The meuse data set: a tutorial for the `gstat` R package

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1 Introduction

The `meuse` data set is a data set comprising of four heavy metals measured in the top soil in a flood plain along the river Meuse. The governing process seems that polluted sediment is carried by the river, and mostly deposited close to the river bank. This document shows a geostatistical analysis of this data set.

This tutorial introduced the functionality of the R package `gstat`, used in conjunction with package `sp`. Package `gstat` provides a wide range of univariable and multivariable geostatistical modelling, prediction and simulation functions, where package `sp` provides general purpose classes and methods for defining, importing/exporting and visualizing spatial data.

2 R geostatistics packages

Package `gstat` (Pebesma, 2004) is an R package that provides basic functionality for univariable and multivariable geostatistical analysis, including

- variogram modelling, residual variogram modelling, and cross variogram modelling using fitting of parametric models to sample variograms
- geometric anisotropy specfied for each partial variogram model
- restricted maximum likelihood fitting of partial sills
- variogram and cross variogram maps
- simple, ordinary, universal and external drift (co)kriging
- (sequential) Gaussian (co)simulation equivalents for each of the kriging varieties
- indicator (co)kriging and sequential indicator (co)simulation
- kriging in a local or global neighbourhood
- block (co)kriging or simulation for each of the varieties, for rectangular or irregular blocks

Other geostatistical packages for R usually lack part of these options (e.g. block kriging, local kriging, or cokriging) but provide others: e.g. package `geoR` and `geoRglm` (by Paulo Ribeiro and Ole Christensen) provide the model-based geostatistics framework described in Diggle et al. (1998), package `fields` (Doug Nychka and others) provides thin plate spline interpolation, covariance functions for spherical coordinates (unprojected data), and routines for network design optimization.

3 Spatial data frames

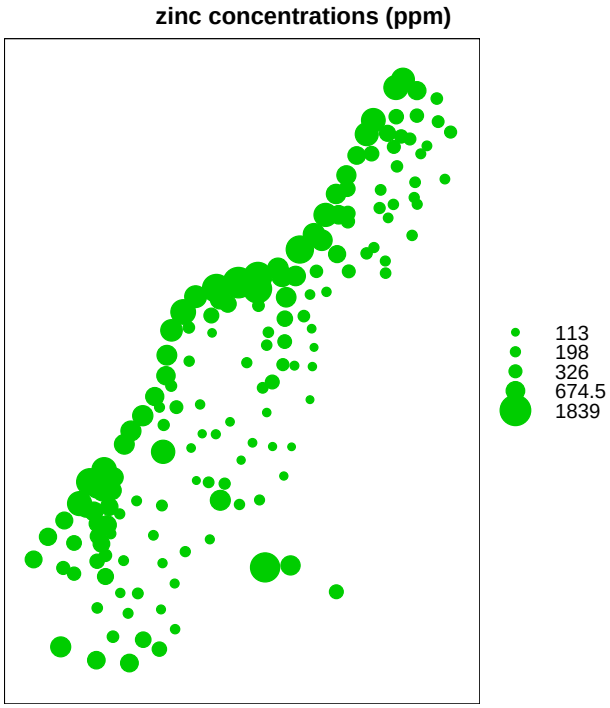
Package `gstat` assumes that data are projected, i.e. they should not be provided as lattitude/longitude. As an example, we will look at the meuse data set, which is a regular data frame that comes with package `gstat`:

```
> library(gstat)

Loading required package: sp

> data(meuse)
> class(meuse)

[1] "data.frame"

> names(meuse)

 [1] "x"       "y"       "cadmium" "copper"  "lead"    "zinc"    "elev"
 [8] "dist"    "om"      "ffreq"   "soil"    "lime"    "landuse" "dist.m"

> coordinates(meuse) = ~x + y
> class(meuse)

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

> summary(meuse)

Object of class SpatialPointsDataFrame
Coordinates:
     min    max
x 178605 181390
y 329714 333611
Is projected: NA
proj4string : [NA]
Number of points: 155
Data attributes:
    cadmium           copper            lead            zinc
 Min.   : 0.200   Min.   : 14.00   Min.   : 37.0   Min.   : 113.0
 1st Qu.: 0.800   1st Qu.: 23.00   1st Qu.: 72.5   1st Qu.: 198.0
 Median : 2.100   Median : 31.00   Median :123.0   Median : 326.0
 Mean   : 3.246   Mean   : 40.32   Mean   :153.4   Mean   : 469.7
```

```
 3rd Qu.: 3.850   3rd Qu.: 49.50   3rd Qu.:207.0   3rd Qu.: 674.5
 Max.   :18.100   Max.   :128.00   Max.   :654.0   Max.   :1839.0

     elev             dist              om         ffreq  soil   lime
 Min.   : 5.180   Min.   :0.00000   Min.   : 1.000   1:84   1:97   0:111
 1st Qu.: 7.546   1st Qu.:0.07569   1st Qu.: 5.300   2:48   2:46   1: 44
 Median : 8.180   Median :0.21184   Median : 6.900   3:23   3:12
 Mean   : 8.165   Mean   :0.24002   Mean   : 7.478
 3rd Qu.: 8.955   3rd Qu.:0.36407   3rd Qu.: 9.000
 Max.   :10.520   Max.   :0.88039   Max.   :17.000
                                    NA's   : 2.000
    landuse       dist.m
 W      :50   Min.   :  10.0
 Ah     :39   1st Qu.:  80.0
 Am     :22   Median : 270.0
 Fw     :10   Mean   : 290.3
 Ab     : 8   3rd Qu.: 450.0
 (Other):25   Max.   :1000.0
 NA's   : 1
```

```
> coordinates(meuse)[1:5, ]

          x      y
[1,] 181072 333611
[2,] 181025 333558
[3,] 181165 333537
[4,] 181298 333484
[5,] 181307 333330
```

```
> bubble(meuse, "zinc", col = c("#00ff0088", "#00ff0088"), main = "zinc concentrations (pp
```



