`GeoModels` Tutorial: analysis of spatial precipitation anomalies using Gaussian and skew Gaussian random fields

Moreno Bevilacqua, Christian Caamaño

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Introduction

In this tutorial we show how to analyze total precipitation anomalies registered at $7,352$ location sites in the USA from 1895 to 1997. A detailed description of the data can be found in Kaufman et al. (2008). The yearly totals have been standardized by the long-run mean and standard deviation for each station from 1962. The size of dataset is large and this tutorial shows how to use the package `GeoModels` in order to perform estimation and prediction using Gaussian and SkewGaussian random fields. We first load the *R* libraries needed in this tutorial.

```
require(devtools)
install_github("vmoprojs/GeoModels")
require(GeoModels)
require(fields)
require(maps)
require(maptools)
require(mapdata)
require(geoR)
require(sn)
library(mapproj)
```

1 Preliminary data analysis

Precipitation anomalies data can be found in the `GeoModels` package. We first import the data:

```
data(anomalies)
head(anomalies)
      lon   lat          z
[1,] -85.25 31.57 -0.4586873
[2,] -87.42 32.23 -0.9253283
[3,] -85.87 32.98 -0.4370817
[4,] -88.13 33.13 -0.6026716
[5,] -86.50 31.32 -0.3519950
[6,] -85.85 33.58  0.5069722
```

and we select the coordinates (given in lon/lat format, decimal degree) and the anomalies data

```
loc=cbind(anomalies[,1],anomalies[,2])
z=cbind(anomalies[,3])
```

A colour map of the anomalies data can be obtained with the following code (see Figure 1).

```
quilt.plot(loc,z,xlab="long",ylab="lat")
map("usa", add = TRUE)
```

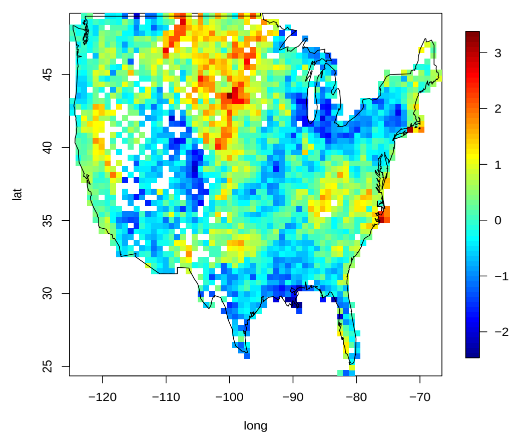

Figure 1: Coloured map of anomalies data.

We first project the spherical coordinates on a two dimensional euclidean space using a projection method. In this example we select a sinusoidal projection. However, the `GeoModels` package allows to handle spherical coordinates given in lon/lat format (decimal degree) and work with geodesic or chordal distances.

```
P.sinusoidal <- mapproject(loc[,1],loc[,2],projection="sinusoidal")
loc<-cbind(P.sinusoidal$x,P.sinusoidal$y)*6371
maxdist=max(dist(loc))
```

Here 6371 is the radius of the earth in KM. The marginal distribution of the data (see the histogram in Figure 2 left part) suggests that the marginal Gaussian assumption seems quite reasonable. However a skew-Gaussian distribution could be more appropriate since it can be appreciated a slight degree of asimmetry. Additionally the h-scatterplot indicate an elliptical dependence for the bivariate distributions (see Figure, 2 left part).

```
hist(z,main="Anomalies␣histogram")
GeoScatterplot(data=z,coordx=loc,maxdist=50,numbins=4)
```

