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.

Meuse analysis using geostat functions

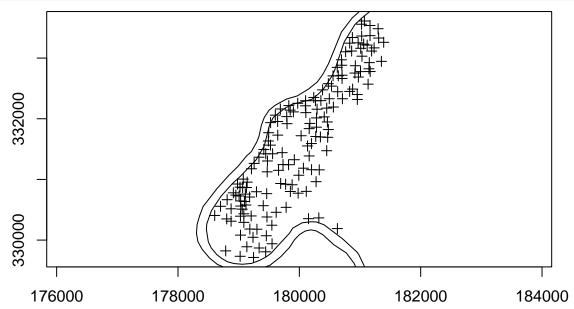
We look at the sampling locations and then examine variograms.

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

pal <- function(n = 9) {
    brewer.pal(n, "Reds")
}
data(meuse)</pre>
```

Zinc: Sampling locations

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



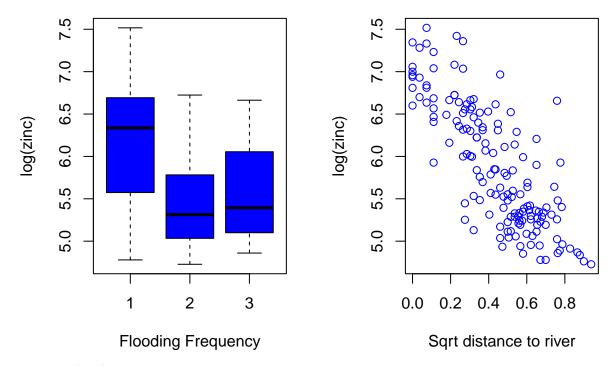
Exploratory analysis

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 two possible covariates:

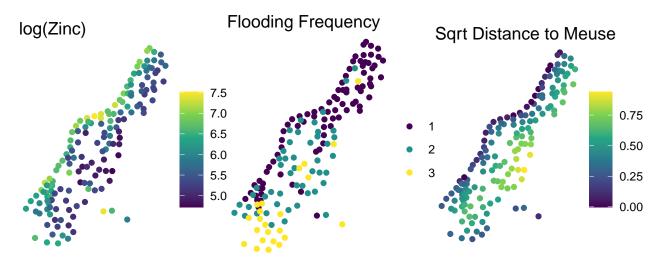
- Flooding frequency (ffreq); 1 = once in two years; 2 = once in ten years; 3 = one in 50 years
- Distance to the Meuse river (dist); normalized to [0, 1]

We focus on these, since they are available across the study region and so can be used for prediction. Following previous authors, we take sqrt(dist) which is closer to linearity.



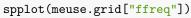
Also map log(zinc) and these covariates.

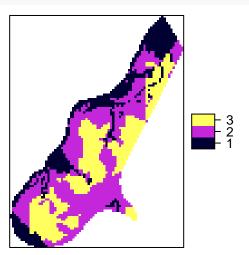
```
m.sf <- sf::st_as_sf(meuse, coords = c("x",</pre>
    "y"))
m.sf$logzinc <- log(m.sf$zinc)</pre>
m.sf$sdist <- sqrt(m.sf$dist)</pre>
a <- ggplot() + geom_sf(data = m.sf[, "logzinc"],</pre>
    aes(color = logzinc)) + theme_void() +
    scale_color_viridis_c() + labs(title = "log(Zinc)",
    color = NULL)
b <- ggplot() + geom_sf(data = m.sf[, "ffreq"],</pre>
    aes(color = ffreq)) + theme_void() +
    scale_color_viridis(discrete = T) + labs(title = "Flooding Frequency",
    color = NULL)
c <- ggplot() + geom_sf(data = m.sf[, "sdist"],</pre>
    aes(color = sdist)) + theme_void() +
    scale_color_viridis_c() + labs(title = "Sqrt Distance to Meuse",
    color = NULL)
ggpubr::ggarrange(a, b, c, nrow = 1, ncol = 3)
```



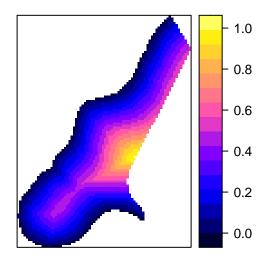
These two covariates are also available for a grid, in the meuse.grid data object. We will make use of this when we get to making predictions. Load in meuse.grid and take a look at the grid covariates.

