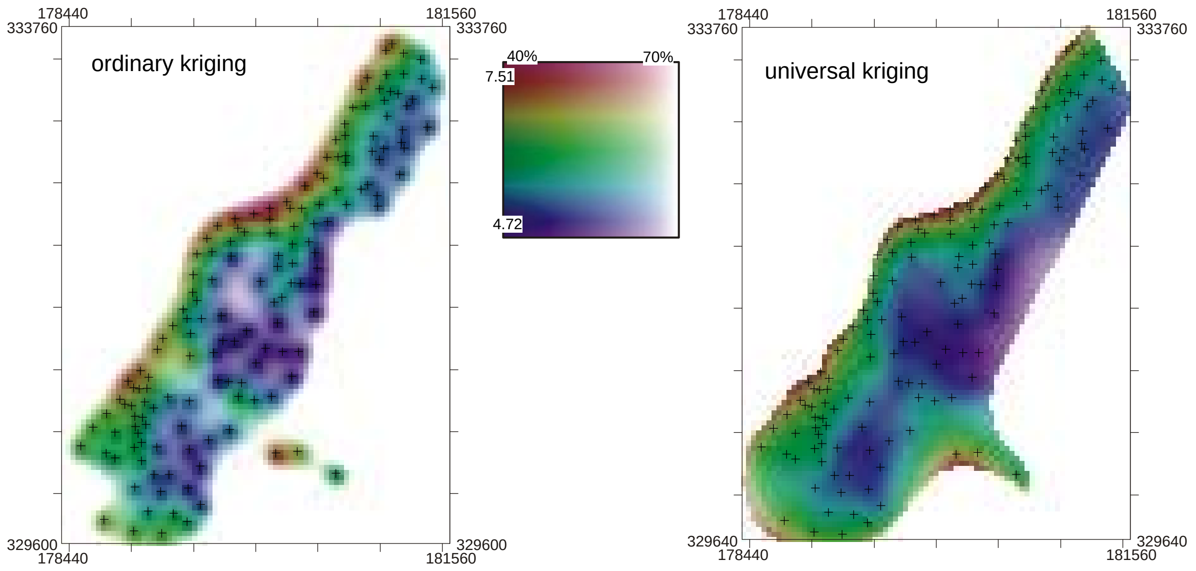


Fig. 5.19: Mapping uncertainty for zinc visualized using whitening: ordinary kriging (left) and universal kriging (right). Predicted values in log-scale. See cover of this book for a color version of this figure.

which is now a spatial object with three RGB bands. To display a true RGB image in R, use the SGDF2PCT method[26]:

```
> RGBimg <- SGDF2PCT(vismaps[c("red", "green", "blue")], ncolors=256, adjust.bands=FALSE)
> vismaps$idx <- RGBimg$idx
> image(vismaps, "idx", col=RGBimg$ct)
> plot(meuse, pch="+", add=TRUE)
```

In the last step (optional), we can set the right georeference and export the map to e.g. GeoTIFF format:

```
> proj4string(vismaps) <- CRS("+init=epsg:28992")
# Export as geoTIFF / or any other format:
> writeGDAL(vismaps[c("red", "green", "blue")], "vismap.tif", drivername="GTiff",
+    type="Byte", options="INTERLEAVE=PIXEL")
```

A comparison of uncertainty for maps produced using ordinary kriging and universal kriging in gstat can be seen in Fig. 5.19. In this case, the universal kriging map is distinctly more precise. You can manually change the lower and upper values for both prediction and error maps depending on your mapping requirements. By default, thresholds of 0.4 and 0.8 (max 1.0) are used for the normalized prediction error values. This assumes that a satisfactory prediction is when the model explains more than 85% of the total variation (normalized error = 40%; see p.23). Otherwise, if the value of the normalized error get above 80%, the model accounts for less than 50% of variability at calibration points and the prediction is probably unsatisfactory.

