2023 554 R Notes on Mapping for Point Data

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Overview

In these notes we will consider mapping and modeling of point data in which the (nominal) exact locations are known.

We will look at modeling a spatially-indexed continuous response via:

- Conventional Kriging via MLE and variants
- A generalized additive model (GAM)
- A Bayesian approach using stochastic partial differential equations (SPDE)

Continuous Response: Motivating Example

We illustrate methods for continuous data using on Zinc levels in the Netherlands.

This data set gives locations and top soil heavy metal concentrations (in ppm), along with a number of soil and landscape variables, collected in a flood plain of the river Meuse, near the village Stein in the South of the Netherlands.

Heavy metal concentrations are bulk sampled from an area of approximately $28 \text{km} \times 39 \text{km}$.

The Meuse data are in a variety of packages. The version in the geoR library are not a spatial object, but can be used with likelihood and Bayes methods.

geoR for geostatistics

```
library(geoR)
library(sp)
library(tidyverse)
library(ggpubr)
library(viridis)
data("meuse")
```

We start the analysis using functions from the geoR library, for which a geodata data type is required. There are 155 observations (sampling locations)

```
zmat <- matrix(cbind(meuse$x, meuse$y, log(meuse$zinc)), ncol = 3, nrow = 155, byrow = F)
geozinc <- as.geodata(zmat, coords.col = c(1, 2), data.col = c(3))</pre>
```

Exploratory analysis

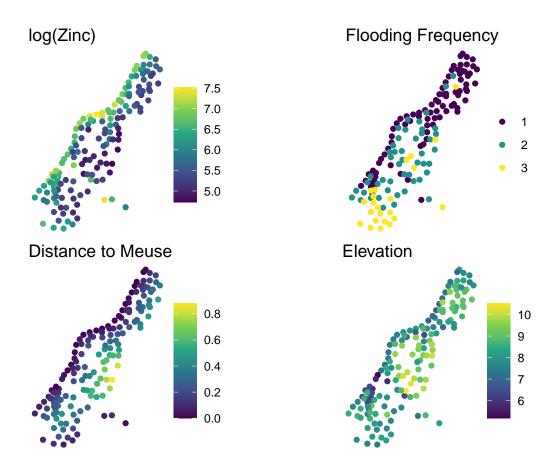
We work with log(zinc) as the distribution is more symmetric than on the original scale, and the variance more constant across levels of covariates.

It's often a good idea to do some exploratory data analysis (EDA), so let's see how log(zinc) varies by three possible covariates:

- Flooding frequency (ffreq); 1 = once in two years; 2 = once in ten years; 3 = one in 50 years
- Distance to the Meuse river (dist); normalized to [0, 1]
- Elevation (elev); relative to the local river bed, in meters.

```
par(mfrow = c(1, 3))
plot(log(meuse$zinc) ~ meuse$ffreq, ylab = "log(zinc)", xlab = "Flooding Frequency",
     col = "blue")
plot(log(meuse$zinc) ~ meuse$dist, ylab = "log(zinc)", xlab = "Scaled distance to river",
     col = "blue")
plot(log(meuse$zinc) ~ meuse$elev, ylab = "log(zinc)", xlab = "Elevation", col = "blue")
      7.5
      7.0
                                                                              7.0
                                          7.0
      6.5
                                          6.5
                                                                              6.5
  log(zinc)
                                                                          log(zinc)
                                      log(zinc)
      6.0
      5.5
                                                                              5.5
                                          5.0
      5.0
                                                                              5.0
              1
                     2
                            3
                                                  0.2 0.4
                                                           0.6
                                                                                  5
                                                                                      6
                                                                                              8
                                                                                                 9
              Flooding Frequency
                                                Scaled distance to river
                                                                                          Elevation
```

Also map these covariates.

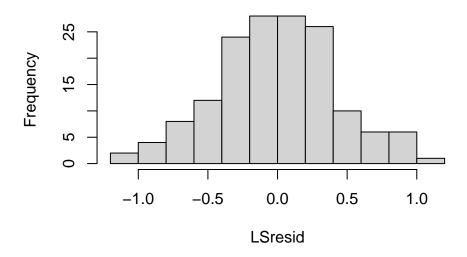


log(zinc) Variogram

First we will be assuming a spatial model on the residuals with elevation and distance in the model. Fit this initial linear model, and view the residuals by histogram and map.