and note the following:

1. the function `coordinates`, when assigned (i.e. on the left-hand side of an `=` or `<-` sign), promotes the `data.frame` meuse into a `SpatialPointsDataFrame`, which knows about its spatial coordinates; coordinates may be specified by a formula, a character vector, or a numeric matrix or data frame with the actual coordinates

2. the function `coordinates`, when not assigned, *retrieves* the spatial coordinates from a `SpatialPointsDataFrame`.

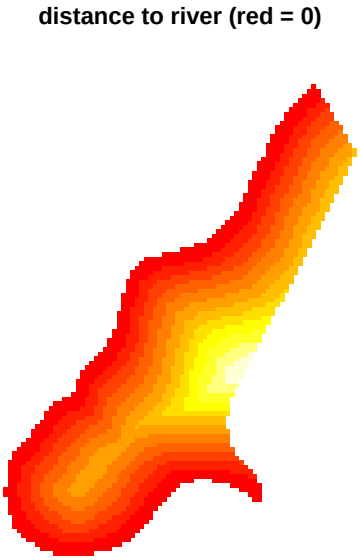
3. the two plotting functions used, `plot` and `bubble` assume that the x- and y-axis are the spatial coordinates, and choose the aspect ratio of the axes such that one unit in x equals one unit in y (i.e., data are map data, projected).

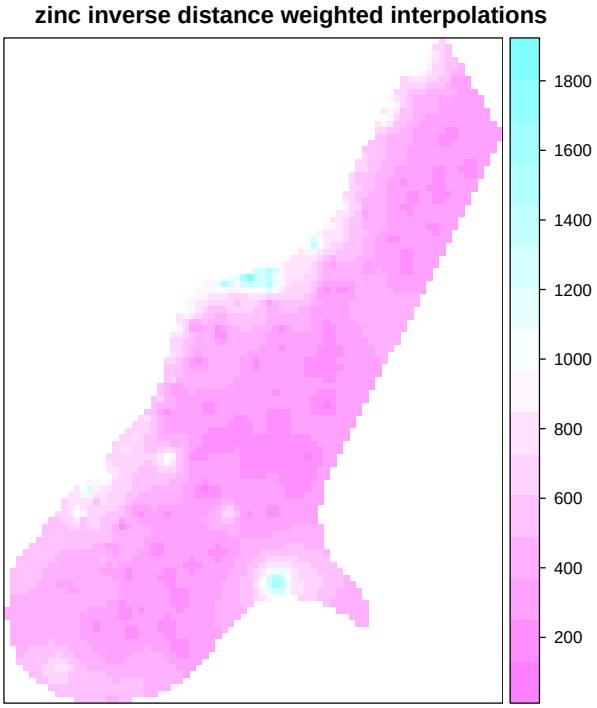
4 Spatial data on a regular grid

```
> data(meuse.grid)
> summary(meuse.grid)
```

```
       x                y             part.a           part.b      
 Min.   :178460   Min.   :329620   Min.   :0.0000   Min.   :0.0000  
 1st Qu.:179420   1st Qu.:330460   1st Qu.:0.0000   1st Qu.:0.0000  
 Median :179980   Median :331220   Median :0.0000   Median :1.0000  
 Mean   :179985   Mean   :331348   Mean   :0.3986   Mean   :0.6014  
 3rd Qu.:180580   3rd Qu.:332140   3rd Qu.:1.0000   3rd Qu.:1.0000  
```

```
 Max.   :181540   Max.   :333740   Max.   :1.0000   Max.   :1.0000
     dist             soil       ffreq
 Min.   :0.0000   Min.   :1.000   1: 779
 1st Qu.:0.1193   1st Qu.:1.000   2:1335
 Median :0.2715   Median :1.000   3: 989
 Mean   :0.2971   Mean   :1.578
 3rd Qu.:0.4402   3rd Qu.:2.000
 Max.   :0.9926   Max.   :3.000

> class(meuse.grid)

[1] "data.frame"

> coordinates(meuse.grid) = ~x + y
> class(meuse.grid)

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

> gridded(meuse.grid) = TRUE
> class(meuse.grid)

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

> image(meuse.grid["dist"])
> title("distance to river (red = 0)")
> zinc.idw = krige(zinc ~ 1, meuse, meuse.grid)

[inverse distance weighted interpolation]

> class(zinc.idw)

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

> spplot(zinc.idw["var1.pred"], main = "zinc inverse distance weighted interpolations")
```