To prepare the 2D legend shown in Fig. 5.19 (100×100 pixels), we use:

```
> legend.2D <- expand.grid(x=seq(.01,1,.01),y=seq(.01,1,.01))
# Hues
> legend.2D$tmpf1 <- -90-legend.2D$y*300
> legend.2D$tmpf2 <- ifelse(legend.2D$tmpf1<=-360, legend.2D$tmpf1+360,
+      legend.2D$tmpf1)
> legend.2D$H <- ifelse(legend.2D$tmpf2>=0, legend.2D$tmpf2, (legend.2D$tmpf2+360))
# Saturation:
> legend.2D$S <- 1-legend.2D$x
# Intensity:
> legend.2D$V <- 0.5+legend.2D$x/2
> gridded(legend.2D) <- ~ x+y
> legend.2D <- as(legend.2D, "SpatialGridDataFrame")
> legendimg <- as(HSV(legend.2D$H, legend.2D$S, legend.2D$V), "RGB")
> legend.2D$red <- as.integer(legendimg@coords[,1]*255)
> legend.2D$green <- as.integer(legendimg@coords[,2]*255)
> legend.2D$blue <- as.integer(legendimg@coords[,3]*255)
# Write as a RGB image:
> legend.2Dimg <- SGDF2PCT(legend.2D[c("red", "green", "blue")], ncolors=256,
+      adjust.bands=FALSE)
> legend.2D$idx <- legend.2Dimg$idx
> writeGDAL(legend.2D[c("red", "green", "blue")], "legend2D.tif",
+      drivername="GTiff", type="Byte", options="INTERLEAVE=PIXEL")
```

Another sophisticated option to visualize the results of (spatio-temporal) geostatistical mapping is the stand-alone visualization software called Aquila[27] (Pebesma et al., 2007). Aquila facilitates interactive exploration of the spatio-temporal **Cumulative Distribution Functions** (CDFs) and allows decision makers to explore uncertainty associated with attaching different threshold or its spatial distribution in the area of interest. It is actually rather simple to use — one only needs to prepare a sample (e.g. 12 slices) of quantile estimates, which are then locally interpolated to produce CDFs.

### 5.6.2 Export of maps to Google Earth

To export maps we have produced to Google Earth, we first need to reproject the maps to the WGS84 coordinate system (the native system for Google Earth). We can first reproject the map of sample points, using the

[26]Note that the results might differ slightly between ILWIS and R, which is mainly due to somewhat different HSI–RGB conversion algorithms. For example, the SGDF2PCT method is limited to 256 colors only!

[27]http://pcraster.geo.uu.nl/projects/aguila/

spTransform method of the sp package, and then export them using writeOGR: 1

```
> meuse.ll <- spTransform(meuse, CRS("+proj=longlat +datum=WGS84"))
> writeOGR(meuse.ll, "meuse.kml", "meuse", driver="KML")
```

You can examine these in Google Earth by opening the KML file meuse.kml which you just wrote. Next, 2
we want to export the predictions of zinc, which means that we first need to reproject the interpolated values 3
onto geographic coordinates. The most efficient way to achieve this is by using the SAGA proj4 module[28]: 4

```
> rsaga.geoprocessor(lib="pj_proj4", 2, param=list(SOURCE_PROJ=paste('"',
+     proj4string(meuse.grid), '"', sep=""), TARGET_PROJ="\"+proj=longlat
+     +datum=WGS84\"", SOURCE="zinc_rk.sgrd", TARGET="zinc_rk_ll.sgrd",
+     TARGET_TYPE=0, INTERPOLATION=1))
```

```
SAGA CMD 2.0.4
library path:   C:/Progra~1/saga_vc/modules
library name:   pj_proj4
module name :   Proj.4 (Command Line Arguments, Grid)
author      :   O. Conrad (c) 2004-8

Load grid: zinc_rk.sgrd...
ready

Parameters

Inverse: no
Source Projection Parameters:  +init=epsg:28992 +proj=sterea
 +lat_0=52.15616055555555 +lon_0=5.38763888888889 +k=0.999908 +x_0=155000
 +y_0=463000 +ellps=bessel +towgs84=565.237,50.0087,465.658,-0.406857,
 0.350733,-1.87035,4.0812 +units=m +no_defs
Target Projection Parameters: +proj=longlat +datum=WGS84
Grid system: 40; 77x 104y; 178500x 329620y
Source: zinc_rk.sgrd
Target: [not set]
Shapes: [not set]
X Coordinates: [not set]
Y Coordinates: [not set]
Create X/Y Grids: no
Target: user defined
Interpolation: Bilinear Interpolation

Source:  +init=epsg:28992 +proj=sterea +lat_0=52.15616055555555
+lon_0=5.38763888888889 +k=0.999908 +x_0=155000 +y_0=463000
+ellps=bessel +towgs84=565.237,50.0087,465.658,-0.406857,0.350733,
-1.87035,4.0812 +units=m +no_defs

Target: +proj=longlat +datum=WGS84

ready
Save grid: zinc_rk_ll.sgrd...
```