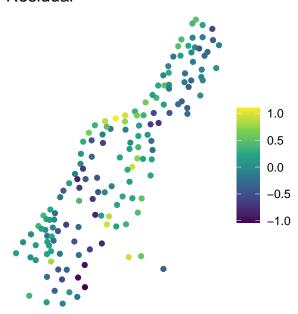
```
LSmod <- lm(log(meuse$zinc) ~ meuse$dist + meuse$elev)
LSresid <- residuals(LSmod)
hist(LSresid)
```

Histogram of LSresid



```
m.sf$resid <- LSresid
ggplot() + geom_sf(data = m.sf[, "resid"], aes(color = resid)) + theme_void() + scale_color_viridis_c()
    labs(title = "Residual", color = NULL)</pre>
```

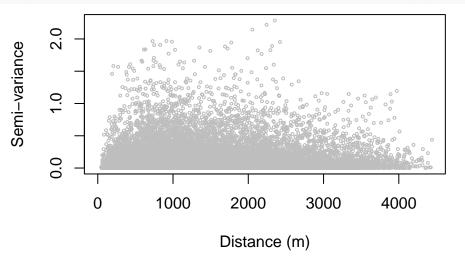
Residual



Cloud

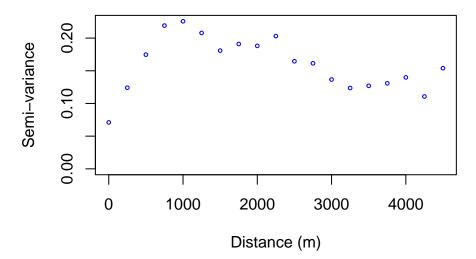
Variogram cloud for log zinc,

```
cloudzinc <- variog(geozinc, option = "cloud", trend = ~meuse$dist + meuse$elev)
## variog: computing omnidirectional variogram
plot(cloudzinc, ylab = "Semi-variance", xlab = "Distance (m)", col = "grey", cex = 0.4)</pre>
```



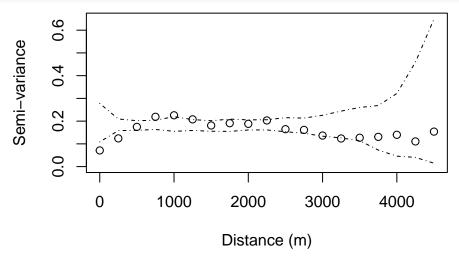
Binned variogram

```
binzinc <- variog(geozinc, uvec = seq(0, 5000, 250), trend = ~meuse$dist + meuse$elev)
## variog: computing omnidirectional variogram
plot(binzinc, ylab = "Semi-variance", xlab = "Distance (m)", cex = 0.5, col = "blue")</pre>
```



Monte Carlo envelopes under no spatial dependence - it is clear there is dependence here.

```
geozinc.env <- variog.mc.env(geozinc, obj = binzinc)
## variog.env: generating 99 simulations by permutating data values
## variog.env: computing the empirical variogram for the 99 simulations
## variog.env: computing the envelops
plot(binzinc, env = geozinc.env, xlab = "Distance (m)", ylab = "Semi-variance")</pre>
```



Parameter estimation from the variogram

We now estimate the parameters of the exponential covariance model which in geoR is parameterized as

$$\tau^2 + \sigma^2 \exp(-d/\phi)$$
,

where d is the distance between the points, σ^2 is the partial sill and τ^2 is the nugget.

The effective range is the distance at which the correlation is 0.05, and if we have a rough estimate of this \tilde{d} (from the binned variogram, for example) then we can solve for an initial estimate $\tilde{\phi} = -\tilde{d}/log(0.05)$.

Maximum likelihood for log(zinc)

We suppress the output from the call.

```
mlfit <- likfit(geozinc, ini = c(0.2, 224), trend = ~meuse$dist + meuse$elev)</pre>
```

We examine the results, specifically point estimates and standard errors.

```
mlfit$parameters.summary
##
            status values
## beta0 estimated 8.6162
## beta1 estimated -2.1072
## beta2 estimated -0.2690
## tausq estimated 0.0010
## sigmasq estimated 0.2065
## phi estimated 241.1982
## kappa
           fixed 0.5000
## psiA
            fixed 0.0000
## psiR
            fixed 1.0000
## lambda
           fixed 1.0000
for (i in 1:3) {
   cat(cbind(mlfit$beta[i], sqrt(mlfit$beta.var[i, i])), "\n")
}
## 8.616183 0.2557962
## -2.107206 0.3414008
## -0.2689692 0.02989409
mlfit$practicalRange
## [1] 722.5653
```

Note that the standard errors change from the least squares fit.

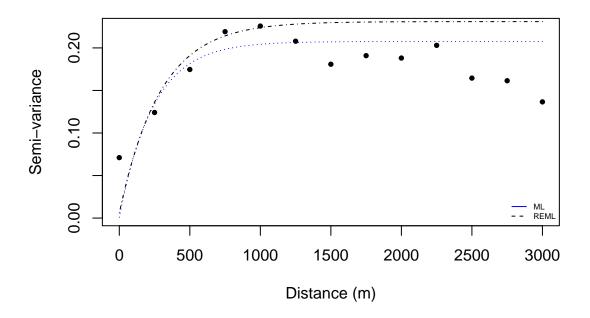
Restricted maximum likelihood for log(zinc)

```
remlfit <- likfit(geozinc, ini = c(0.55, 224), lik.method = "RML", trend = ~meuse$dist +
    meuse$elev)</pre>
```

The results: slight differences from ML.