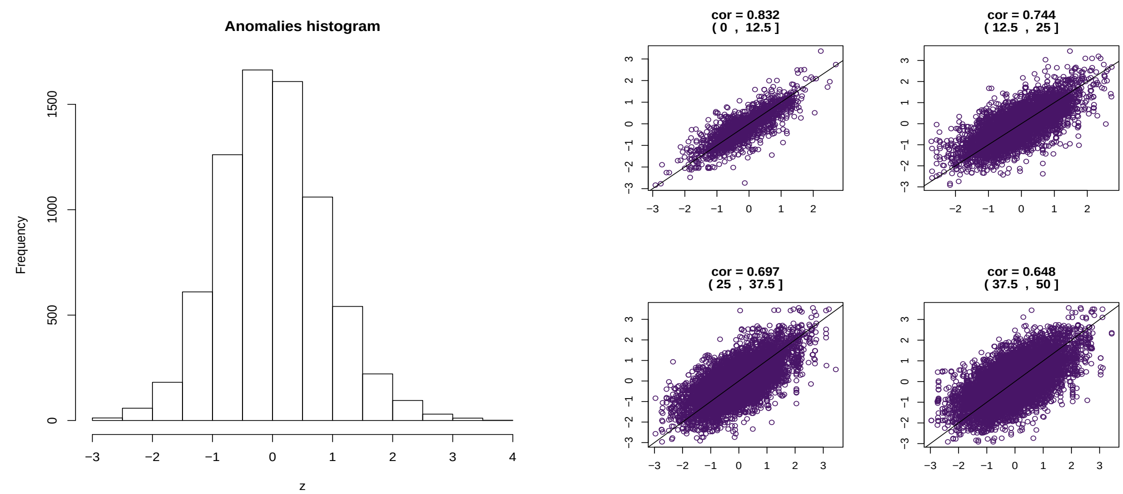

Figure 2: From left to right: histrogram of anomalies data and associated $h-$scatterlplot.

Finally, the empirical semivariogram in Figure 3 suggests the presence of a non-negligible nugget effect.

```
evariog=GeoVariogram(data=z,coordx=loc,maxdist=maxdist/4)
plot(evariog$centers,evariog$variograms,ylim=c(0,1),
                         pch=20,xlab="Km",ylab="Semi-variogram")
```

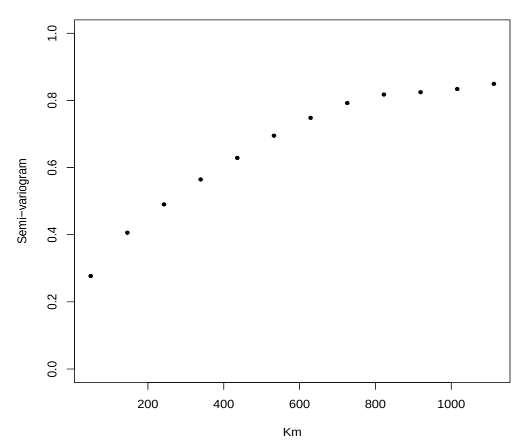

Figure 3: Empirical semi-variogram of anomalies data.

This preliminary graphical analysis suggest the use of a Gaussian and a skew-Gaussian random field with a covariance model with a nugget effect.

2 Gaussian and skew-Gaussian random fields

We first consider a zero mean, unit variance and weakly stationary standard Gaussian random field $G = \{G(\boldsymbol{s}), \quad \boldsymbol{s} \in S\}$, where $\boldsymbol{s}$ represents a location in the domain $S \subset \mathrm{I\!R}^2$ with isotropic reparametrized (special case of) generalized Wendland function as proposed in Bevilacqua et al. (2020) with a nugget effect that is:

$$\rho(\boldsymbol{h}) = \begin{cases} 1 & ||\boldsymbol{h}|| = 0 \\ (1-\tau^2)(1-\frac{||\boldsymbol{h}||}{(\alpha\beta)})^{\beta} & 0 < ||\boldsymbol{h}|| \leq \alpha\beta \\ 0 & ||\boldsymbol{h}|| > \alpha\beta \end{cases} \cdot \tag{1}$$

Here $||\boldsymbol{h}||$ is the Euclidean distance and $0 \leq \tau^2 < 1$ represents the nugget parameter. Additionally $\alpha > 0$ is a spatial depedendence parameter and $\beta \geq 3/2$ is a parameter that allows to switch from compact support to global support dependence. In particular when $\beta \to \infty$ then the exponential model is achieved. The model is compactly supported which is a nice feature from computational point of view since algorithms for sparse matrices can be used to handle the associated covariance matrix.