```
library(sp)
data(meuse.grid)
coordinates(meuse.grid) = ~x + y
proj4string(meuse.grid) <- CRS("+init=epsg:28992")
gridded(meuse.grid) = TRUE</pre>
```



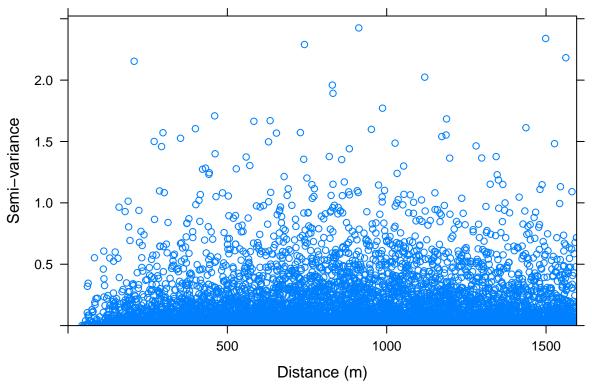


spplot(meuse.grid["dist"])

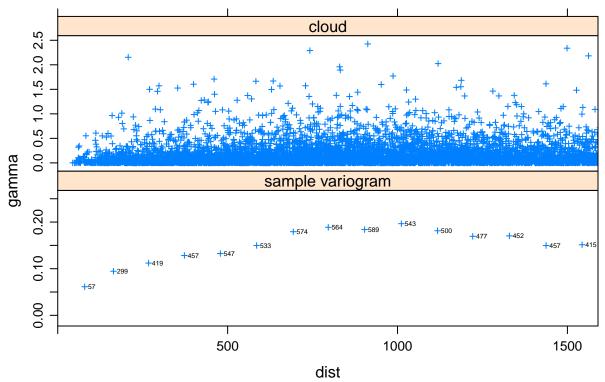


log(zinc): Variogram cloud, trend removed

```
library(gstat)
cld <- variogram(log(zinc) ~ sqrt(meuse$dist) +
    as.factor(meuse$ffreq), meuse, cloud = TRUE)
plot(cld, ylab = "Semi-variance", xlab = "Distance (m)")</pre>
```



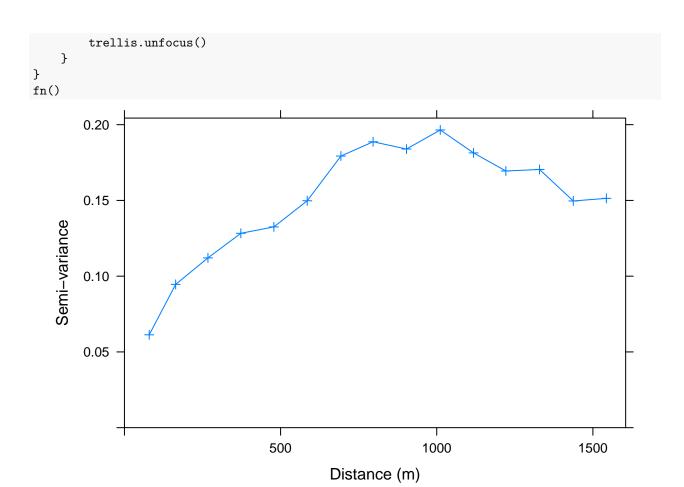
More variograms, with sample sizes



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) ~ sqrt(meuse$dist) +
    as.factor(meuse$ffreq), 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")</pre>
```



