

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

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1 Introduction

The `meuse` data set provided by package `sp` is a data set comprising of four heavy metals measured in the top soil in a flood plain along the river Meuse, along with a handful of covariates. The process governing heavy metal distribution seems that polluted sediment is carried by the river, and mostly deposited close to the river bank, and areas with low elevation. This document shows a geostatistical analysis of this data set. The data set was introduced by Burrough and McDonnell, 1998.

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 specified 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 spatial sampling design optimization.

3 Spatial data frames

As an example, we will look at the `meuse` data set, which is a regular data frame that comes with package `gstat` (remove the 88 from the colour strings to make a plot without alpha transparency on windows or X11):

```
> library(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
```

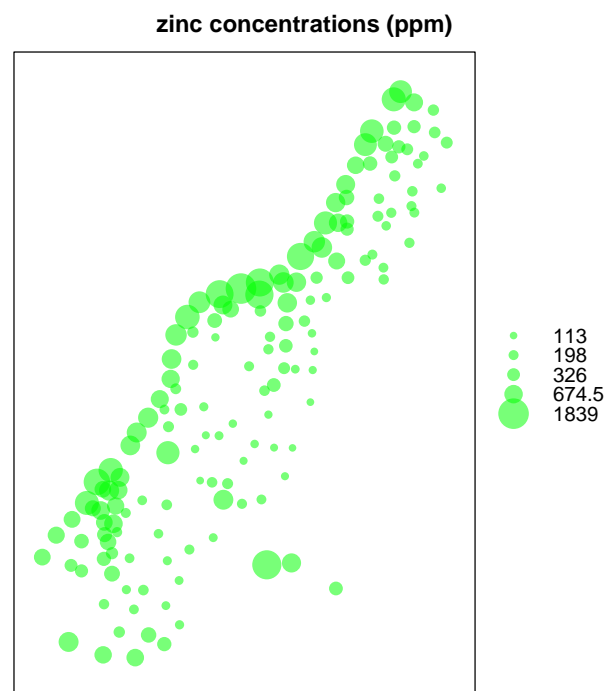
elev	dist	om	ffreq	soil	lime
Min. : 5.180	Min. : 0.00000	Min. : 1.000	1:84	1:97	0:111
1st Qu.: 7.546	1st Qu.: 0.07569	1st Qu.: 5.300	2:48	2:46	1: 44
Median : 8.180	Median : 0.21184	Median : 6.900	3:23	3:12	
Mean : 8.165	Mean : 0.24002	Mean : 7.478			
3rd Qu.: 8.955	3rd Qu.: 0.36407	3rd Qu.: 9.000			
Max. : 10.520	Max. : 0.88039	Max. : 17.000			
		NA's : 2			

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 (ppm)")
```



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.

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	1:1665	1: 779
1st Qu.:0.1193	2:1084	2:1335
Median :0.2715	3: 354	3: 989
Mean :0.2971		
3rd Qu.:0.4402		
Max. :0.9926		

```
> 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)")
> library(gstat)
> zinc.idw = idw(zinc~1, meuse, meuse.grid)

[inverse distance weighted interpolation]

> class(zinc.idw)

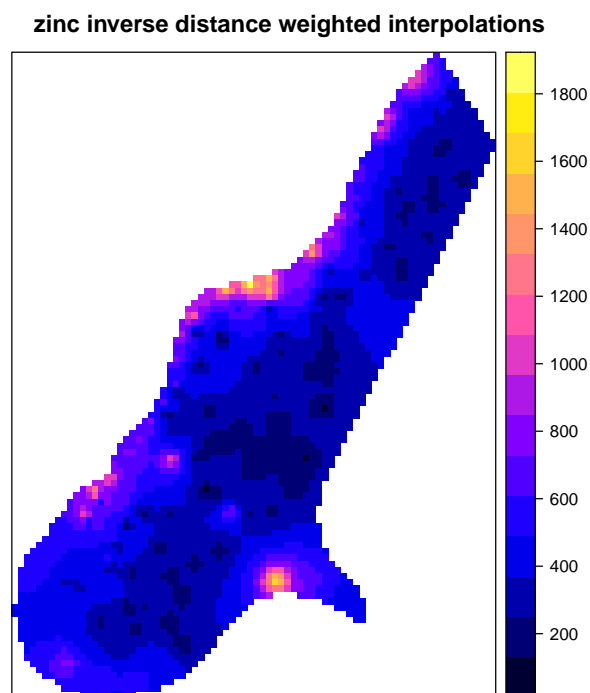
[1] "SpatialPixelsDataFrame"
attr(,"package")
[1] "sp"