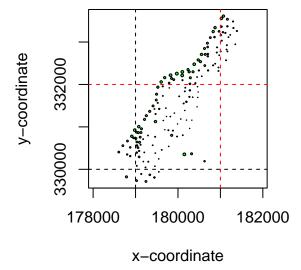
```
remlfit$parameters.summary
##
            status values
## beta0 estimated 8.6396
## beta1 estimated -2.1215
## beta2 estimated -0.2701
## tausq estimated 0.0061
## sigmasq estimated 0.2248
## phi estimated 289.1468
## kappa
           fixed 0.5000
            fixed 0.0000
## psiA
## psiR
            fixed 1.0000
             fixed 1.0000
## lambda
remlfit$practicalRange
## [1] 866.2064
```

Comparison of estimates



Prediction for log(zinc) by Kriging

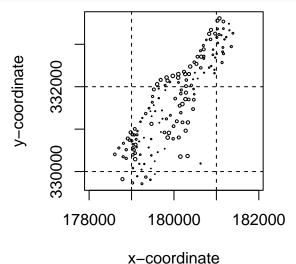
First we plot the data along with the region within which we shall carry out prediction.



We now fit a linear model in distance and elevation to log(zinc). We then form a geodata object with the residuals as the response.

```
lmfit <- lm(geozinc$data ~ meuse$dist + meuse$elev)
lmfit</pre>
```

```
## Call:
## lm(formula = geozinc$data ~ meuse$dist + meuse$elev)
## Coefficients:
## (Intercept)
                 meuse$dist
                               meuse$elev
##
        8.4845
                    -1.9600
                                  -0.2607
detrend <- as.geodata(cbind(geozinc$coords, lmfit$residuals))</pre>
points(detrend, pt.divide = "rank.prop", xlab = "x-coordinate",
    ylab = "y-coordinate", cex.min = 0.1, cex.max = 0.5)
abline(h = 330000, lty = 2)
abline(h = 332000, lty = 2)
abline(v = 179000, lty = 2)
abline(v = 181000, lty = 2)
```



Next carry out MLE on the detrended data.

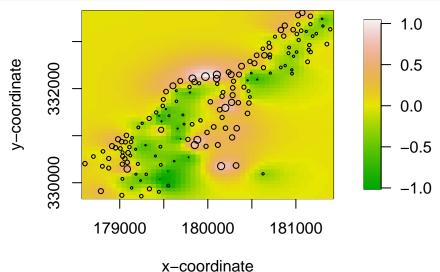
```
mlfit2 \leftarrow likfit(detrend, ini = c(0.2, 224))
## likfit: likelihood maximisation using the function optim.
## likfit: Use control() to pass additional
##
           arguments for the maximisation function.
           For further details see documentation for optim.
## likfit: It is highly advisable to run this function several
           times with different initial values for the parameters.
##
## likfit: WARNING: This step can be time demanding!
## likfit: end of numerical maximisation.
mlfit2
## likfit: estimated model parameters:
         beta
                tausq
                         sigmasq
## " 0.0306" " 0.0000" " 0.2076" "238.0914"
## Practical Range with cor=0.05 for asymptotic range: 713.2582
## likfit: maximised log-likelihood = -54.82
```

Finally, we can obtain spatial predictions on a grid, using the parameter estimates from the ML fit to the

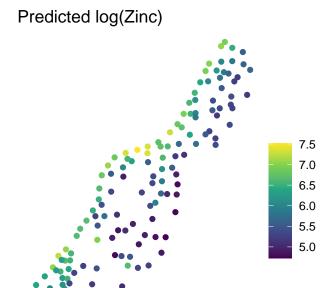
residuals. Ordinary Kriging is used for this prediction.