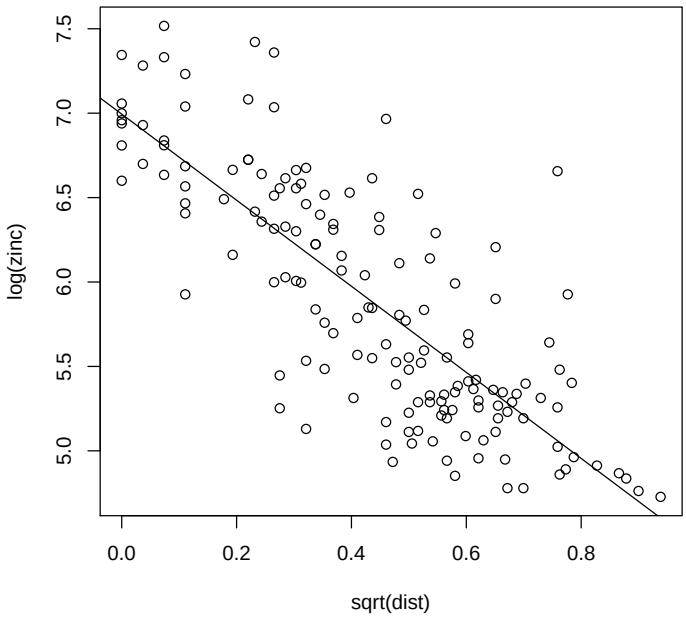




If you compare the bubble plot of zinc measurements with the map with distances to the river, it becomes evident that the larger concentrations are measured at locations close to the river. This relationship can be linearized by

log-transforming the zinc concentrations, and taking the square root of distance to the river:

```
> plot(log(zinc) ~ sqrt(dist), meuse)
> abline(lm(log(zinc) ~ sqrt(dist), meuse))
```



5 Variograms

Variograms are calculated using the function `variogram`, which takes a formula as its first argument: `log(zinc)~1` means that we assume a constant trend for the variable log(zinc).

```
> lzn.vgm = variogram(log(zinc) ~ 1, meuse)
> lzn.vgm
```