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

```

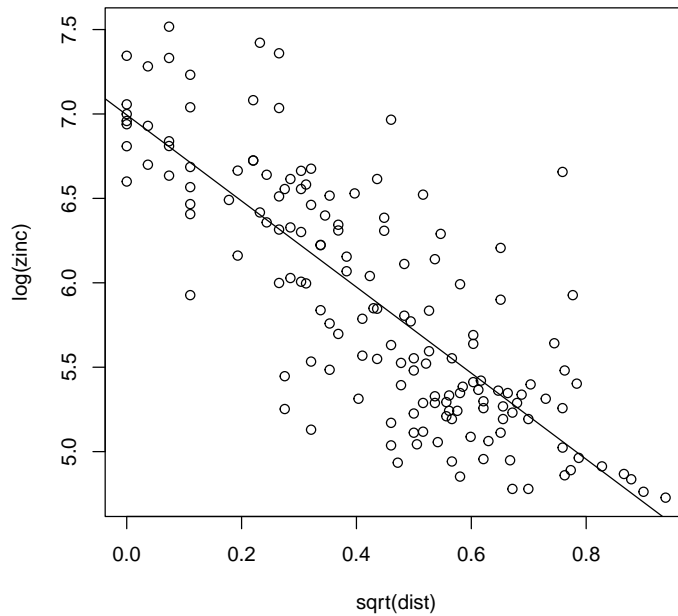
distance to river (red = 0)





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

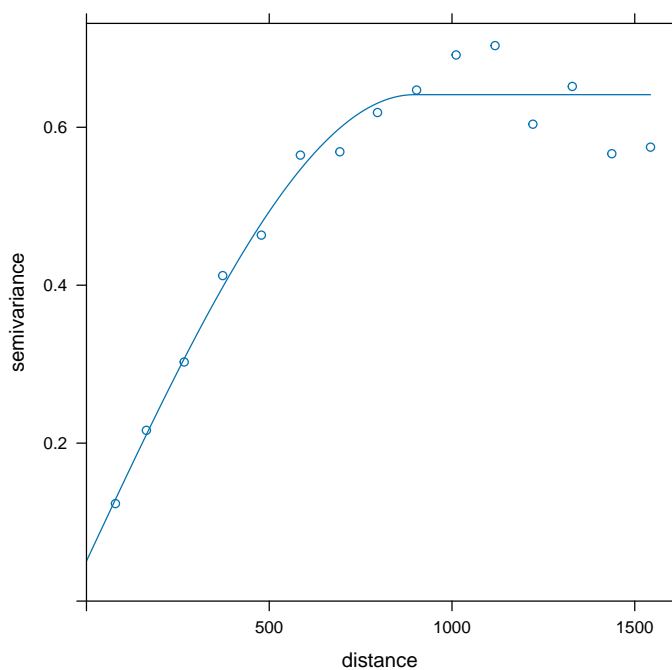
```

> 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 $\sim \text{sqrt}(\text{dist})$ as a predictor variable:

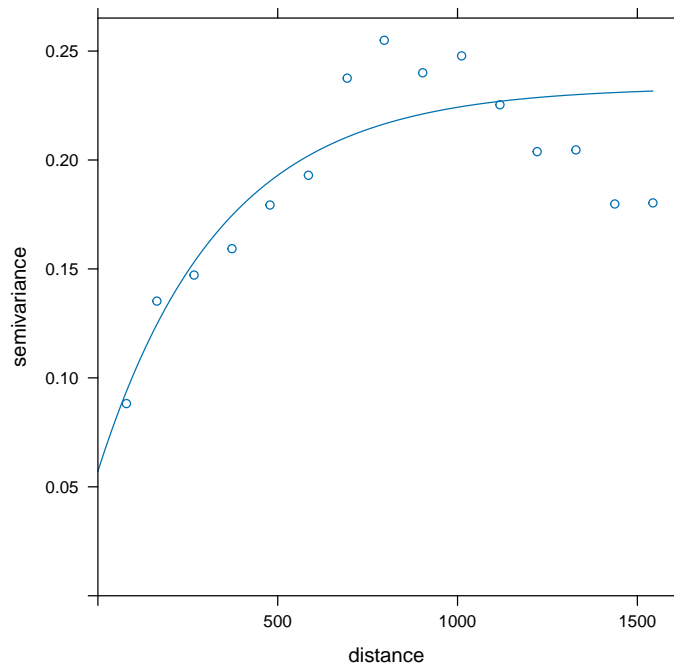
```

> 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)