To view the results produce an image plot of the predictions, with the data superimposed.

```
library(fields)
image.plot(x = pred.grid[["Var1"]][1:51], y = unique(pred.grid[["Var2"]]),
    z = matrix(kc$predict, nrow = 51, ncol = 51), col = terrain.colors(100),
    xlab = "x-coordinate", ylab = "y-coordinate")
symbols(detrend$coords[, 1], detrend$coords[, 2], circles = (detrend$data -
    min(detrend$data))/1, add = T, inches = 0.04)
```



However, since we're predicting the residuals, to get back to the original task of predicting log(zinc), we can add this value back onto our predictions from lmfit, which yields the following:



Standard deviations of prediction for log(zinc)

We now plot the Kriging standard deviations of the predictions.

```
image.plot(x = pred.grid[["Var1"]][1:51], y = unique(pred.grid[["Var2"]]),
    z = matrix(sqrt(kc$krige.var), nrow = 51, ncol = 51),
    col = cm.colors(100), xlab = "x-coordinate", ylab = "y-coordinate")
points(detrend$coords[, 1], detrend$coords[, 2], cex = 0.5,
    pch = 16)
                                                                          0.45
                                                                          0.40
              y-coordinate
                    332000
                                                                          0.35
                                                                          0.30
                                                                          0.25
                                                                          0.20
                                                                          0.15
                    330000
                                                                          0.10
                            179000
                                         180000
                                                      181000
                                      x-coordinate
```

The standard deviation is smallest close to the datapoints, as expected.

Another example, using categorical flooding frequency covariate

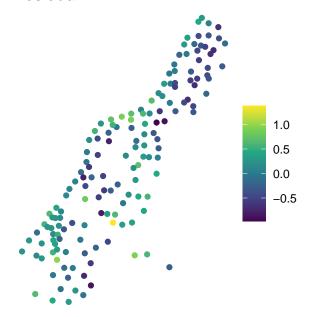
Now, we'll repeat, but use categorical flooding frequency and distance to the Meuse River as covariates.

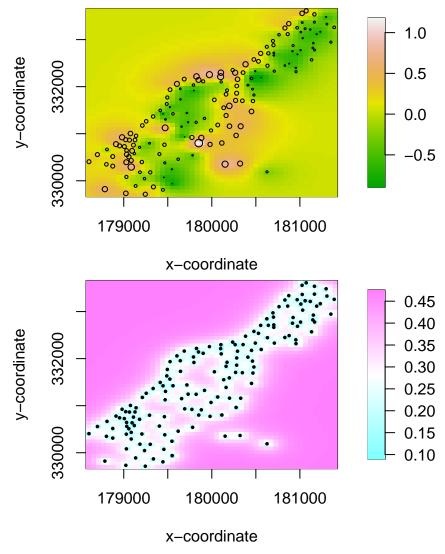
```
# repeat, using distance to Meuse and flood frequency covariates (label objects
# associated with this version with a '3')
lmfit3 <- lm(geozinc$data ~ meuse$dist + meuse$ffreq)</pre>
detrend3 <- as.geodata(cbind(geozinc$coords, lmfit3$residuals))</pre>
mlfit3 \leftarrow likfit(detrend3, ini = c(0.2, 224))
## -----
## likfit: likelihood maximisation using the function optim.
## likfit: Use control() to pass additional
           arguments for the maximisation function.
          For further details see documentation for optim.
## likfit: It is highly advisable to run this function several
          times with different initial values for the parameters.
## likfit: WARNING: This step can be time demanding!
## likfit: end of numerical maximisation.
pred.grid3 \leftarrow expand.grid(seq(178600, 181400, 1 = 51), seq(329700, 333620, 1 = 51))
kc3 <- krige.conv(detrend3, loc = pred.grid3, krige = krige.control(obj.m = mlfit3))</pre>
## krige.conv: model with constant mean
## krige.conv: Kriging performed using global neighbourhood
```

Again, map the residuals from the linear model first, then map predictions and standard deviation.

```
m.sf$resid3 <- lmfit3$residuals
ggplot() + geom_sf(data = m.sf[, "resid3"], aes(color = resid3)) + theme_void() +
    scale_color_viridis_c() + labs(title = "Residual", color = NULL)</pre>
```

Residual





Notice that there are visible differences in the predicted surface, as compared to the first model, but the standard deviation is similar in the two.

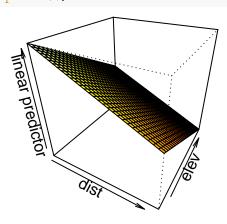
GAM model for log(zinc)

We now model the log(zinc) surface as linear in distance and elevation, and with the spatial surface modeled with a thin plate regression spline, with the smoothing parameter estimated using REML.

```
## Family: gaussian
## Link function: identity
## Formula:
## lzinc \sim s(x, y, bs = "tp") + dist + elev
## Parametric coefficients:
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 8.52282 0.30738 27.727 < 2e-16 ***
                       0.62631 -2.508 0.0134 *
             -1.57105
## dist
## elev
              -0.27677
                         0.03361 -8.235 1.71e-13 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Approximate significance of smooth terms:
          edf Ref.df
                         F p-value
## s(x,y) 22.66 26.52 6.264 <2e-16 ***
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## R-sq.(adj) = 0.833 Deviance explained = 86%
## -REML = 67.057 Scale est. = 0.087094 n = 155
```