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

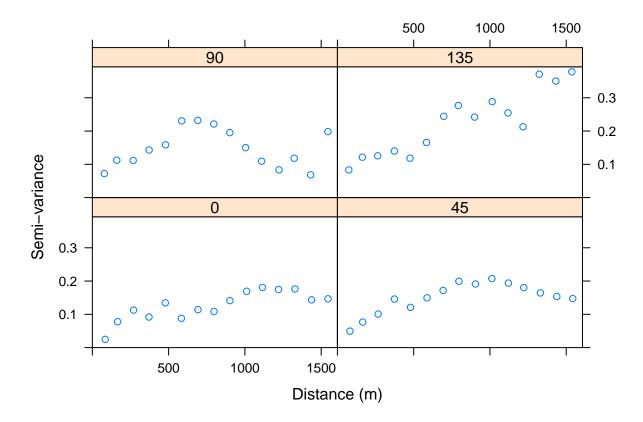
Directional variogram with linear trend removed

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) ~ sqrt(meuse$dist) +
    as.factor(ffreq), meuse, alpha = c(0,
    45, 90, 135))

plot(dircld, xlab = "Distance (m)", ylab = "Semi-variance")</pre>
```



Other capabilities in gstat

See

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

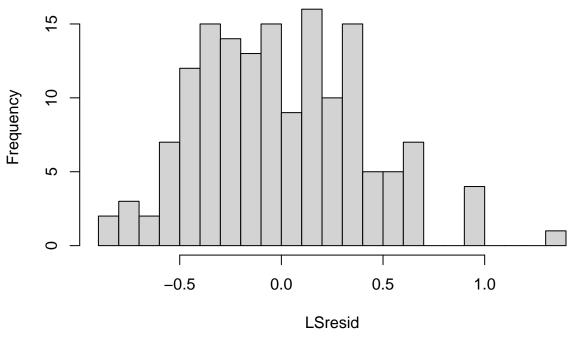
geoR for geostatistics

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

First we will be assuming a spatial model on the residuals with ffreq and sqrt(dist) in the model. Fit this initial linear model, and view the residuals by histogram and map.

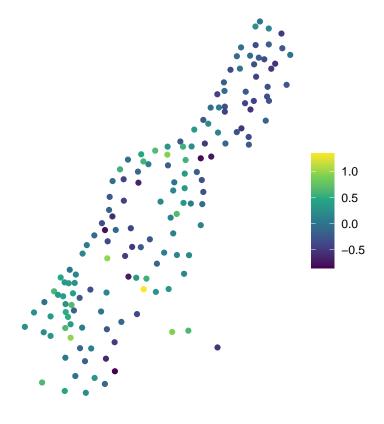
```
LSmod <- lm(log(meuse$zinc) ~ sqrt(meuse$dist) +
    as.factor(meuse$ffreq))
LSresid <- residuals(LSmod, type = "pearson")
hist(LSresid, nclass = 25)</pre>
```

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 = "Residuals from Linear Model",
    color = NULL)</pre>
```

Residuals from Linear Model



Moran's I

We can calculate Moran's I to see the strength of spatial dependence in the residuals. Our results show that we can reject the null hypothesis that there is zero spatial autocorrelation present in LSresid at the $\alpha=0.05$ level.

```
library(ape)
dists <- as.matrix(dist(cbind(geozinc[1]$coords[,</pre>
    1], geozinc[1]$coords[, 2])))
dists.inv <- 1/dists</pre>
diag(dists.inv) <- 0</pre>
dists.inv[1:5, 1:5]
               1
                                         3
## 1 0.000000000 0.014116748 0.008414063 0.003857440 0.002729898
## 2 0.014116748 0.000000000 0.007063831 0.003535423 0.002757553
## 3 0.008414063 0.007063831 0.000000000 0.006984644 0.003983684
## 4 0.003857440 0.003535423 0.006984644 0.000000000 0.006482446
## 5 0.002729898 0.002757553 0.003983684 0.006482446 0.000000000
Moran.I(LSresid, dists.inv)
## $observed
## [1] 0.1210698
##
## $expected
## [1] -0.006493506
##
## $sd
## [1] 0.01060145
```

```
##
## $p.value
## [1] 0
```

Maximum likelihood for log(zinc)

We fit with the Matern covariance model with

$$\rho(h) = \frac{1}{2^{\kappa - 1} \Gamma(\kappa)} \left(\frac{h}{\phi} \right)^{\kappa} K_{\kappa} \left(\frac{h}{\phi} \right),$$

where h is the distance between 2 points and we take $\kappa = 0.5$ so that ϕ is the only estimated parameter. The other parameters estimated are τ^2 , the nugget, and σ^2 , the spatial variance. The practical range reported is the distance at which the correlations drop to 0.05, and is a function of ϕ .