```

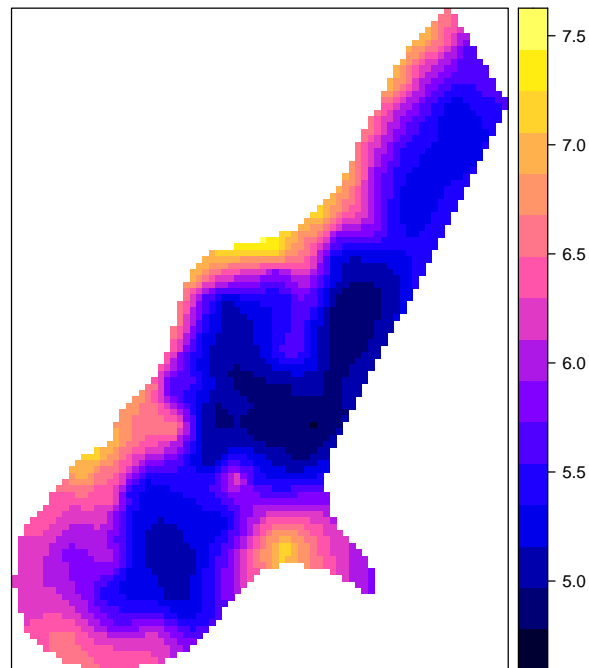
In this case, the variogram of residuals with respect to a fitted mean function are shown. Residuals were calculated using ordinary least squares.

6 Kriging

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

[using ordinary kriging]

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

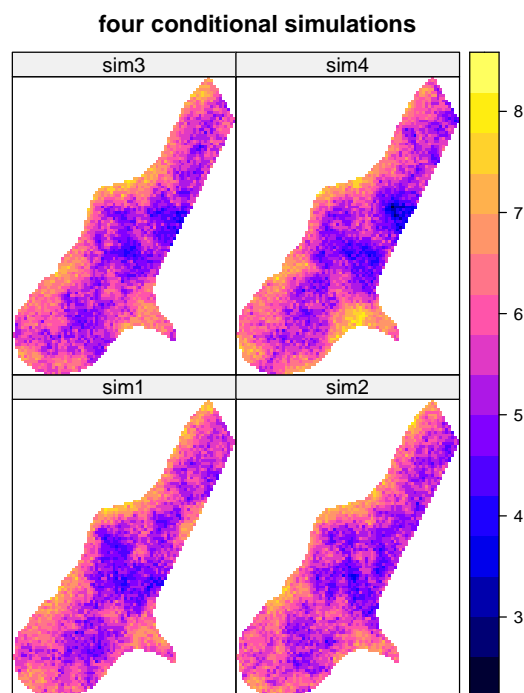


7 Conditional simulation

```
> 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 = "four conditional simulations")
```