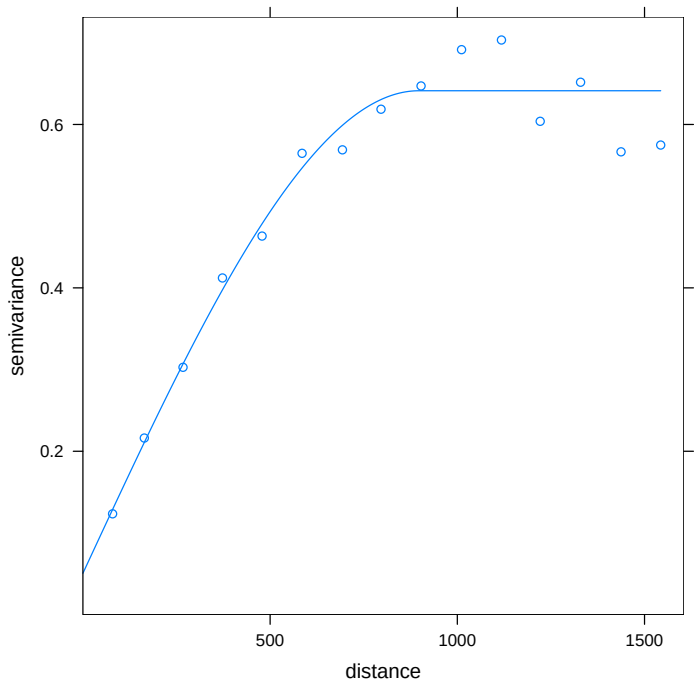
```
    np       dist     gamma dir.hor dir.ver   id
1   57   79.29244 0.1234479       0       0 var1
2  299  163.97367 0.2162185       0       0 var1
3  419  267.36483 0.3027859       0       0 var1
4  457  372.73542 0.4121448       0       0 var1
5  547  478.47670 0.4634128       0       0 var1
6  533  585.34058 0.5646933       0       0 var1
7  574  693.14526 0.5689683       0       0 var1
8  564  796.18365 0.6186769       0       0 var1
9  589  903.14650 0.6471479       0       0 var1
10 543 1011.29177 0.6915705       0       0 var1
```

```
11 500 1117.86235 0.7033984       0       0 var1
12 477 1221.32810 0.6038770       0       0 var1
13 452 1329.16407 0.6517158       0       0 var1
14 457 1437.25620 0.5665318       0       0 var1
15 415 1543.20248 0.5748227       0       0 var1
```

```
> lzn.fit = fit.variogram(lzn.vgm, model = vgm(1, "Sph", 900, 1))
> lzn.fit
```

```
  model      psill    range
1   Nug 0.05066243   0.0000
2   Sph 0.59060780 897.0209
```

```
> plot(lzn.vgm, lzn.fit)
```

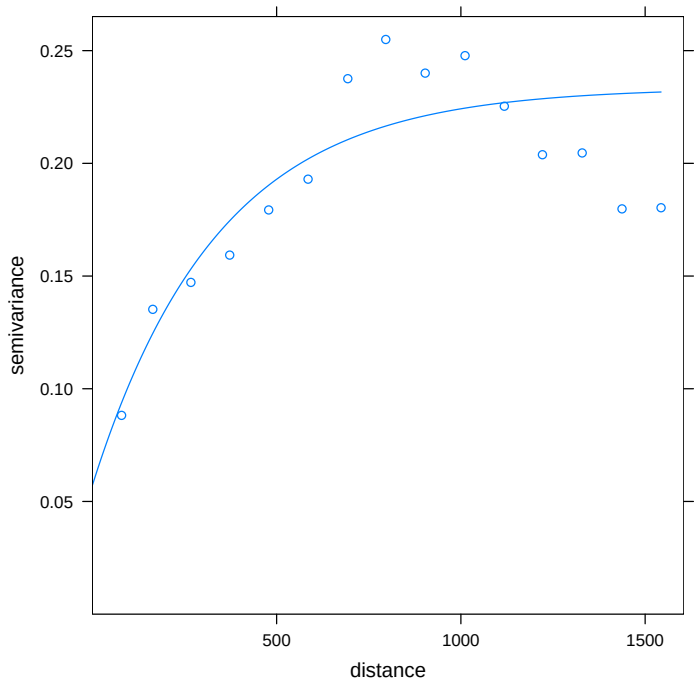


Instead of the constant mean, denoted by `~1`, we can specify a mean function, e.g. using `~sqrt(dist)` as a predictor variable:

```
> lznr.vgm = variogram(log(zinc) ~ sqrt(dist), meuse)
> lznr.fit = fit.variogram(lznr.vgm, model = vgm(1, "Exp", 300,
+     1))
> lznr.fit
```

```
  model      psill    range
1   Nug 0.05712231   0.0000
2   Exp 0.17641559 340.3201
```