We suppress the output from the call.

```
mlfit <- likfit(geozinc, cov.model = "matern",
    ini = c(0.2, 224), trend = ~sqrt(meuse$dist) +
        as.factor(meuse$ffreq))</pre>
```

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

```
mlfit$parameters.summary
##
              status
                       values
## beta0
                       7.0712
           estimated
           estimated -2.1208
## beta1
## beta2
           estimated -0.5154
           estimated -0.5266
## beta3
## tausq
           estimated
                      0.0372
## sigmasq estimated
                     0.1316
           estimated 300.5381
## phi
## kappa
               fixed
                       0.5000
## psiA
               fixed
                       0.0000
               fixed
## psiR
                       1.0000
## lambda
               fixed
                       1.0000
for (i in 1:3) {
    cat(cbind(mlfit$beta[i], sqrt(mlfit$beta.var[i,
        i])), "\n")
}
## 7.071249 0.1326244
## -2.120796 0.2365602
## -0.5153624 0.06780136
mlfit$practicalRange
## [1] 900.3318
```

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

Restricted maximum likelihood for log(zinc)

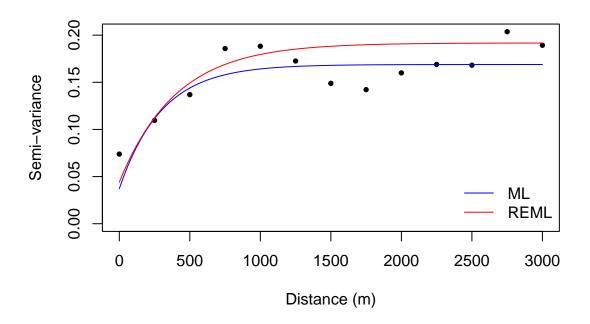
Restricted MLE is preferable in general for estimation when there are variance parameters.

```
remlfit <- likfit(geozinc, cov.model = "matern",
    ini = c(0.55, 224), lik.method = "RML",
    trend = ~sqrt(meuse$dist) + as.factor(meuse$ffreq))</pre>
```

The results show slight differences from ML.

```
remlfit$parameters.summary
    status values
## beta0 estimated 7.0823
## beta1 estimated -2.1109
## beta2 estimated -0.5280
## beta3 estimated -0.5455
## tausq estimated 0.0442
## sigmasq estimated 0.1476
## phi estimated 401.4313
## kappa fixed 0.5000
## psiA
            fixed 0.0000
## psiR
            fixed 1.0000
## lambda
            fixed 1.0000
remlfit$practicalRange
## [1] 1202.581
for (i in 1:3) {
   cat(cbind(mlfit$beta[i], sqrt(mlfit$beta.var[i,
       i]), remlfit$beta[i], sqrt(remlfit$beta.var[i,
       i])), "\n")
}
## 7.071249 0.1326244 7.082279 0.1527493
## -2.120796 0.2365602 -2.110917 0.2515499
## -0.5153624 0.06780136 -0.5280202 0.06913553
```

Comparison of estimates



Prediction for log(zinc) by Kriging

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.

