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 to model the spatial distribution of a disease, as in Azevedo et al. 2020[1]. 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 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 simulated risk maps of COVID-19, median risk map and risk uncertainty map. All tools needed - 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.

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

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 = ".")
```

```
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 are 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()`

```
irates() =
```

```
## 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

```
rates = irates(dfobj = covid, oid = "id_region", xx = "xcoord", yy = "ycoord", zz = "zcoord",
               cases = "ncases", pop = "poprisk", casesNA = 2, day = "20200601")
```

The function `irates()` 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
```

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

4.4 Create block data with `blockfile()`

Function `blockfile()`

```
## 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
##   ..$ 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()

Function `maskfile()`

```
## 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()`.

```r
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.

```r
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()

Function `varexp()`

```
## 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.

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

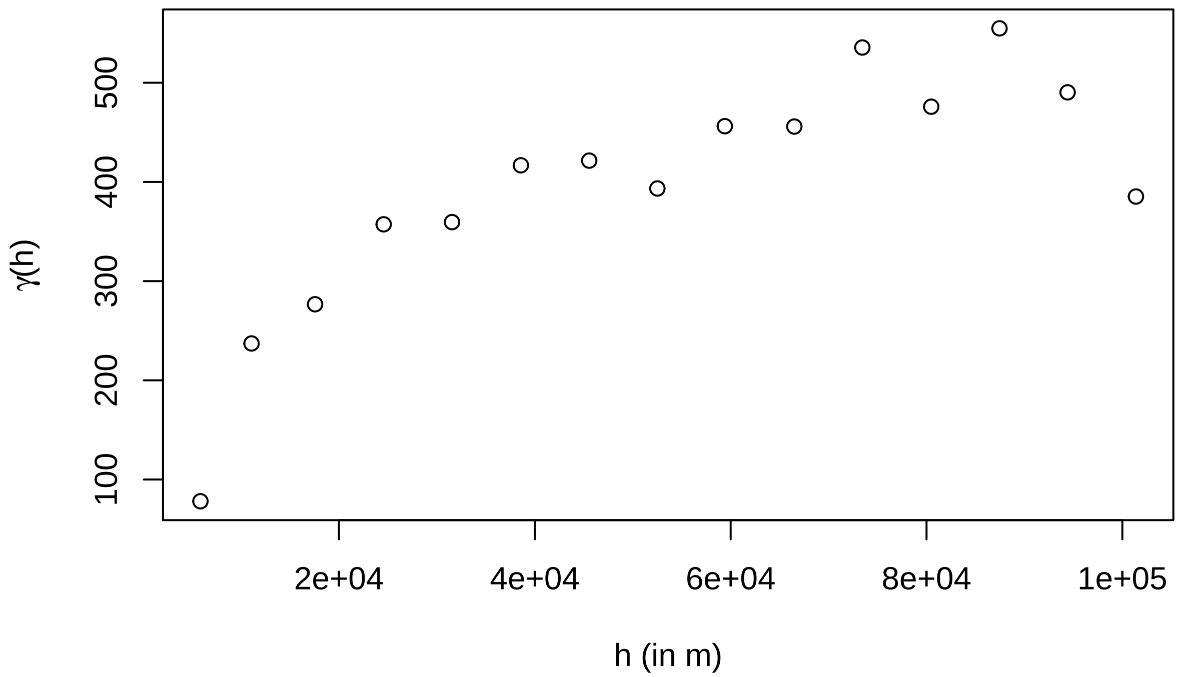
The function returns a list with the weighted variance (by population size) and variogram estimates at nlags.