GAM output: The fitted distance by elevation surface

```
vis.gam(gam.mod, theta = 30, phi = 30)
```



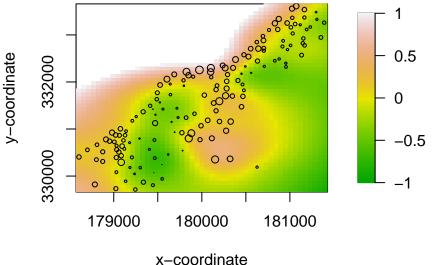
GAM prediction

```
pred.grid.gam <- expand.grid(seq(178600, 181400, 1 = 51),
    seq(329700, 333620, 1 = 51))

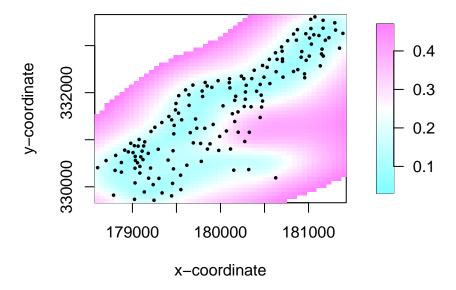
pred.dat.gam <- data.frame(x = pred.grid.gam[, 1],
    y = pred.grid.gam[, 2], dist = mean(meuse$dist),
    elev = mean(meuse$elev))

zinc.pred.gam <- predict.gam(gam.mod, pred.dat.gam,
    type = "terms")[, 3]

zinc.pred.gam.sd <- predict.gam(gam.mod, se.fit = T,</pre>
```



Standard deviations of prediction from GAM



Meuse analysis using geostat functions

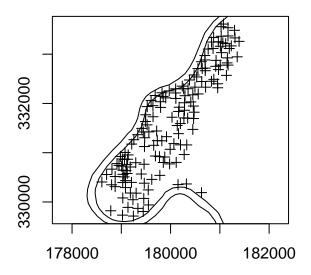
The sp package functions can make full use of the GIS capabilities of R more readily.

```
pal <- function(n = 9) {
    brewer.pal(n, "Reds")
}

data(meuse)
coords <- SpatialPoints(meuse[, c("x", "y")])
meuse1 <- SpatialPointsDataFrame(coords, meuse)
data(meuse.riv)
river_polygon <- Polygons(list(Polygon(meuse.riv)),
    ID = "meuse")
rivers <- SpatialPolygons(list(river_polygon))
coordinates(meuse) = ~x + y</pre>
```

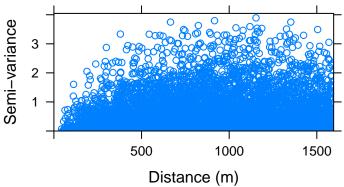
Zinc: Sampling locations

```
plot(meuse1, axes = T)
plot(rivers, add = T)
```



log(zinc): Variogram cloud, no trend removed

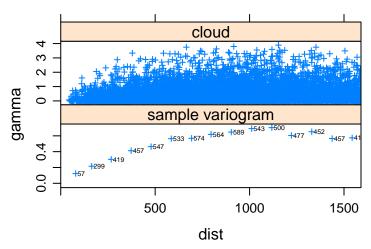
```
library(gstat)
cld <- variogram(log(zinc) ~ 1, meuse, cloud = TRUE)
plot(cld, ylab = "Semi-variance", xlab = "Distance (m)")</pre>
```



More variograms, with sample sizes

```
xlim = c(0, 1590),
cex = .5, pch = 3
)
```

More variograms

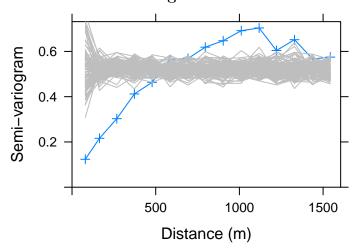


Monte Carlo simulations of semi-variogram

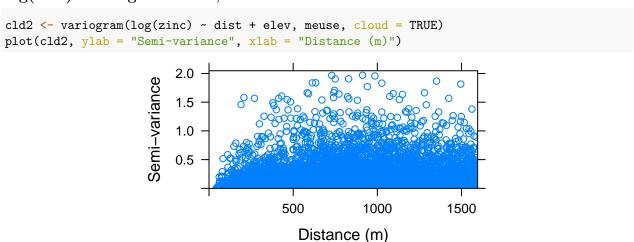
We simulate 100 datasets with random relabeling of points, and then form variograms for each.

```
v <- variogram(log(zinc) ~ 1, meuse)
plot(v, type = "b", pch = 3, xlab = "Distance (m)",
    ylab = "Semi-variance")
fn = function(n = 100) {
    for (i in 1:n) {
        meuse$random = sample(meuse$zinc)
        v = variogram(log(random) ~ 1, meuse)
        trellis.focus("panel", 1, 1, highlight = FALSE)
        llines(v$dist, v$gamma, col = "grey")
        trellis.unfocus()
    }
}
fn()</pre>
```

