Geostatistical COVID-19 infection risk maps with R

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1 Introduction

This tutorial shows how to do block sequential simulation to model the spatial distribution of a disease, as in Azevedo et al. 2020[1], using R. For that purpose we will run an example using COVID-19 data.

The R code in this tutorial calculates parameters and generate files to be read by an .exe program (dss.c.64.exe) performing block sequential simulation (using direct sequential simulation algorithm, Soares 2000[2]).

2 Data and R code

A set of functions written in R will generate the required files and call dss.c.64.exe for block sequential simulation.

To run the code, you will need :

- a COVID-19 datafile and,
- a grid with id region values at all simulation locations.

3 Basic instructions

Make sure to put all data and R functions in default (working) directory. Inside that directory create a folder called "input" and put the dss.c.64.exe inside.

4 COVID-19 example

For our example we will use a COVID-19 dataset for Portugal mainland with all cases notified to health authorities on 01/06/2020. The example is a step-by-step guide to obtain geostatistical maps of COVID-19. All tools needed to run this task (R functions, datasets and .exe) are available on github to reproduce example.

4.1 Source functions

Start by running the code via source. I created separate files for each function:

```
source("f1_irates.R", echo = T)
source("f2_blockfile.R", echo = T)
source("f3_maskfile.R", echo = T)
source("f4_varexp.R", echo = T)
source("f5_varmodel.R", echo = T)
source("f6_ssdpars.R", echo = T)
source("f7_outraster.R", echo = T)
```

4.2 Import COVID-19 data

As input you should provide a data frame with id of region, x, y and z cartesian coordinates at region mass center, number of COVID-19 cases by region and population at risk by region.

Therefore we start by reading an ascii file with the COVID-19 data (available on github) and create a data frame from it.

[1] https://doi.org/10.1186/s12942-020-00221-5
[2] https://doi.org/10.1023/A:1012246006212

```
covid = read.table("covid19_data.txt", header = TRUE, sep = "\t", dec = ".")
```

```
head(covid)
```

```
##   id_region        name_region     xcoord     ycoord zcoord poprisk ncases
## 1         1           Abrantes  -5332.936  -18739.44      0   35377     17
## 2         2             Agueda -24009.776  100641.94      0   45992     65
## 3         3    Aguiar da Beira  50540.025  122094.85      0    4740     NA
## 4         4           Alandroal  60012.722 -116382.18      0    5064     NA
## 5         5 Albergaria-a-Velha -29294.848  113819.38      0   24128     91
## 6         6           Albufeira  -8581.783 -285532.71      0   41123     76
```

```
str(covid)
```

```
## 'data.frame':    278 obs. of  7 variables:
##  $ id_region  : int  1 2 3 4 5 6 7 8 9 10 ...
##  $ name_region: Factor w/ 278 levels "Abrantes","Agueda",..: 1 2 3 4 5 6 7 8 9 10 ...
##  $ xcoord     : num  -5333 -24010 50540 60013 -29295 ...
##  $ ycoord     : num  -18739 100642 122095 -116382 113819 ...
##  $ zcoord     : int  0 0 0 0 0 0 0 0 0 0 ...
##  $ poprisk    : int  35377 45992 4740 5064 24128 41123 11712 12860 53641 19505 ...
##  $ ncases     : int  17 65 NA NA 91 76 7 9 40 23 ...
```

You may see the dataset contains regions where number of cases is missing (id regions 3 and 4). These NA must be replaced by an integer, for kriging to run. Function `irates()` (next section) includes an argument to overcome this limitation.