Once we have created this gridded result, we can plot the maps and export the plots to Google Earth. First 5
we need to set up metadata in the form of a SpatialGrid object for defining the size and placing of a PNG 6
image overlay in Google Earth; this is the job of the GE_SpatialGrid method of the maptools package: 7

```
# read back into R:
> rsaga.sgrd.to.esri(in.sgrds="zinc_rk_ll.sgrd", out.grids="zinc_rk_ll.asc",
+        out.path=getwd())
> zinc_rk.ll <- readGDAL("zinc_rk_ll.asc")
```

[28]SAGA will automatically estimate both the grid cell size and the bounding box in geographical coordinates. Compare with section 10.6.3.

```
  zinc_rk_ll.asc has GDAL driver AAIGrid
  and has 105 rows and 122 columns
```

```
> proj4string(zinc_rk.ll) <- CRS("+proj=longlat +datum=WGS84")
> zinc_rk.kml <- GE_SpatialGrid(zinc_rk.ll)
```

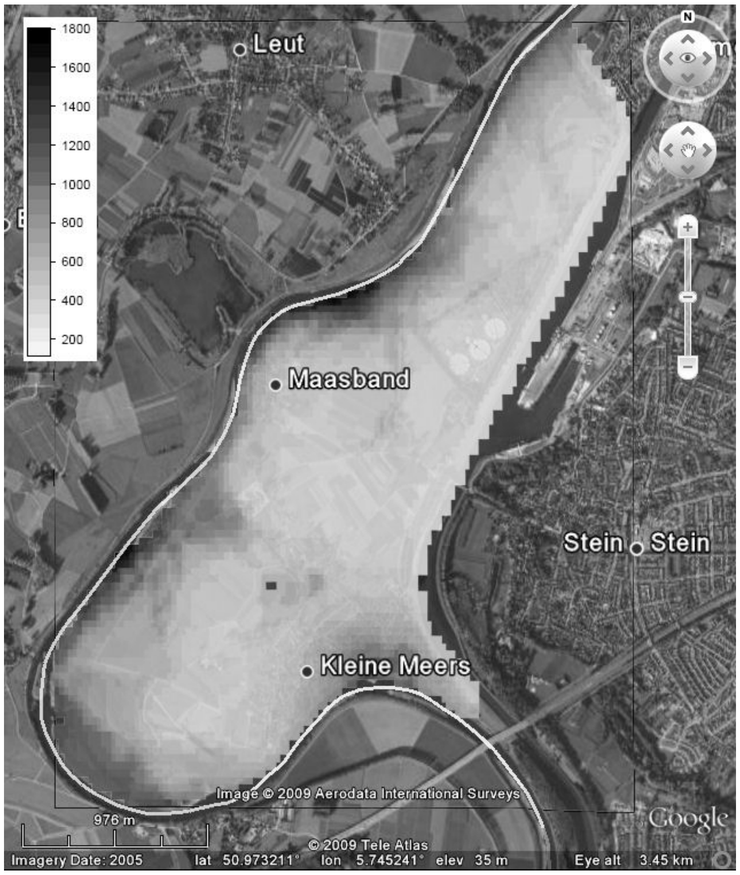


Fig. 5.20: RK predictions of zinc for Meuse area — as visualized in Google Earth.