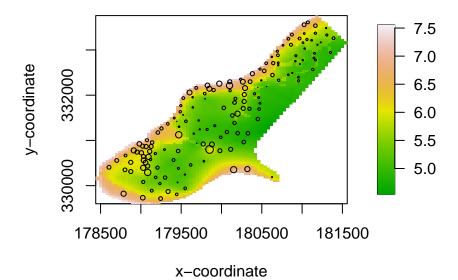
```
lmdata <- data.frame(logzinc = geozinc$data,</pre>
    sqrtdist = sqrt(meuse$dist), ffreq = as.factor(meuse$ffreq))
lmfit <- lm(logzinc ~ sqrtdist + ffreq, data = lmdata)</pre>
lmfit
##
## Call:
## lm(formula = logzinc ~ sqrtdist + ffreq, data = lmdata)
## Coefficients:
## (Intercept)
                   sqrtdist
                                   ffreq2
                                                ffreq3
                    -2.2660
                                  -0.3605
                                               -0.3167
detrend <- as.geodata(cbind(geozinc$coords,</pre>
    lmfit$residuals))
likfit(geozinc, ini = c(1000, 50))
## 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.
## likfit: estimated model parameters:
##
          beta
                               sigmasq
                    tausq
       6.6360" " 0.0347" "
                              1.8478" "2142.6170"
## Practical Range with cor=0.05 for asymptotic range: 6418.707
```

```
##
## likfit: maximised log-likelihood = -99.13
```

We can obtain spatial predictions on a grid, using the parameter estimates from the ML fit.

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:

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

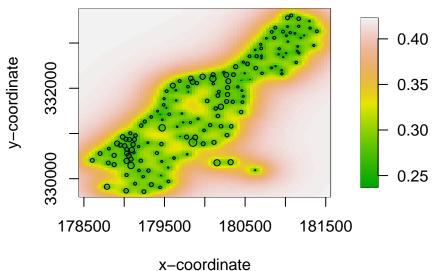


```
# library(sf) df <- st_as_sf(zinc.dat,
# coords=c('x', 'y')) ggplot() + geom_sf(data =
# df, col = 'black', fill = NA) + theme_bw() +
# coord_sf() + xlab('') + ylab('') +
# theme(legend.title = element_blank(),
# panel.grid = element_blank(), panel.border =
# element_blank(), axis.ticks = element_blank(),
# axis.text = element_blank())</pre>
```

Standard deviations of prediction for log(zinc)

We now plot the Kriging standard deviations of the predictions.

```
image.plot(x = unique(pred.grid[["Var1"]]), y = unique(pred.grid[["Var2"]]),
    z = matrix(sqrt(kc$krige.var), nrow = 78, ncol = 104),
    col = terrain.colors(100), xlab = "x-coordinate",
    ylab = "y-coordinate")
symbols(detrend$coords[, 1], detrend$coords[, 2], circles = (detrend$data -
    min(detrend$data))/1, add = T, inches = 0.04)
```



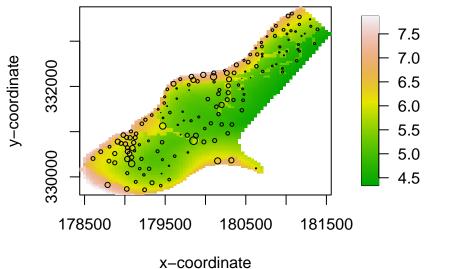
The standard deviation is smallest close to the datapoints, as expected.

GAM model for log(zinc)

We now model the log(zinc) surface as linear in the square root of distance to the Meuse and flooding frequency, and with the spatial surface modeled with a thin plate regression spline, with the smoothing parameter estimated using REML.

```
library(mgcv)
library(lattice)
library(latticeExtra)
library(RColorBrewer)
zinc.dat <- data.frame(x = meuse$x, y = meuse$y, lzinc = log(meuse$zinc),</pre>
    sqrtdist = sqrt(meuse$dist), ffreq = as.factor(meuse$ffreq))
gam.mod \leftarrow gam(lzinc \sim s(x, y, bs = "tp") + sqrtdist +
   ffreq, data = zinc.dat, method = "REML")
summary(gam.mod)
##
## Family: gaussian
## Link function: identity
##
## Formula:
## lzinc \sim s(x, y, bs = "tp") + sqrtdist + ffreq
## Parametric coefficients:
             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 6.9831 0.1522 45.869 < 2e-16 ***
## sqrtdist -1.8917 0.3496 -5.411 2.87e-07 ***
              -0.5879 0.0721 -8.154 2.43e-13 ***
## ffreq2
                       0.1129 -5.530 1.66e-07 ***
## ffreq3
              -0.6241
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Approximate significance of smooth terms:
## edf Ref.df F p-value
## s(x,y) 19.27 24.06 5.803 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) = 0.835 Deviance explained = 85.9%
## -REML = 58.733 Scale est. = 0.085927 n = 155
```