We consider two RFs in our analysis. The first is a location-scale transformation of G that is a RF $Y = \{Y(\boldsymbol{s}), \boldsymbol{s} \in A\}$ defined as:

$$Y(\boldsymbol{s}) := \mu(\boldsymbol{s}) + \sigma G(\boldsymbol{s}) \tag{2}$$

with $\mathrm{I\!E}(Y(\boldsymbol{s})) = \mu(\boldsymbol{s}) \in \mathrm{I\!R}$ and $Var(Y(\boldsymbol{s})) = \sigma^2 > 0$.

The second is a location-scale transformation of the skew Gaussian RF proposed in Zhang and El-Shaarawi (2010) that is:

$$U_\eta(\boldsymbol{s}) = \mu(\boldsymbol{s}) + \sigma\left(\frac{\eta}{\sigma}|G_1(\boldsymbol{s})| + G_2(\boldsymbol{s})\right) \tag{3}$$

with $\mathrm{I\!E}(U_\eta(\boldsymbol{s})) = \mu(\boldsymbol{s}) + \eta\sqrt{2/\pi}$ and $Var(U_\eta(\boldsymbol{s})) = \sigma^2 + \eta^2(1-2/\pi)$ where $\eta \in \mathbb{R}$ is the asymmetry parameter, $\sigma > 0$ and G_i $i = 1, 2$ are two independents copies of a process G. More precisely, G_1 is a Gaussian RF with correlation (1) (assuming zero nugget) and G_2 is an independent Gaussian RF with correlation (1). Note that if $\eta = 0$ the Gaussian RF in (2) is obtained. As a consequence (3) is a generalization of (2). The correlation function of the Skew-Gaussian RF is given by (Zhang and El-Shaarawi, 2010)

$$\rho_{U_\eta}(\boldsymbol{h}) = \frac{2\eta^2}{\pi\sigma^2 + \eta^2(\pi-2)}\Big((1-\rho_1^2(\boldsymbol{h}))^{1/2} + \rho_1(\boldsymbol{h})\arcsin(\rho_1(\boldsymbol{h})) - 1\Big) + \frac{\sigma^2\rho(\boldsymbol{h})}{\sigma^2 + \eta^2(1-2/\pi)}. \tag{4}$$

where $\rho_1(\boldsymbol{h})$ is the correlation function in (1) with $\tau^2 = 0$.

For both RFs we assume a constant mean $\mu(\boldsymbol{s}) = \mu$, even if the `GeoModels` package allows to specify a model regression for the spatial mean.

To obtain the names of the correlation parameters of the correlation models and the names of the nuisance parameters of the Gaussian and Skew-Gaussian models, two useful functions are `CorrParam` and `NuisParam`:

```
CorrParam("GenWend_Matern")
[1] "power2" "scale"  "smooth"
 NuisParam("Gaussian")
[1] "mean"   "nugget" "sill"
 NuisParam("SkewGaussian")
[1] "mean"   "nugget" "sill"   "skew"
```

Here `nugget` is the τ^2 parameter, `sill` is the σ^2 parameter and `skew` is the η parameter. For the the special case of the generalized Wendland model in equation (1) `scale`, `power2` are the α and β parameters respectively. Finally `smooth` is the smoothness parameter of the Generalized Wendland model and when this parameter is set to zero then we obtain (1) (Bevilacqua et al., 2020).