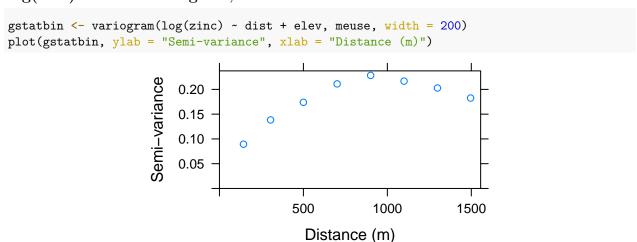
Monte Carlo simulations of semi-variogram



log(zinc): Variogram cloud, detrended



log(zinc): Binned variogram, detrended



Zinc: Directional variogram with linear trend removed

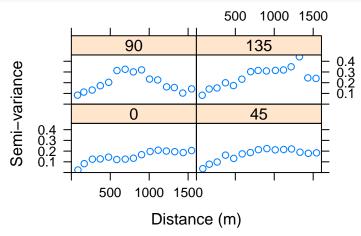
We form 4 variograms with data taken from different directions, with 0 and 90 corresponding to north and east, respectively.

Note that 0 is the same as 180.

```
dircld <- variogram(log(zinc) ~ dist + elev, meuse, alpha = c(0, 45, 90, 135))
```

Zinc: Directional variogram with linear trend removed

```
plot(dircld, xlab = "Distance (m)", ylab = "Semi-variance")
```

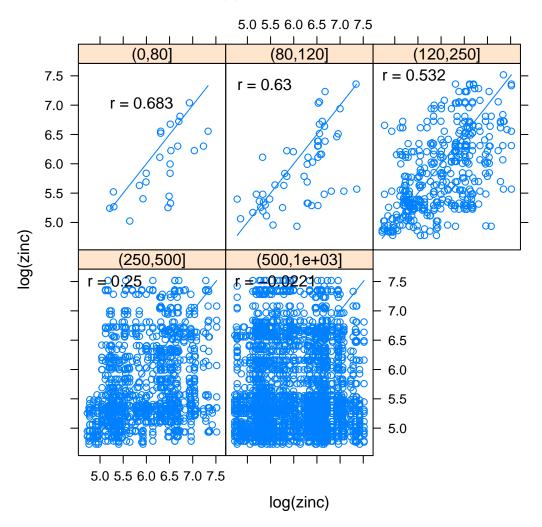


Zinc: Lagged scatterplots

We examine scatterplots of points within different distances of each other. This is another way of assessing whether spatial dependence exists.

```
hscat(log(zinc) \sim 1, meuse, c(0, 80, 120, 250, 500, 1000), cex = 0.1)
```

lagged scatterplots



Other capabilities in gstat

See

- $\bullet\,$ fit.variogram for estimation from the variogram
- krige (and associated functions) for Kriging,
- vgm generates variogram models

SPDE model

Next we illustrate kriging via SPDE using data on log(zinc) levels in the meuse dataset.

```
library(INLA)
zincdf = data.frame(y = log(meuse$zinc), locx = meuse$x,
    locy = meuse$y, dist = meuse$dist, elev = meuse$elev)
```

Mesh construction

The mesh is the discretization of the domain (study area). The domain is divided up into small triangles.

Can use the function meshbuilder() to learn about mesh construction.

The function inla.mesh.2d() requires at least 2 of the following 3 arguments to run

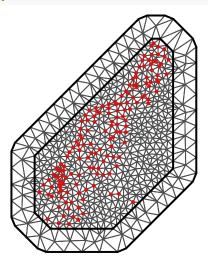
- loc or loc.domain: the function requires informations about the spatial domain given by spatial points or given by the domain extent.
- max.edge: the maximum edge length must be specified. If it is a two-dimensional vector then the first component is for the internal and the second for the part outside the boundary. Note that it uses the same scale unit as the coordinates.

Optional arguments:

- offset: specifies how much the domain will be extended in the outer and inner part. If negative it is interpreted as a factor relative to the approximate data diameter. If positive it is the extension distance on same scale unit to the coordinates provided.
- cutoff: it specifies the minimum distance allowed between points. It means that if the distance between two points is less than the supplied value then they are replaced by a single vertex. It is very useful in case of clustered data points because it avoids building many small triangles arround clustered points.
- min.angle: it specifies the minimum internal angle of the triangles. This could be a two-dimensional vector with the same meaning as previously. We would like to have a mesh with triangles as regular as possible.