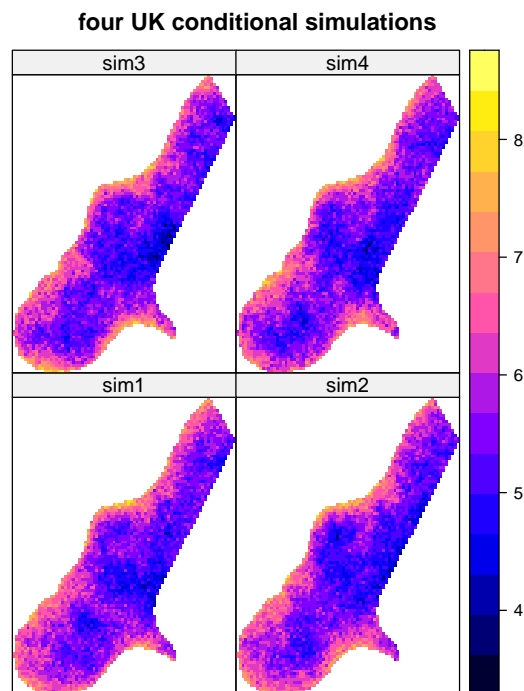


For UK/residuals:

```
> 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]

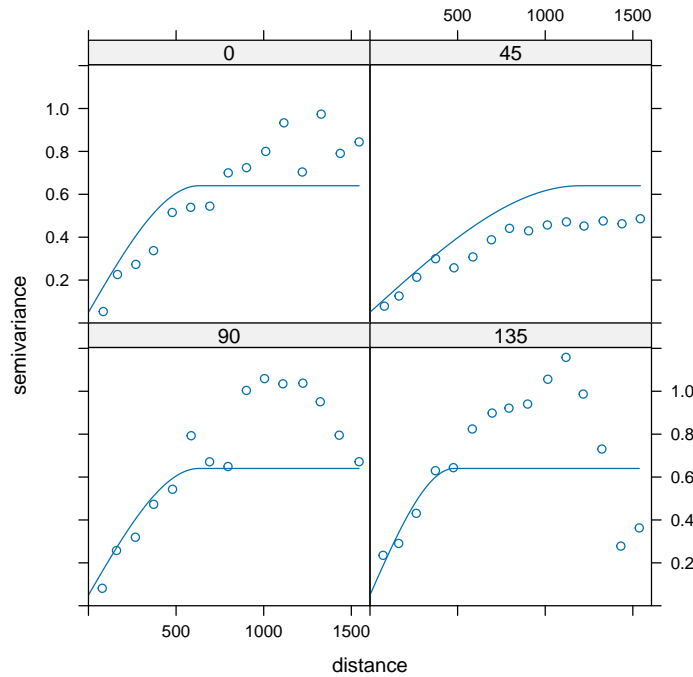
```
> spplot(lzn.condsim2, main = "four UK conditional simulations")
```



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(.59, "Sph", 1200, .05, anis = c(45, .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: $(Z(s) - Z(s + h))^2 = (Z(s + h) - Z(s))^2$.

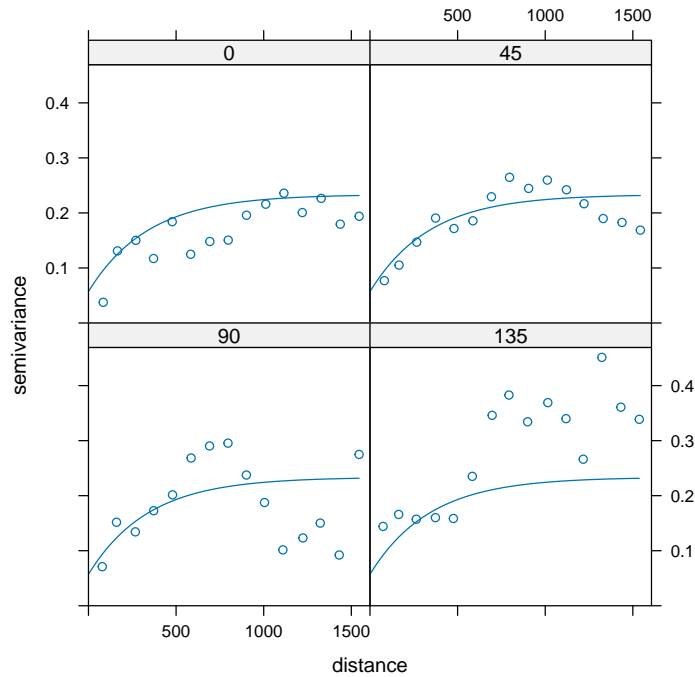
The first plot gives the variogram in the zero direction, which is North; 90 degrees is East. By default, point pairs are assigned to the directional variogram panel with their nearest direction, so North contains everything between -22.5 and 22.5 degrees (North-West to North-East). After classifying 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°), 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 dimensions, and want to further 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).

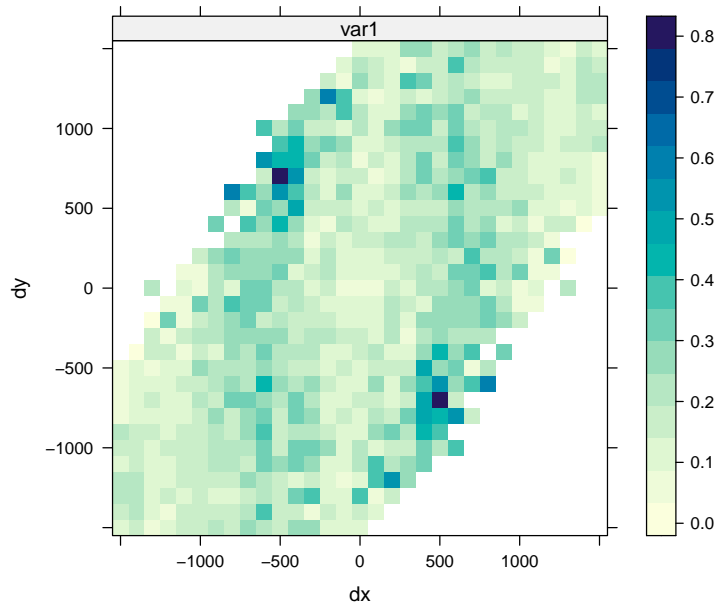
```
> lznr.dir = variogram(log(zinc)~sqrt(dist), meuse, alpha = c(0, 45, 90, 135))
> plot(lznr.dir, lznr.fit, as.table = TRUE)
```



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-dimensional 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