```r
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:

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



4.7 Fit variogram model with `varmodel()`

Function `varmodel()`

```
## 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:

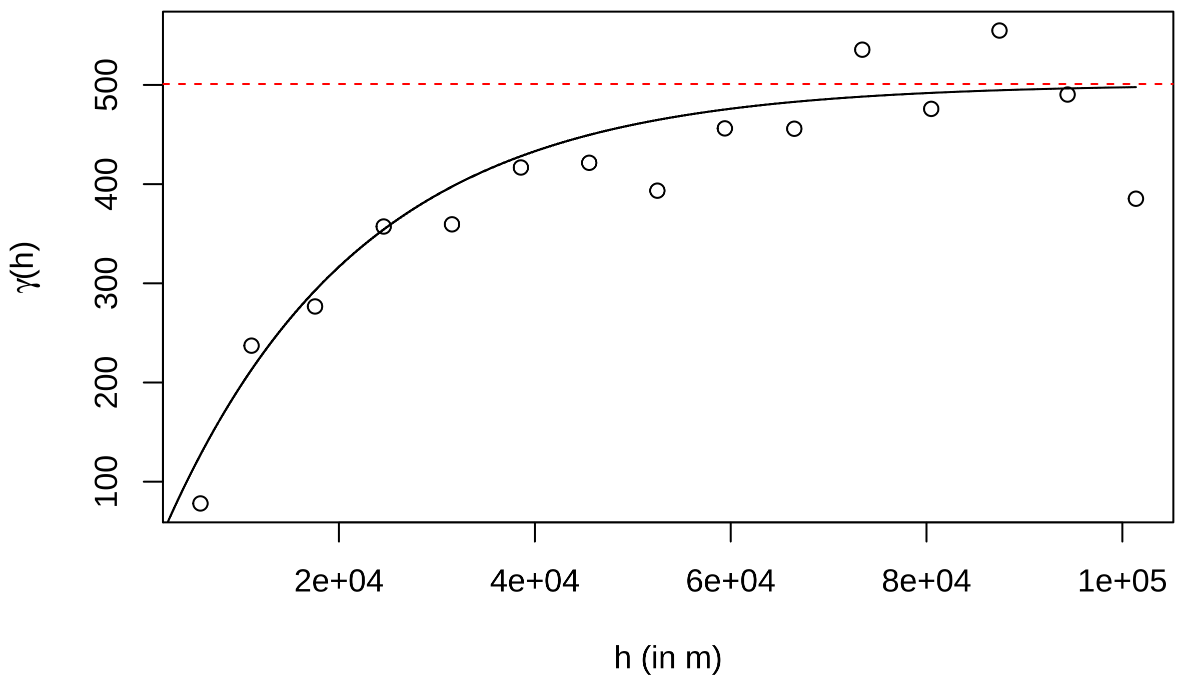
- `varexp`, string, name of object, output of function varexp()
- `mod`, character, the variogram model type (available are: "Sph" or "Exp")
- `nug`, numeric, nugget-effect value of the variogram
- `ran`, numeric, range value of the variogram
- `sill`, numeric, sill (or partial sill) value of the variogram

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

```
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 ...
```

```r
# 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()`

```
## 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()` 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`, 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)

```
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 Obtain risk maps with `outraster()`.

```
outraster()
```

```
## 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 (and respective .gri) 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"
```

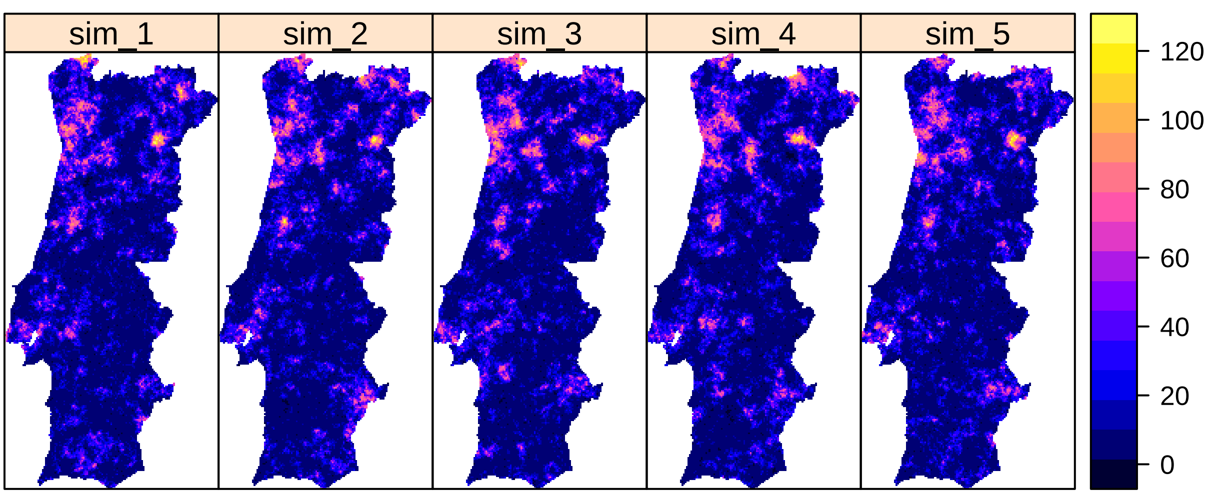
```
str(maps, max.level = 3)
```

```
## 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
##   .. ..@ crs     :Formal class 'CRS' [package "sp"] with 1 slot
##   .. ..@ history : list()
##   .. ..@ z       : list()
##  $ etype      :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
```