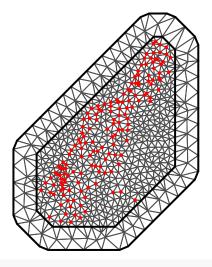
By specifying loc we obtain a mesh with observations lying at the vertices.

```
max.edge = 200
mesh <- inla.mesh.2d(loc = zincdf[, c("locx", "locy")], offset = c(100, 500), max.edge = c(max.edge,
    max.edge * 3))
plot(mesh, asp = 1, main = "")
points(zincdf[, c("locx", "locy")], col = "red", cex = 0.4)</pre>
```



We visualize the mesh below.

```
plot(mesh, asp = 1, main = "")
points(zincdf[, c("locx", "locy")], col = "red", cex = 0.5, pch = 16)
```



```
# axis(1); axis(2)
```

To connect the measurement locations to the mesh representation, the A-matrix is needed. We create the A-matrix below.

The observed data lie on the vertices.

We now create *the stack*. The stack is a complicated way of supplying the data (and covariates and effects) to INLA. For more complex spatial models, the stack is incredibly helpful, as the alternative is worse (you would have to construct the total model A matrix by hand). The stack allows different matrices to be combined (in more complex problems).

```
Xcov = data.frame(intercept = 1, dist = zincdf$dist,
        elev = zincdf$elev)
# - expands the factor covariates
Xcov = as.matrix(Xcov)
colnames(Xcov)
## [1] "intercept" "dist" "elev"
```

See ?inla.stack for lots of examples of the flexibility.

```
# - second is for 'fixed effects'
)
```

The name s is arbitrary, but it must correspond to the letter we use in the formula (later).

We specify PC priors for the spatial SD and the spatial range.

Now we specify the model – the intercept is in Xcov so we use -1 in the formula.

We finally fit the SPDE model below.

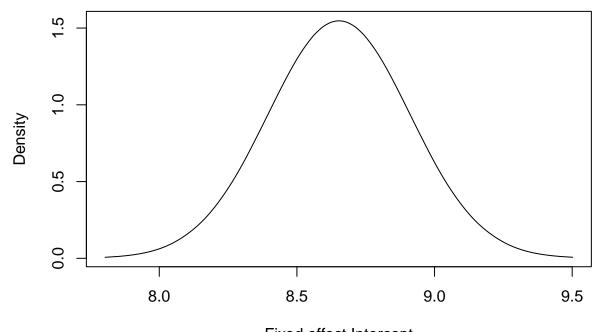
See ?inla.spde2.result for extracting results.

```
summary(res)
##
## Call:
      c("inla.core(formula = formula, family = family, contrasts = contrasts,
##
##
      ", " data = data, quantiles = quantiles, E = E, offset = offset, ", "
      scale = scale, weights = weights, Ntrials = Ntrials, strata = strata,
##
##
      ", " lp.scale = lp.scale, link.covariates = link.covariates, verbose =
##
      verbose, ", " lincomb = lincomb, selection = selection, control.compute
##
      = control.compute, ", " control.predictor = control.predictor,
##
      control.family = control.family, ", " control.inla = control.inla,
      control.fixed = control.fixed, ", " control.mode = control.mode,
##
      control.expert = control.expert, ", " control.hazard = control.hazard,
##
      control.lincomb = control.lincomb, ", " control.update =
##
##
      control.update, control.lp.scale = control.lp.scale, ", "
##
      control.pardiso = control.pardiso, only.hyperparam = only.hyperparam,
##
      ", " inla.call = inla.call, inla.arg = inla.arg, num.threads =
##
      num.threads, ", " blas.num.threads = blas.num.threads, keep = keep,
      working.directory = working.directory, ", " silent = silent, inla.mode
##
```

```
= inla.mode, safe = FALSE, debug = debug, ", " .parent.frame =
##
      .parent.frame)")
## Time used:
      Pre = 1.57, Running = 0.402, Post = 0.0194, Total = 1.99
## Fixed effects:
          mean
                 sd 0.025quant 0.5quant 0.975quant mode kld
## Xcov1 8.653 0.258 8.148
                                8.653
                                            9.158 8.653
## Xcov2 -2.147 0.370
                         -2.872 -2.147
                                            -1.422 -2.147
## Xcov3 -0.270 0.031
                       -0.331 -0.270
                                           -0.209 -0.270 0
## Random effects:
## Name
           Model
##
      s SPDE2 model
## Model hyperparameters:
                                            mean
                                                      sd 0.025quant 0.5quant
## Precision for the Gaussian observations 29.601 11.214
                                                            14.584
                                                                    27.316
## Range for s
                                         673.355 172.690
                                                            387.028 655.890
## Stdev for s
                                           0.424 0.062
                                                              0.316
                                                                      0.419
##
                                          0.975quant mode
                                             57.87 23.277
## Precision for the Gaussian observations
## Range for s
                                            1062.85 624.084
## Stdev for s
                                               0.56 0.408
## Marginal log-Likelihood: -81.11
## is computed
## Posterior summaries for the linear predictor and the fitted values are computed
## (Posterior marginals needs also 'control.compute=list(return.marginals.predictor=TRUE)')
print("MLE SE BAYES SD")
## [1] "MLE SE BAYES SD"
for (i in 1:3) {
   cat(cbind(mlfit$beta[i], sqrt(mlfit$beta.var[i, i])), res$summary.fixed[i, 1],
       res$summary.fixed[i, 2], "\n")
}
## 8.616183 0.2557962 8.65295 0.2578743
## -2.107206 0.3414008 -2.146916 0.3699748
## -0.2689692 0.02989409 -0.2701416 0.03098174
```