Estimation of Anomalies data

Given a realization $\boldsymbol{Y} = (y(\boldsymbol{s}_1), y(\boldsymbol{s}_2), \ldots, y(\boldsymbol{s}_N))^T$ from a Gaussian random field with correlation (1), the estimation of the parameters can be performed using maximum likelihood method that is maximizing the Gaussian multivariate pdf

$$f_{\boldsymbol{Y}}(y_1, \ldots, y_N; \boldsymbol{\theta}_Y) = (2\pi)^{-N/2}|\sigma^2 R|^{-1/2}\exp\left\{-\frac{(\boldsymbol{Y}-\mu\mathbf{1}_N)^T R^{-1}(\boldsymbol{Y}-\mu\mathbf{1}_N)}{2\sigma^2}\right\} \tag{5}$$

with respect to $\boldsymbol{\theta}_Y = (\mu, \sigma^2, \alpha, \beta, \tau^2)^T$. Here $R = [\rho(\boldsymbol{s}_i - \boldsymbol{s}_j)]_{i,j=1}^N$ is the correlation matrix.

However, since maximum likelihood method is computationally expensive for large datasets, in this example we focus on pairwise likelihood estimation method, an estimation method that involves only the pdf of the generic random pair $\boldsymbol{Y}_{ij} = (Y(\boldsymbol{s}_i), Y(\boldsymbol{s}_j)$ that is $f_{\boldsymbol{Y}_{ij}}(y_i, y_j; \boldsymbol{\theta}_Y)$

Similarly, given a realization $\boldsymbol{U}_\eta = (u_\eta(\boldsymbol{s}_1), u_\eta(\boldsymbol{s}_2), \ldots, u_\eta(\boldsymbol{s}_N))^T$, from a skew-Gaussian random field the pairwise likelihood estimation method involves the bivariate pdf of the bivariate random vector $\boldsymbol{U}_{\eta;ij} = (U_\eta(\boldsymbol{s}_i), U_\eta(\boldsymbol{s}_j))^T$ given by Alegria et al. (2017):

$$f_{\boldsymbol{U}_{\eta;ij}}(u_i, u_j; \boldsymbol{\theta}_{U_\eta}) = 2\sum_{l=1}^{2} \phi_2(\boldsymbol{u}_{ij} - \boldsymbol{\mu}_{ij}; \boldsymbol{A}_l)\Phi_n(\boldsymbol{c}_l; \boldsymbol{0}, \boldsymbol{B}_l) \tag{6}$$

where $\boldsymbol{\theta}_{U_\eta} = (\mu, \sigma^2, \eta, \alpha, \beta, \tau^2)^T$, $\boldsymbol{\mu}_{ij} = (\mu, \mu)^T$ and $\boldsymbol{A}_l$, $\boldsymbol{B}_l$, $\boldsymbol{c}_l$ are specific quantities depending on the correlation and the parameters (see Alegria et al. (2017) for details).

The pairwise likelihood function associated to Y is given by

$$pl(\boldsymbol{\theta}_Y) = \sum_{i=i}^{N-1} \sum_{j=i+1}^{N} log(f_{\boldsymbol{Y}_{ij}}(y_i, y_j))w_{ij} \tag{7}$$

and the pairwise likelihood function associated to U_η is given by

$$pl(\boldsymbol{\theta}_{U_\eta}) = \sum_{i=i}^{N-1} \sum_{j=i+1}^{N} log(f_{\boldsymbol{U}_{\eta;ij}}(u_i, u_j))w_{ij} \tag{8}$$

where w_{ij} are non-negative weights, not depending on $\boldsymbol{\theta}$, specified as:

$$w_{ij} = \begin{cases} 1 & ||\boldsymbol{s}_i - \boldsymbol{s}_j|| < d \\ 0 & \text{otherwise} \end{cases}. \tag{9}$$

The pairwise likelihood estimator $\hat{\boldsymbol{\theta}}_{pl}$ of the Gaussian and skew-Gaussian random fields is obtained maximizing (7) and (8) with respect to $\boldsymbol{\theta}_Y$ and $\boldsymbol{\theta}_{U_\eta}$ respectively.