4.3 Compute rates (/10^4) and variance-error terms with `irates()`

Use `irates()` to compute rates (/10^4), variance-error terms by region. The arguments of the function are:

- `dfobj`, string, dataframe name with COVID-19 data
- `id`, character, field name for region id
- `x`, character, field name for x-coordinates
- `y`, character, field name for y-coordinates
- `z`, character, field name for z-coordinates
- `cases`, character, field name for number of cases
- `pop`, character, field name for population size
- `casesNA`, numeric, an integer used to replace rows with cases = NA,
- `day`, character, string indicating date (format "yyyymmdd") of COVID-19 data

```
rates = irates(df = covid, oid = "id_region", x = "xcoord", y = "ycoord", z = "zcoord",
               cases = "ncases", pop = "poprisk", casesNA = 2, day = "20200601")
```

The function writes a text file (.out) with rates and store it in input folder. `irates()` also returns the following list of objects:

```
str(rates)
```

```
## List of 4
##  $ rates    :'data.frame':   278 obs. of  7 variables:
##   ..$ id  : int [1:278] 1 2 3 4 5 6 7 8 9 10 ...
##   ..$ x   : num [1:278] -5333 -24010 50540 60013 -29295 ...
##   ..$ y   : num [1:278] -18739 100642 122095 -116382 113819 ...
##   ..$ z   : int [1:278] 0 0 0 0 0 0 0 0 0 0 ...
##   ..$ rate: num [1:278] 4.81 14.13 4.22 3.95 37.72 ...
##   ..$ err : num [1:278] 0.000885 0.000681 0.006607 0.006184 0.001298 ...
##   ..$ pop : int [1:278] 35377 45992 4740 5064 24128 41123 11712 12860 53641 19505 ...
```

```
##  $ mrisk    : num 31.3
##  $ file     :List of 3
##   ..$ day   : chr "20200601"
##   ..$ name  : chr "20200601notified.out"
##   ..$ folder: chr "Z:/pos_doc/covid/bkrig/tutorial_example/input"
##  $ ssdirpars:List of 7
##   ..$ nvars  : int 4
##   ..$ xcolumn: int 1
##   ..$ ycolumn: int 2
##   ..$ zcolumn: int 3
##   ..$ varcol : int 4
##   ..$ minval : num 1.31
##   ..$ maxval : num 122
```

4.4 Create block data with `blockfile()`

Use `blockfile()` to transform grid file in block format. The function requires some libraries to be loaded. If not installed they will be first installed.

You should provide a georeferenced grid file with id region values at simulation locations. The arguments of the function are:

- rateobj, character, name of list, output of function `irates()`.
- gridimage, character, name of georeferenced grid file (e.g. tif)
- na.value, numeric, integer with grid value for "No data"

```
block = blockfile(rates, "grid2k.tif")
```

The grid file values should refer to the region id's at simulation locations (nodes). All regions in covid data should be represented by 1 or more node.

The function writes a text file (.out) with blockdata and store it in input folder. `blockfile()` also returns the following list of objects:

```
str(block, max.level = 2)
```

```
## List of 4
##  $ gridpars:List of 4
##   ..$ nodes     : int [1:2] 141 288
##   ..$ resolution: num [1:2] 2000 2000
##   ..$ origin    : num [1:2] -119191 -300405
##   ..$ NAs       : num -999
##  $ outgrid :List of 3
##   ..$ values : num [1:40608] -999 -999 -999 -999 -999 -999 -999 -999 -999 -999 ...
##   ..$ idblock: int [1:278] 1 2 3 4 5 6 7 8 9 10 ...
##   ..$ nblock : int 278
##  $ file    :List of 3
##   ..$ day   : chr "20200601"
##   ..$ name  : chr "20200601blockdata.out"
##   ..$ folder: chr "Z:/pos_doc/covid/bkrig/tutorial_example/input"
##  $ ingrid  :Formal class 'RasterLayer' [package "raster"] with 12 slots
```

4.5 Create mask file with `maskfile()`

The function `maskfile()` creates a mask for the block file. The only argument of the function is the name of list, output of function `blockfile()`.

```
mask = maskfile(block)
```