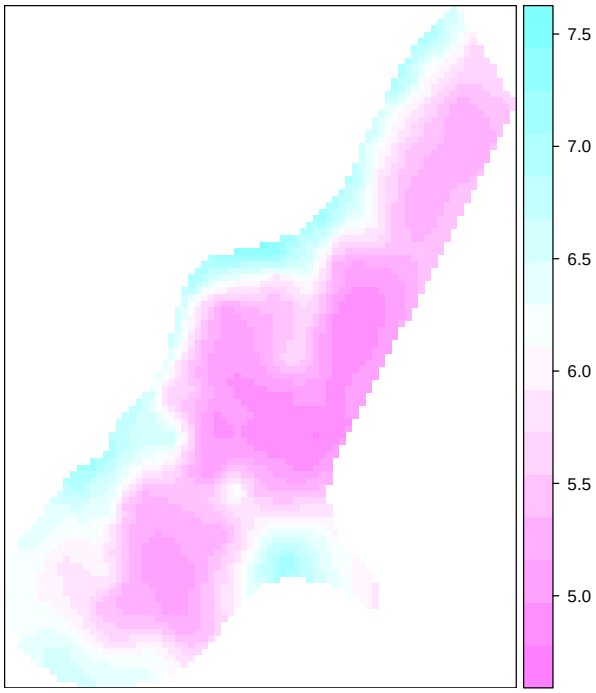
```
> plot(lznr.vgm, lznr.fit)
```



In this case, the variogram of residuals with respect to a fitted mean function are shown. Residuals were calculated using ordinary least squares.

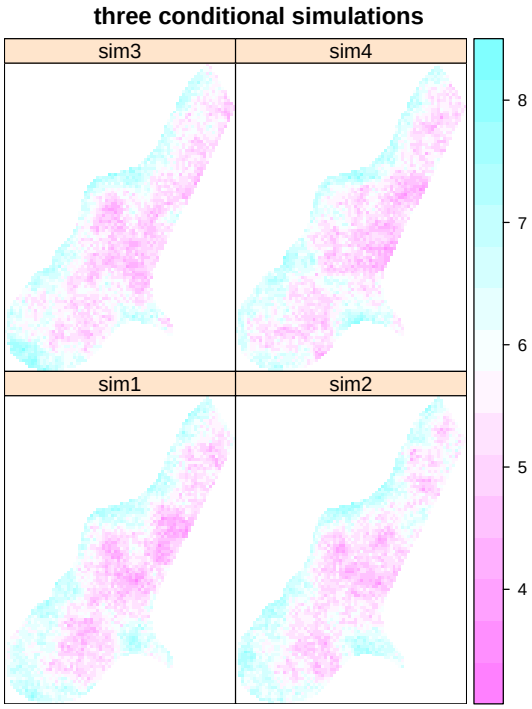
6 Kriging

```
> lzn.kriged = krige(log(zinc) ~ 1, meuse, meuse.grid, model = lzn.fit)

[using ordinary kriging]

> spplot(lzn.kriged["var1.pred"])
```



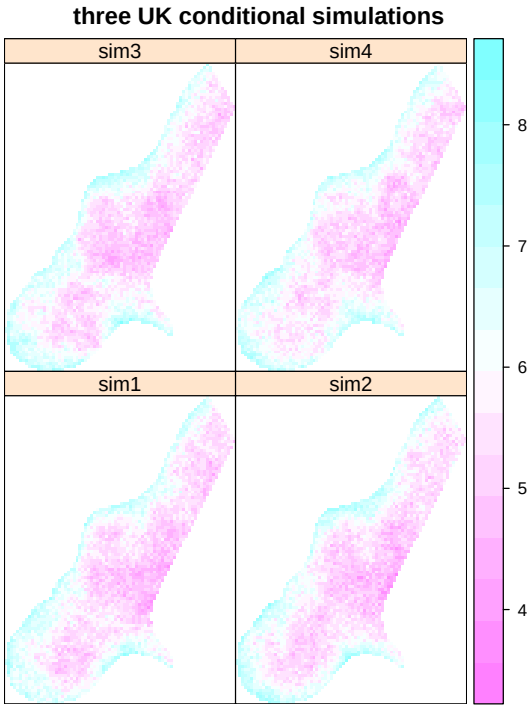
7 Conditional simulation

```
> lzn.condsim = krige(log(zinc) ~ 1, meuse, meuse.grid, model = lzn.fit,
+     nmax = 30, nsim = 4)

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

> spplot(lzn.condsim, main = "three conditional simulations")
```



For UK/residuals:

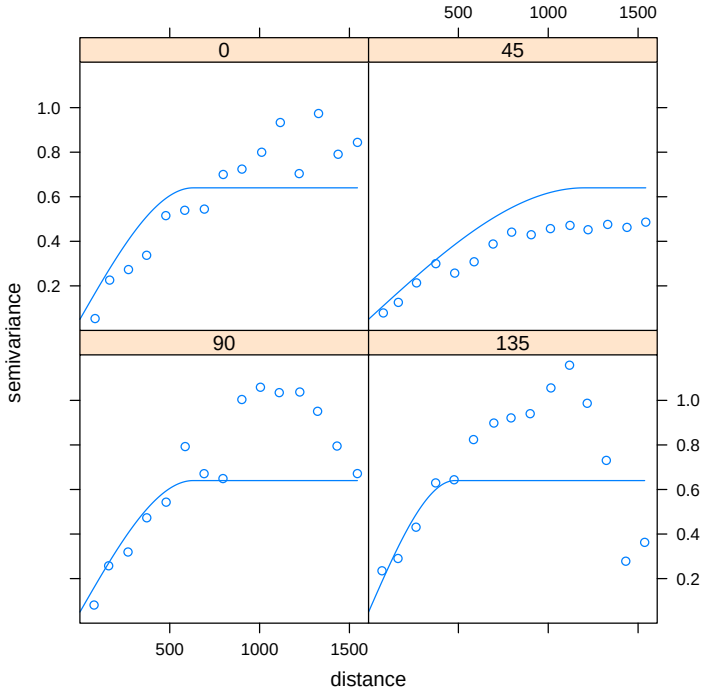
```
> lzn.condsim2 = krige(log(zinc) ~ sqrt(dist), meuse, meuse.grid,
+     model = lznr.fit, nmax = 30, nsim = 4)

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

> spplot(lzn.condsim2, main = "three UK conditional simulations")
```



8 Directional variograms

The following command calculates a directional sample variogram, where directions are binned by direction angle alone. For two point pairs, $Z(s)$ and $Z(s+h)$, the separation vector is h, and it has a direction. Here, we will classify directions into four direction intervals:

```
> lzn.dir = variogram(log(zinc) ~ 1, meuse, alpha = c(0, 45, 90,
+     135))
> lzndir.fit = vgm(0.59, "Sph", 1200, 0.05, anis = c(45, 0.4))
> plot(lzn.dir, lzndir.fit, as.table = TRUE)
```



Looking at directions between 180 and 360 degrees will repeat the image shown above, because the variogram is a symmetric measure: $(Z(s) - Z(s + h))^2 = (Z(s + h) - Z(s))^2$.

The first plot gives the variogram in the zero direction, which is North; 90 degrees is East. By default, point pairs are assigned to the directional variorgram panel with their nearest direction, so North contains everything between -22.5 and 22.5 degrees (North-West to North-East). After classifying by direction, point pairs are binned by separation distance class, as is done in the usual omnidirectional case.

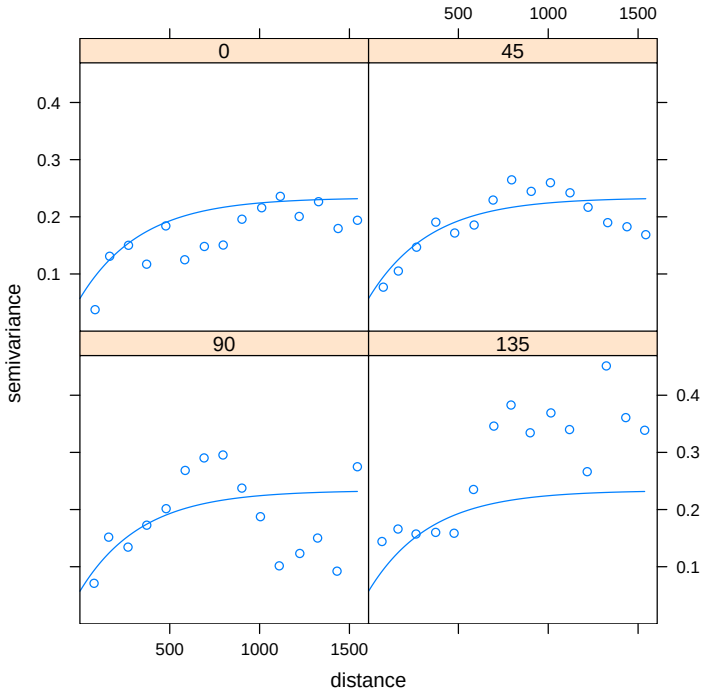
In the figure, the partial sill, nugget and model type of the model are equal to those of the omnidirectional model fitted above; the range is that in the direction with the largest range (45^o), and the anisotropy ratio, the range in the 135 direction and the range in the 45 direction, estimated "by eye" by comparing the 45 and 135 degrees sample variograms. Gstat does not fit anisotropy parameters automatically.

We do not claim that the model fitted here is "best" in some way; in order to get to a better model we may want to look at more directions, other directions (e.g. try `alpha = c(22, 67, 112, 157)`), and to variogram maps (see below). More elaborate approaches may use directions in three dimentions, and want to furnter control the direction tolerance (which may be set such that direction intervals overlap).