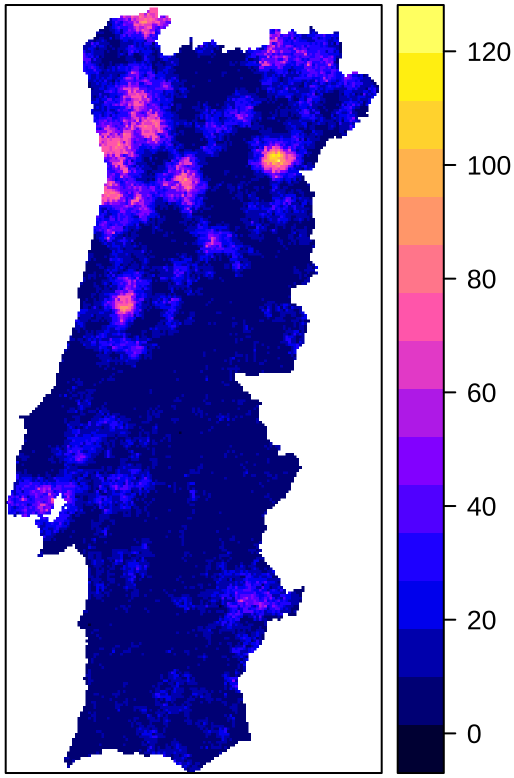
```
##   .. ..@ legend  :Formal class '.RasterLegend' [package "raster"] with 5 slots
##   .. ..@ title   : chr(0)
##   .. ..@ extent  :Formal class 'Extent' [package "raster"] with 4 slots
##   .. ..@ rotated : logi FALSE
##   .. ..@ rotation:Formal class '.Rotation' [package "raster"] with 2 slots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

You may plot results:

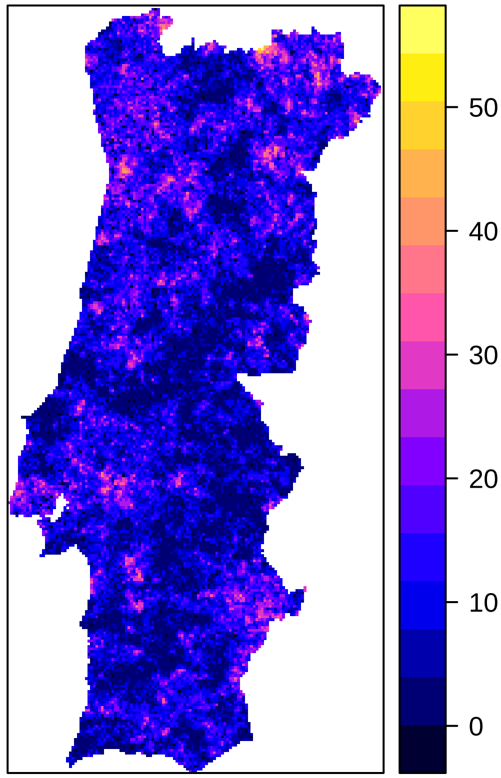
```
spplot(maps[["simulations"]])
```



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




```r
spplot(maps[["uncertainty"]])
```



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