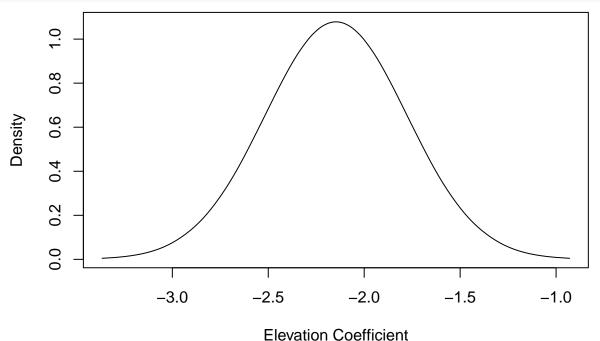
Visual summarization

```
tmp = inla.tmarginal(function(x) x, res$marginals.fixed[[1]])
plot(tmp, type = "1", xlab = "Fixed effect Intercept", ylab = "Density")
```



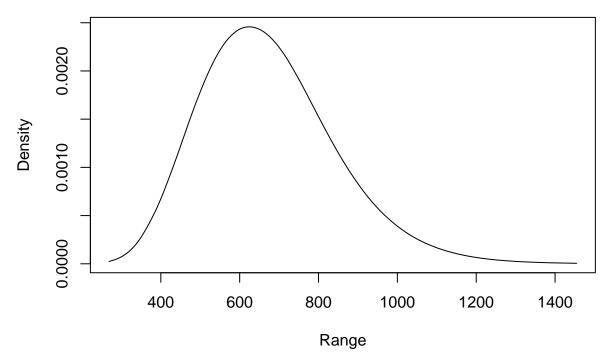
Fixed effect Intercept

```
tmp = inla.tmarginal(function(x) x, res$marginals.fixed[[2]])
plot(tmp, type = "l", xlab = "Elevation Coefficient", ylab = "Density")
```



We plot summaries of the marginal posteriors for hyperparameters below.

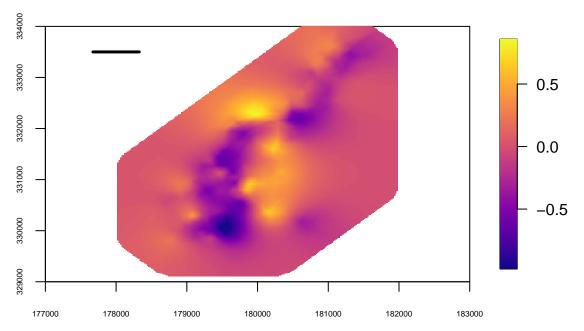
```
range = inla.tmarginal(function(x) x, res$marginals.hyperpar[[2]])
plot(range, type = "l", xlab = "Range", ylab = "Density")
```



We define a function for plotting spatial fields for this application.

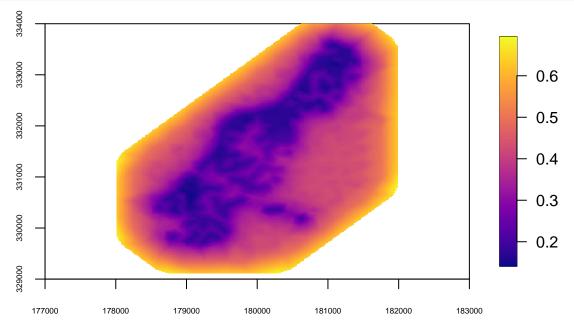
We now plot the predictive mean of the spatial field.

```
local.plot.field(res$summary.random[["s"]][["mean"]], mesh, cex.axis = 0.5)
lines(178000 + c(-0.5, 0.5) * (res$summary.hyperpar[2, "0.5quant"]), c(333500, 333500),
    lwd = 3) # add on the estimated range
```



We now plot the predictive standard deviation of the spatial field.

local.plot.field(res\$summary.random\$s\$sd, mesh, cex.axis = 0.5)



And finally, we plot the fitted values.

Fitted values

