Geostatistical COVID-19 infection risk maps with R

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1 Introduction

This tutorial shows how to run block sequential simulation with R modeling the spatial distribution of a disease, as in Azevedo et al. 2020¹. For that purpose we will follow an example using COVID-19 data where simulated risk maps, median risk map and risk uncertainty map are obtained in the end.

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 2000²).

2 R functions and packages

Some of the functions written will require other functions available in external packages raster, sp, rgdal and data.table. If not installed, these packages will be downloaded and installed from CRAN repositories.

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 simulated risk maps of COVID-19, median risk map and risk uncertainty map. All tools needed - R functions, datasets and .exe - are available on the github repository to reproduce the example.

The following data are needed to run the example:

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

 $^{^{1}}$ https://doi.org/10.1186/s12942-020-00221-5

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

Supported file types for the grid map are the 'native' raster package format and those that can be read via rgdal.

4.1 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 (*centroid*), 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 and create a data frame from it.

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

0 0 0 0 0 0 0 0 0 0 ...

17 65 NA NA 91 76 7 9 40 23 ...

```
head(covid)
##
     id_region
                      name_region
                                      xcoord
                                                  ycoord zcoord poprisk ncases
## 1
             1
                         Abrantes
                                  -5332.936
                                              -18739.44
                                                              0
                                                                  35377
                                                                            17
## 2
             2
                                                                  45992
                           Agueda -24009.776
                                               100641.94
                                                              0
                                                                            65
## 3
             3
                  Aguiar da Beira 50540.025
                                               122094.85
                                                              0
                                                                   4740
                                                                            NA
## 4
             4
                        Alandroal 60012.722 -116382.18
                                                              0
                                                                   5064
                                                                            NA
             5 Albergaria-a-Velha -29294.848 113819.38
                                                                            91
## 5
                                                              0
                                                                  24128
## 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
                        -18739 100642 122095 -116382 113819 ...
                 : num
```

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

35377 45992 4740 5064 24128 41123 11712 12860 53641 19505 ...

4.2 Source functions

\$ zcoord

\$ poprisk

\$ ncases

: int

: int

: int

I created separate files for each function. Beacause code needs to run in a certain order, functions are numbered. Start by running the following code via source:

```
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)
```

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

Syntax:

##

##

```
## function (dfobj = NA, oid = NA, xx = NA, yy = NA, zz = NA, cases = NA, ## pop = NA, casesNA = 2, day = "20200301")
```

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

- oid, character, field name for region id
- xx, character, field name for x-coordinates
- yy, character, field name for y-coordinates
- zz, 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 irates() returns the following list of objects:

```
str(rates)
```

```
## List of 4
##
   $ rates
                                278 obs. of 7 variables:
               :'data.frame':
     ..$ 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/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
```

It also writes a text file (.out) with rates and store it in input folder.

4.4 Create block with blockfile()

Syntax:

```
## function (rateobj, gridimage, na.value = -999)
```

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, string, 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
              : num [1:2] -119191 -300405
##
    ..$ origin
##
    ..$ 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
            : chr "20200601"
##
    ..$ day
    ..$ name : chr "20200601blockdata.out"
##
    ..$ folder: chr "Z:/pos_doc/covid/bkrig/codigo/input"
## $ ingrid :Formal class 'RasterLayer' [package "raster"] with 12 slots
```

4.5 Create mask with maskfile()

Syntax:

```
## function (blockobj)
```

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)
```

The function returns the following a list of objects and generates a text file (.out) with values {-1,0} where -1 are assigned to nodata locations and 0 are assigned to nodes with values (id region). The file is 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/input"
## $ zones:List of 2
## ..$ nzones : int 2
## ..$ zoneval: num [1:2] -1 0
```

4.6 Calculate experimental variogram with varexp()

Syntax:

```
## function (dfobj, lag, nlags)
```

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

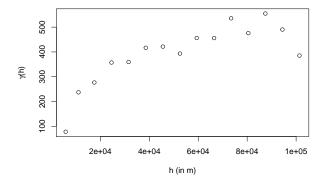
• dfobj, string, name of list, output of function irates()

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



4.7 Fit variogram model with varmodel()

Syntax:

```
## function (varexp, mod = c("Exp", "Sph"), nug, ran, sill)
```

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, string, 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

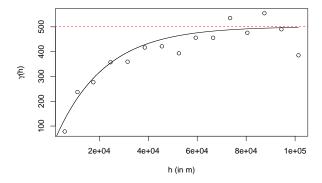
```
vmod = varmodel(vexp, mod = "Exp", nug = 0, ran = 60000, sill = vexp[["weightsvar"]])
```

varmodel() returns the following list of objects:

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



4.8 Create parameters file with ssdpars()

Syntax:

```
## function (blockobj, maskobj, dfobj, varmobj, simulations = 1, nrbias = 20,
## biascor = c(1, 1), ndMin = 1, ndMax = 32, nodMax = 12, radius1, radius2,
## radius3 = 1, ktype = 0)
```

Function ssdpars() generates a parameters file (.par) and the simulated maps in .out format. Function ssdpars() invokes dss.c.64.exe specified by the parameters file.

Arguments include names of lists and parameter values required for simulation processes:

- blockobj, string, name of list, output of function blockfile()
- maskobj, string, name of list, output of function maskfile()
- dfobj, string, name of list, output of function irates()
- varmobj, string, 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)

Note that this process may take a while, depending mostly on the number of simulation nodes and number of simulations specified.

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

4.9 Obtain risk maps with outraster()

Syntax:

```
## function (blockobj, grids = F, emaps = T)
```

Function outraster() read simulation files (.out) returned by ssdpars() and returns a list with simulated maps (rasterstack object), e-type and uncertainty maps (rasterlayers).

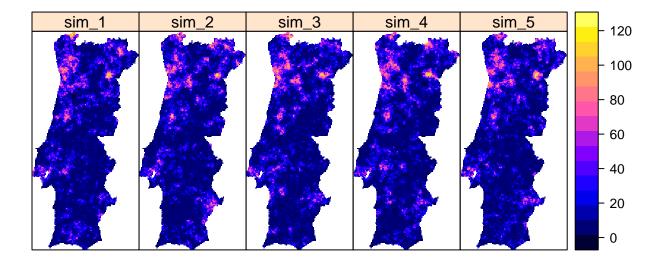
The arguments of the function:

- blockobj, string, name of list, output of function blockfile(),
- if grids = T, saves simulated maps in 'native' raster package format .grd,
- if emaps = T (default), saves e-type and uncertainty maps in format .grd.

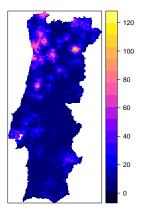
All .grd files are stored in input folder.

```
maps = outraster(block)
## [1] "20200601sim_1.out"
## [1] "20200601sim 2.out"
## [1] "20200601sim_3.out"
## [1] "20200601sim_4.out"
## [1] "20200601sim_5.out"
str(maps, max.level = 3)
## List of 3
## $ simulations:Formal class 'RasterStack' [package "raster"] with 11 slots
     .. ..@ filename: chr ""
##
##
     .. .. @ layers :List of 5
##
     .. ..@ title : chr(0)
     .. .. @ extent :Formal class 'Extent' [package "raster"] with 4 slots
##
     .. .. @ rotated : logi FALSE
##
     ....@ rotation:Formal class '.Rotation' [package "raster"] with 2 slots
##
##
     .. .. @ ncols : int 141
##
     .. .. @ nrows : int 288
                    :Formal class 'CRS' [package "sp"] with 1 slot
##
     .. ..@ crs
##
     .. .. @ history : list()
##
                  : list()
     .. ..@ z
                 :Formal class 'RasterLayer' [package "raster"] with 12 slots
##
   $ etype
                :Formal class '.RasterFile' [package "raster"] with 13 slots
##
     .. ..@ file
##
     .. ..@ data
                    :Formal class '.SingleLayerData' [package "raster"] with 13 slots
     ....@ legend :Formal class '.RasterLegend' [package "raster"] with 5 slots
##
     .. ..@ title
                    : chr(0)
##
##
     ....@ extent :Formal class 'Extent' [package "raster"] with 4 slots
##
     .. .. @ rotated : logi FALSE
##
     ....@ rotation:Formal class '.Rotation' [package "raster"] with 2 slots
                    : int 141
##
     .. ..@ ncols
##
     .. ..@ nrows
                   : int 288
##
                   :Formal class 'CRS' [package "sp"] with 1 slot
     .. ..@ crs
##
     .. .. @ history : list()
##
     .. ..@ z
                    : list()
```

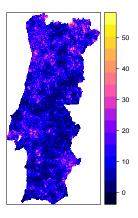
```
$ uncertainty:Formal class 'RasterLayer' [package "raster"] with 12 slots
    .. .. @ file :Formal class '.RasterFile' [package "raster"] with 13 slots
##
     ....@ data :Formal class '.SingleLayerData' [package "raster"] with 13 slots
##
##
     ....@ legend :Formal class '.RasterLegend' [package "raster"] with 5 slots
     ....@ title : chr(0)
     ....@ extent :Formal class 'Extent' [package "raster"] with 4 slots
##
     .. .. @ rotated : logi FALSE
     ....@ rotation:Formal class '.Rotation' [package "raster"] with 2 slots
##
     .. .. @ ncols : int 141
##
##
     ....@ nrows : int 288
     ....@ crs :Formal class 'CRS' [package "sp"] with 1 slot
##
     .. .. @ history : list()
     .. ..@ z
                   : list()
spplot(maps[["simulations"]])
```



```
spplot(maps[["etype"]])
```



spplot(maps[["uncertainty"]])



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