Generates a file with values {-1,0} where -1 are assigned to nodata locations and 0 are assigned to nodes with values (id region). A text file (.out) with mask data is created and stored in input folder.

```
str(mask)
```

```
## List of 2
##  $ file :List of 3
##   ..$ day   : chr "20200601"
##   ..$ name  : chr "20200601mask.out"
##   ..$ folder: chr "Z:/pos_doc/covid/bkrig/tutorial_example/input"
##  $ zones:List of 2
##   ..$ nzones : int 2
##   ..$ zoneval: num [1:2] -1 0
```

4.6 Calculate experimental variogram with `varexp()`

Use `varexp()` to calculate experimental variogram from COVID-19 rates. Only implemented in omnidirectional case. The arguments are:

- dfobj, character, name of object, output of function `irates()`
- lag, numeric, the lag distance used for variogram estimates
- nlags, numeric, the number of lags to calculate variogram.

```
vexp = varexp(rates, lag = 7000, nlags = 15)
```

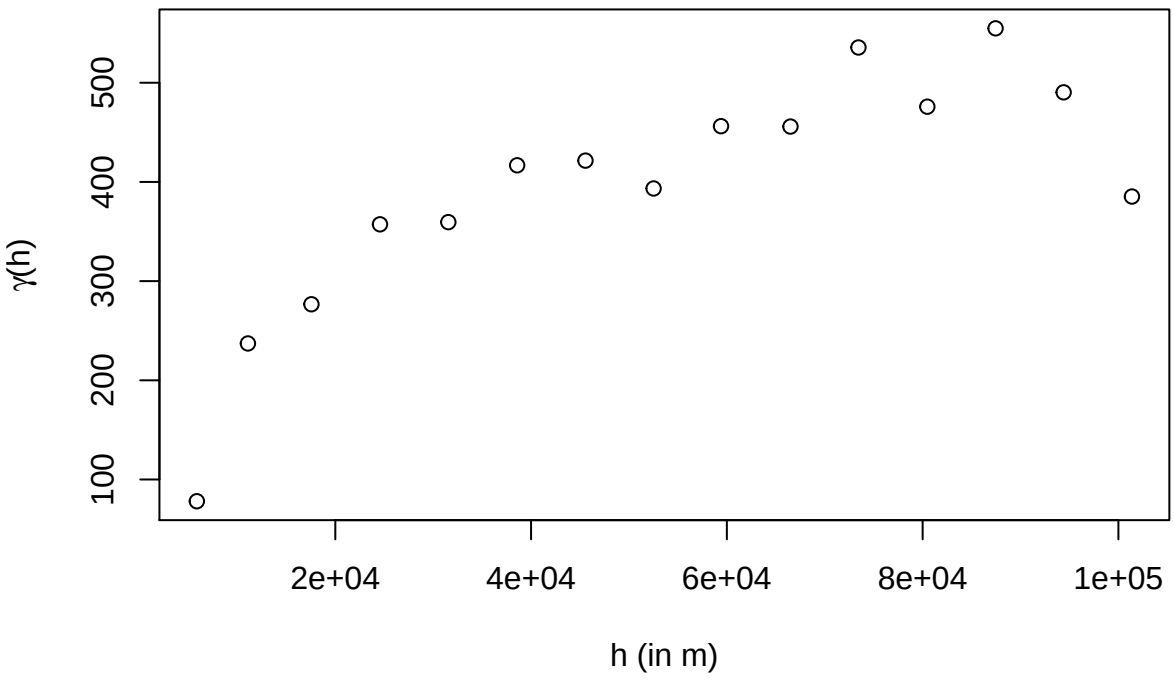
The function returns a list with the weighted variance (by population size) and variogram estimates at nlags.

```
str(vexp)
```

```
## List of 2
##  $ weightsvar: num 501
##  $ semivar   :'data.frame':  15 obs. of  2 variables:
##   ..$ dist        : num [1:15] 5855 11072 17561 24565 31547 ...
##   ..$ semivariance: num [1:15] 78.1 237.1 276.7 357.3 359.5 ...
```