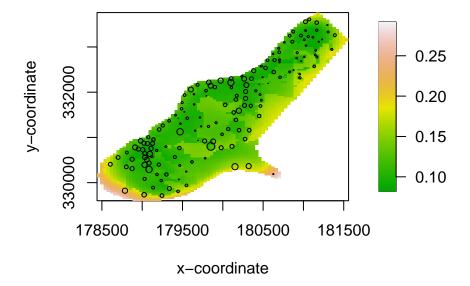
GAM prediction



Standard deviations of prediction from GAM

```
image.plot(x = pred.grid.gam[["Var1"]][1:78], y = unique(pred.grid.gam[["Var2"]]),
    z = matrix(zinc.pred.gam.sd, nrow = 78, ncol = 104),
    col = terrain.colors(100), xlab = "x-coordinate",
    ylab = "y-coordinate")

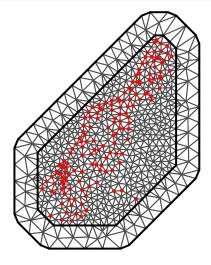
symbols(detrend$coords[, 1], detrend$coords[, 2], circles = (detrend$data -
    min(detrend$data))/1, add = T, inches = 0.04)
```



SPDE Model for log(zinc)

We now create a Bayesian SPDE model for $\log(\text{zinc})$.

We can visualize the mesh we created as follows:



Next, we create an A matrix and the stack, which we need in order to define our model.

```
A <- inla.spde.make.A(mesh = mesh, loc = data.matrix(zincdf[, c("locx", "locy")]))
# Define X matrix
Xcov <- data.frame(intercept = 1,</pre>
                    sqrtdist = zincdf$sqrtdist)
Xcov <- as.matrix(Xcov)</pre>
colnames(Xcov)
## [1] "intercept" "sqrtdist"
# Create the stack
stack <- inla.stack(</pre>
 tag = "est",
  # - Name (nametag) of the stack
  # - Here: est for estimating
 data = list(y = zincdf$y),
  effects = list(
   # - The Model Components
   s = 1:mesh$n,
   Xcov = Xcov
 ),
  # - The second is all fixed effects
 A = list(A, 1)
 # - First projector matrix is for 's'
  # - second is for 'fixed effects'
)
```

Next, we can set a prior and define our model.

Finally, we can fit our model:

```
res <- inla(formula,
  data = inla.stack.data(stack, spde = spde),
  control.predictor = list(A = inla.stack.A(stack), compute = T),
  # compute=T to get posterior for fitted values
  family = family,
  control.family = control.family,
  # control.compute = list(config=T, dic=T, cpo=T, waic=T),
  # if Model comparisons wanted</pre>
```

```
control.inla = list(int.strategy = "eb"),
  # - faster computation
  # control.inla = list(int.strateqy='qrid'),
  # - More accurate integration over hyper-parameters
  verbose = F
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 = 1.56, Running = 0.377, Post = 0.0179, Total = 1.96
## Fixed effects:
                   sd 0.025quant 0.5quant 0.975quant
          mean
## Xcov1 6.994 0.117
                         6.764
                                 6.994
                                              7.224 6.994
## Xcov2 -2.576 0.242
                          -3.050 -2.576
                                              -2.102 -2.576
## Random effects:
## Name
             Model
       s SPDE2 model
##
## Model hyperparameters:
                                                        sd 0.025quant 0.5quant
                                              mean
## Precision for the Gaussian observations 12.387
                                                    3.203
                                                                7.314
                                                                      11.974
                                           564.083 163.987
                                                              306.962 542.425
## Range for s
## Stdev for s
                                             0.328 0.055
                                                                0.233
                                                                       0.323
                                           0.975quant
                                                        mode
## Precision for the Gaussian observations
                                               19.845 11.178
## Range for s
                                              947.579 501.801
## Stdev for s
                                                0.449 0.314
## Marginal log-Likelihood: -93.88
## 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)')
```