Tutorial for Geostatistical COVID-19 infection risk maps

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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. 2020¹. 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 kriging simulation (using direct sequential simulation algorithm, Soares 2000²).

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 kriging calculations.

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_ssdir.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.

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

¹https://doi.org/10.1186/s12942-020-00221-5

 $^{^{2}}$ https://doi.org/10.1023/A:1012246006212

head(covid)

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

str(covid)

```
278 obs. of 7 variables:
   'data.frame':
    $ 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 ...
##
                        -5333 -24010 50540 60013 -29295 ...
##
    $ xcoord
                 : num
    $ ycoord
                   nıım
                        -18739 100642 122095 -116382 113819 ...
                        0 0 0 0 0 0 0 0 0 0 ...
##
    $ zcoord
                   int
##
                        35377 45992 4740 5064 24128 41123 11712 12860 53641 19505 ...
    $ poprisk
                   int
                        17 65 NA NA 91 76 7 9 40 23 ...
    $ ncases
                 : int
```

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 (/10⁴) 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

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 ...
##
##
             : num [1:278] -5333 -24010 50540 60013 -29295 ...
             : num [1:278] -18739 100642 122095 -116382 113819 ...
##
             : int [1:278] 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/codigo_back/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 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
    ##
    ..$ 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/codigo_back/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/codigo_back/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.

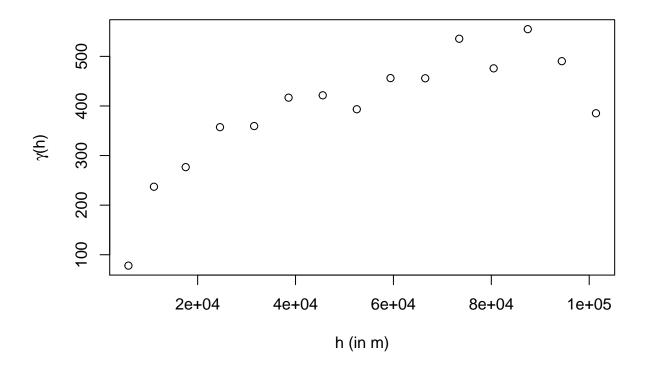
```
vexp = varexp(rates, lag = 7000, nlags = 15)
```

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)")
```



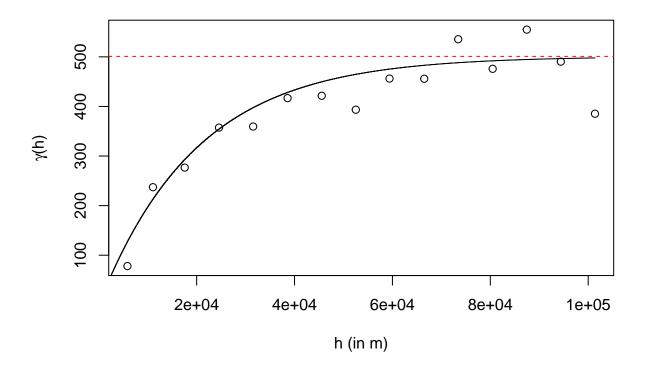
4.7 Fit variogram model with varmodel()

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:
##
                  : Factor w/ 1 level "Exp": 1
     ..$ model
##
     ..$ modeltype: num 2
##
     ..$ nugget
                  : num 0
##
     ..$ range
                  : num 60000
                  : num 501
##
     ..$ psill
    $ 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)")
```

```
# 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 kriging 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)

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.