You may plot results to evaluate main structural patterns in the data:

```
plot(vexp[["semivar"]], ylab = expression(paste(gamma, "(h)")), xlab = "h (in m)")
```



4.7 Fit variogram model with `varmodel()`

Funtion `varmodel()` fits (manually) a theoretical variogram. You should provide the experimental variogram data to evaluate fit by visual inspection, the variogram model type and the variogram parameters. The arguments of `varmodel()` are:

- varexp, character, name of object, output of function varexp()
- mod, character, the variogram model type (available are: "Sph" or "Exp")
- nug, numeric, nugget-effect value of the variogram
- ran, numeric, range value of the variogram
- sill, numeric, sill (or partial sill) value of the variogram

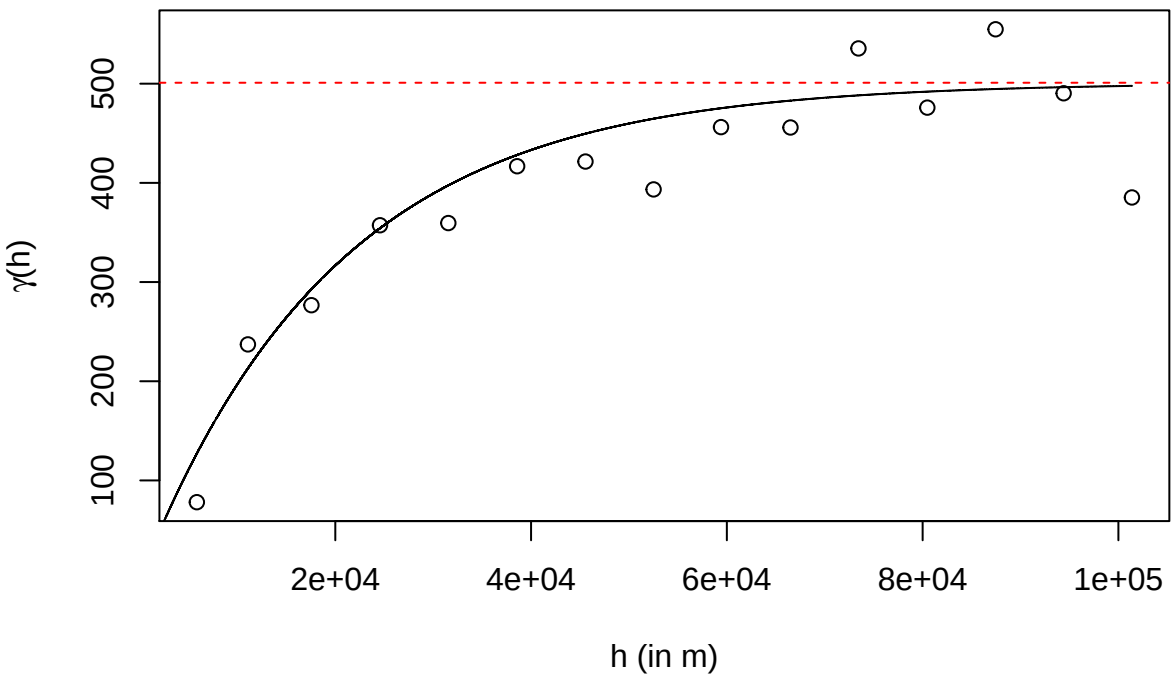
```
vmod = varmodel(vexp, mod = "Exp", nug = 0, ran = 60000, sill = vexp[["weightsvar"]])
```

```
str(vmod)
```

```
## List of 3
##  $ structures: num 1
##  $ parameters:'data.frame':  1 obs. of  5 variables:
##   ..$ model    : Factor w/ 1 level "Exp": 1
##   ..$ modeltype: num 2
##   ..$ nugget   : num 0
##   ..$ range    : num 60000
##   ..$ psill    : num 501
##  $ fittedval : num [1:101385] 0 0.025 0.0501 0.0751 0.1002 ...
```

```
# plot experimental variogram
plot(vexp[["semivar"]], ylab = expression(paste(gamma, "(h)")), xlab = "h (in m)")
```

```r
# add sill
abline(h = vexp[["weightsvar"]], col ="red", lty = 2)
# add theoretical model
lines(vmod[["fittedval"]])
```