For the residual variogram from the linear regression model using sqrt(dist) as covariate, the directional dependence is much less obvious; the fitted model here is the fitted isotropic model (equal in all directions).

```
> lznr.dir = variogram(log(zinc) ~ sqrt(dist), meuse, alpha = c(0,
+     45, 90, 135))
```

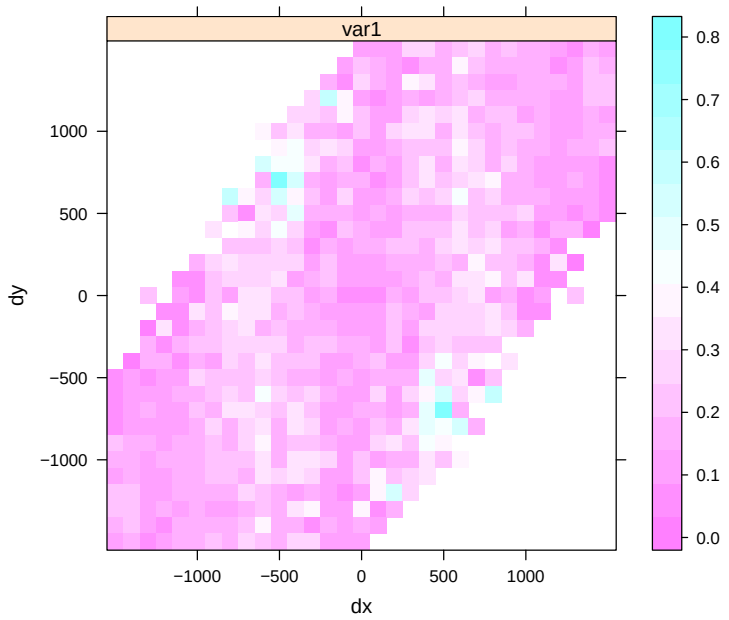
```
> plot(lznr.dir, lznr.fit, as.table = TRUE)
```



9 Variogram maps

Another means of looking at directional dependence in semivariograms is obtained by looking at variogram maps. Instead of classifying point pairs $Z(s)$ and $Z(s+h)$ by direction and distance class *separately*, we can classify them *jointly*. If $h = \{x, y\}$ be the two-dimentional coordinates of the separation vector, in the variogram map the semivariance contribution of each point pair $(Z(s) - Z(s+h))^2$ is attributed to the grid cell in which h lies. The map is centered around $(0, 0)$, as h is geographical distance rather than geographical location. Cutoff and width correspond to some extent to map extent and cell size; the semivariance map is point symmetric around $(0, 0)$, as $\gamma(h) = \gamma(-h)$.

```
> vgm.map = variogram(log(zinc) ~ sqrt(dist), meuse, cutoff = 1500,
+     width = 100, map = TRUE)
> plot(vgm.map, threshold = 5)
```



The threshold assures that only semivariogram map values based on at least 5 point pairs are shown, removing too noisy estimation.