```

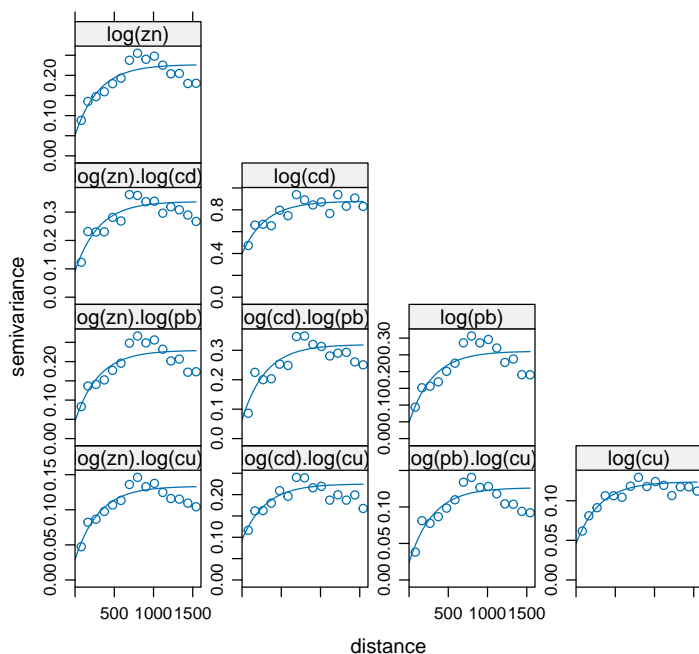
log(pb) [1]      Nug 0.04770893      0
log(pb) [2]      Exp 0.21323027    300
log(cu) [1]      Nug 0.04577523      0
log(cu) [2]      Exp 0.07827374    300
log(zn).log(cd) [1] Nug 0.09190848      0
log(zn).log(cd) [2] Exp 0.24542024    300
log(zn).log(pb) [1] Nug 0.04528367      0
log(zn).log(pb) [2] 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

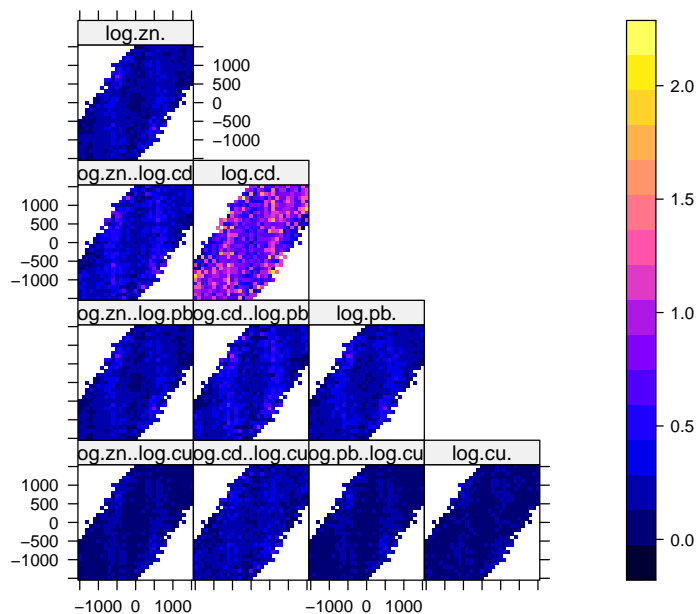
```

```

> 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

- Burrough, P.A., R.A. McDonnell, 1998. Principles of Geographical Information Systems, 2nd Edition. Oxford University Press.
- 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.