4.8 Create parameters file with `ssdpars()` and calls dss.c.64.exe

Function `ssdpars()` writes the parameters file (.par) for .exe and runs block sequential simulations Function arguments are the names of objects returned above and parameter values for block-kriging and simulation processes:

- blockobj, character, name of list, output of function blockfile()
- maskobj, character, name of list, output of function maskfile()
- dfobj, character, name of list, output of function irates()
- varmobj,character, name of list, output of function varmodel()
- simulations, numeric, number of simulations
- nrbias, numeric, nr simulations for bias correction
- biascor, num vector, flag for (mean, variance) correction (yes = 1, no = 0)
- ndMin, numeric, min number of neighbour observations used in kriging
- ndMax, numeric, max number of neighbour observations used in kriging
- nodMax, numeric, max number of previously simulated nodes used in kriging
- radius1, numeric, search radii in the major horizontal axe
- radius2, numeric, search radii in the axe orthogonal (horizontal) to radius1
- radius3, numeric, search radii in the vertical axe
- ktype, numeric, the kriging type to be used (available are: 0 = simple, 1 = ordinary)

```
ssdpars(blockobj = block, maskobj = mask, dfobj = rates, varmobj = vmod,
        simulations = 5, radius1 = 60000, radius2 = 60000)
```

The function generates a text file (.par), calls dss.c.64.exe, run block simulations and returns the simulated maps (.out). This process may take a while depending mostly on the number of simulation nodes and number of simulations.

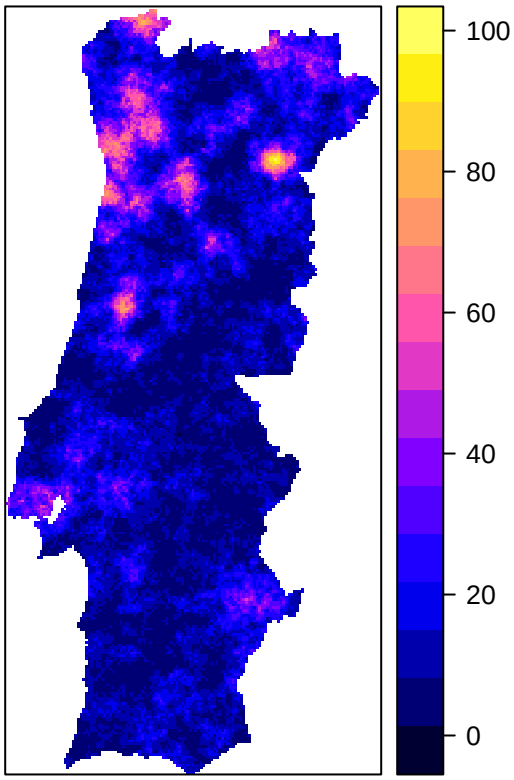
Both text file (.par) and simulations files (.out) are stored in input folder.

4.9 Export simulations from .out format to raster format

Function `outraster()` transforms simulations .out returned by `ssdpars()` into grid (raster) files. Argument `blockobj =` is the name (string) of the object returned by `blockfile()`. If argument `emaps = T`, the function also computes e-type and uncertainty maps and plots e-type map.

```
outraster(block, emaps = T)
```

```
## [1] "20200601sim_1.out"
## [1] "20200601sim_2.out"
## [1] "20200601sim_3.out"
## [1] "20200601sim_4.out"
## [1] "20200601sim_5.out"
```



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