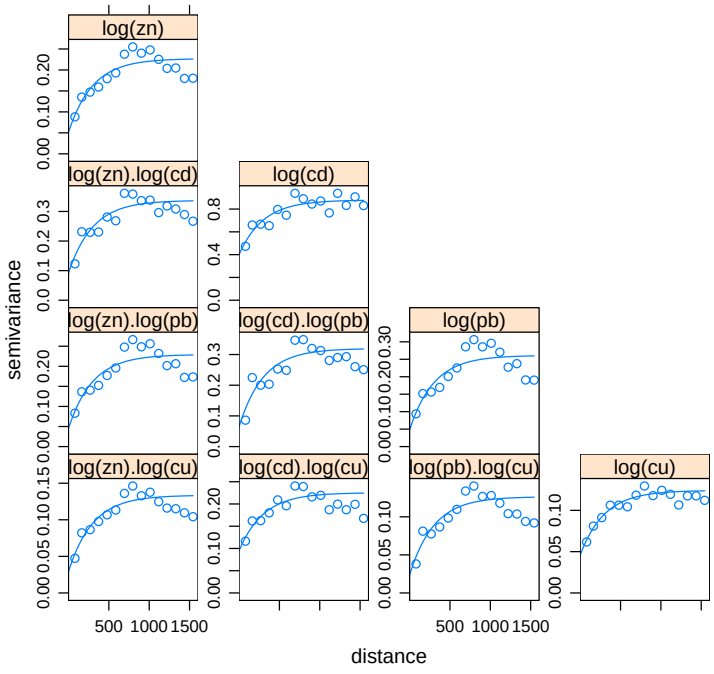
10 Cross variography

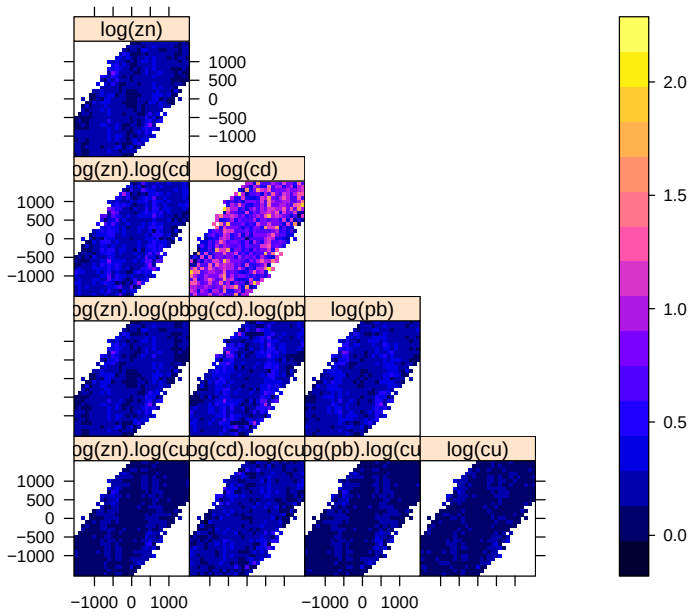
Fitting a linear model of coregionalization.

```
> g = gstat(NULL, "log(zn)", log(zinc) ~ sqrt(dist), meuse)
> g = gstat(g, "log(cd)", log(cadmium) ~ sqrt(dist), meuse)
> g = gstat(g, "log(pb)", log(lead) ~ sqrt(dist), meuse)
> g = gstat(g, "log(cu)", log(copper) ~ sqrt(dist), meuse)
> v = variogram(g)
> g = gstat(g, model = vgm(1, "Exp", 300, 1), fill.all = TRUE)
> g.fit = fit.lmc(v, g)
> g.fit

data:
log(zn) : formula = log(zinc)`~`sqrt(dist) ; data dim = 155 x 12
log(cd) : formula = log(cadmium)`~`sqrt(dist) ; data dim = 155 x 12
log(pb) : formula = log(lead)`~`sqrt(dist) ; data dim = 155 x 12
log(cu) : formula = log(copper)`~`sqrt(dist) ; data dim = 155 x 12
variograms:
                  model      psill range
log(zn)[1]          Nug 0.05141798     0
log(zn)[2]          Exp 0.17556219   300
log(cd)[1]          Nug 0.39996573     0
log(cd)[2]          Exp 0.47893816   300
```

```
log(pb)[1]            Nug 0.04770893     0
log(pb)[2]            Exp 0.21323027   300
log(cu)[1]            Nug 0.04577523     0
log(cu)[2]            Exp 0.07827374   300
log(zn).log(cd)[1]    Nug 0.09190848     0
log(zn).log(cd)[2]    Exp 0.24542024   300
log(zn).log(pb)[1]    Nug 0.04528367     0
log(zn).log(pb)[2]    Exp 0.18407011   300
log(cd).log(pb)[1]    Nug 0.06425412     0
log(cd).log(pb)[2]    Exp 0.25525359   300
log(zn).log(cu)[1]    Nug 0.02912806     0
log(zn).log(cu)[2]    Exp 0.10438748   300
log(cd).log(cu)[1]    Nug 0.09441635     0
log(cd).log(cu)[2]    Exp 0.13073936   300
log(pb).log(cu)[1]    Nug 0.02369778     0
log(pb).log(cu)[2]    Exp 0.10267516   300
```

```
> plot(v, g.fit)
> vgm.map = variogram(g, cutoff = 1500, width = 100, map = TRUE)
> plot(vgm.map, threshold = 5, col.regions = bpy.colors(), xlab = "",
+     ylab = "")
```





References

- Diggle, P.J., J.A. Tawn, R.A. Moyeed, 1998. Model-based geostatistics. Applied Statistics 47(3), pp 299-350.
- Pebesma, E.J., 2004. Multivariable geostatistics in S: the gstat package. Computers & Geosciences 30: 683-691.
- Wackernagel, H., 1998. Multivariate Geostatistics; an introduction with applications, 2nd edn., Springer, Berlin, 291 pp.