1 where zinc_rk.kml is the name of R object, which carries only a definition of the ground overlay frame and
2 not the data to be exported. Next we create a PNG (Portable Network Graphics) file (the format recognized as
3 an overlay by Google Earth) using the png graphics device:

```
> png(file="zinc_rk.png", width=zinc_rk.kml$width, height=zinc_rk.kml$height, bg="transparent")
> par(mar=c(0,0,0,0), xaxs="i", yaxs="i")
> image(as.image.SpatialGridDataFrame(zinc_rk.ll[1]),
+     col=grey(rev(seq(0,0.95,1/length(at.zinc)))),
+     xlim=zinc_rk.kml$xlim, ylim=zinc_rk.kml$ylim)
```

4 which will plot the map over the whole area of the plotting space, so that border coordinates exactly match
5 the borders of the plot. We then create the overlay itself, from the PNG file, with the kmlOverlay method,
6 specifying the SpatialGrid object that orients the map in Google Earth:

```
> kmlOverlay(zinc_rk.kml, kmlfile="zinc_rk.kml", imagefile="zinc_rk.png", name="zinc")
```

```
  [1] "<?xml version='1.0' encoding='UTF-8'?>"
  [2] "<kml xmlns='http://earth.google.com/kml/2.0'>"
  [3] "<GroundOverlay>"
```

```
[4] "<name>zinc (RK)</name>"
[5] "<Icon><href>zinc_rk.png</href><viewBoundScale>0.75</viewBoundScale></Icon>"
[6] "<LatLonBox><north>50.992973</north><south>50.955488</south>
+     <east>5.76502299201062</east><west>5.721466</west></LatLonBox>"
[7] "</GroundOverlay></kml>"
```

```
> dev.off()
```

When you open the resulting KML in Google Earth, you will see a display shown in Fig. 5.20. This allows you to orient yourself and make an interpretation of the produced maps. Open the final map in Google Earth and visually explore how many areas next to the populated areas show high concentrations of zinc.

**Self-study exercises:**

(1.) How many pixels in the `meuse.grid` are available for spatial prediction? (HINT: Number of pixels that do not have missing values for any of the variables.)

(2.) What is the correlation coefficient between maps `dist` and `ahn`? (HINT: use the `cor` method.) Is the default Pearson's parametric correlation appropriate? (HINT: Make a scatterplot of the two maps using the `plot` method. Compute also a non-parametric Spearman correlation.)

(3.) How much of the variation in Zinc does the RK model explains, and which are the most significant predictors? (HINT: Look at the R-square and the `Pr(>|t|)`.)

(4.) Up to which distance from the points are the predictions improved by the ordinary kriging model (rather than just by using an average of all the observations)? (HINT: look at the original variance, and then find at which distance does the semivariance exceeds the original variance.)

(5.) Up to which distance is zinc spatially auto-correlated based on this model? Provide R code to support your answer.

(6.) Is there significant difference in the accuracy of the predictions between OK and RK?

(7.) Up to which distance from the points are the predictions improved by the model? (HINT: At which distance does the regression-kriging prediction variance exceed the global variance?)

(8.) Generate geostatistical simulations of zinc by using only ordinary kriging model and compare your results with Fig 5.12. Which simulation produces higher variability of values (HINT: derive standard deviation and range) — with RK or OK model?

(9.) Randomly split the meuse points in two data sets. Then repeat OK and RK using the same procedure explained in section 5.3.1 and see if the difference in accuracy at validation points is still the same?

(10.) If you had more funds available to locate additional 50 points, and then sample soil again, where would you put them? (HINT: use the sampling optimization algorithm implemented in the intamapInteractive package.)

**Further reading:**

★ Bivand, R., Pebesma, E., Rubio, V., 2008. **Applied Spatial Data Analysis with R**. Use R Series. Springer, Heidelberg.

★ Ribeiro Jr, P. J., Christensen, O. F. and Diggle, P. J., 2003. geoR and geoRglm: Software for Model-Based Geostatistics. In: Hornik, K. and Leisch, F. and Zeileis, A. (eds) **Proceedings of the 3rd International Workshop on Distributed Statistical Computing** (DSC 2003), Technical University Vienna, pp. 517–524.

★ Kutner, M. H., Nachtsheim, C. J., Neter, J., Li, W. (Eds.), 2004. **Applied Linear Statistical Models**, 5th Edition. McGraw-Hill.

★ Pebesma, E. J., 2004. Multivariable geostatistics in S: the gstat package. Computers & Geosciences 30(7), 683–691.

★ `http://leg.ufpr.br/geoR/` — The geoR package project.

★ `http://www.gstat.org` — The gstat package project.