In the `GeoModels` package we can choose the fixed parameters and the parameters that must be estimated. Pairwise likelihood estimation is performed with the function `GeoFit`:

In this example, we perform optimization of (7) and (8) using the function `BFGS`. However other type of optimization algorithms can be used (`nlminb` or `BFGS-LB` or `Nelder-Mead` for instance). We use the following code to estimate the parameters $\boldsymbol{\theta}_Y$ of the Gaussian random fields (note that the fixed parameter β of the correlation model (1) is reparametrized with its inverse in the `GeoModels` package, following a suggestion in Bevilacqua et al. (2020))

```
model="Gaussian"
dd=120
start=list(mean=mean(z) ,sill=var(z),nugget=0.10,scale=200)
fixed=list(smooth=0,power2=1/3.5)
pcl1=GeoFit(coordx=loc,corrmodel=corrmodel,data=z,model=model,
 maxdist=dd,optimizer="BFGS", start=start,fixed=fixed)
```

Note that the option *maxdist=120* set the compact support of the weight function i.e. $d = 120$ in (9). This specific arbitrary choice of d in the weight function (9) allows to improve the computational efficiency of the method. The object `pcl1` include information about the pairwise likelihood estimation:

```
pcl1
#################################################################
Maximum  Composite-Likelihood Fitting of Gaussian Random Fields
Setting: Marginal Composite-Likelihood
Model: Gaussian
Type of the likelihood objects: Pairwise
Covariance model: GenWend_Matern
Optimizer: BFGS
Number of spatial coordinates: 7352
Number of dependent temporal realisations: 1
Type of the random field: univariate
Number of estimated parameters: 4
Type of convergence: Successful
Maximum log-Composite-Likelihood value: -427763.58
Estimated parameters:
     mean      nugget       scale        sill
 -0.06536     0.16975   205.51929     0.69028
#################################################################
```

Similarly, we use the following code to estimate the parameters $\boldsymbol{\theta}_{U_\eta}$ of the skew-Gaussian random fields.

```
model="SkewGaussian"
dd=120
start=list(mean=mean(z),sill=var(z),nugget=0.1,skew=0.7,scale=200)
fixed=list(smooth=0, power2=1/3.5)
pcl2=GeoFit(coordx=loc,corrmodel=corrmodel,data=z,
    model=model,maxdist=dd,optimizer="BFGS",start=start,fixed=fixed)
```

The object `pcl2` include informations about the pairwise likelihood estimation:

```
pcl2
#################################################################
Maximum  Composite-Likelihood Fitting of Skew Gaussian Random Fields
```

```
Setting: Marginal Composite-Likelihood
Model: SkewGaussian
Type of the likelihood objects: Pairwise
Covariance model: GenWend_Matern
Optimizer: BFGS
Number of spatial coordinates: 7352
Number of dependent temporal realisations: 1
Type of the random field: univariate
Number of estimated parameters: 5
Type of convergence: Successful
Maximum log-Composite-Likelihood value: -426729.45
Estimated parameters:
    mean     nugget      scale       sill       skew
 -0.6895     0.2446   284.9527     0.4665     0.7827
#################################################################
```

The estimation of the skew parameter shows the presence of negative asymmetry in the anomalies data. Additionally, it can be appreciated that the skew Gaussian case shows a better maximum log-(Composite) Likelihood value, as expected, since the Gaussian RF is a special case of the skew Gaussian RF.

Checking model assumptions

Given the estimation of the Gaussian and skew-Gaussian random fields, the estimated residuals are

$$\widehat{Y(\boldsymbol{s}_i)} = \frac{y(\boldsymbol{s}_i) - \widehat{\mu}}{(\widehat{\sigma}^2)^{\frac{1}{2}}} \quad i = 1, \dots N \tag{10}$$

and

$$\widehat{U_\eta(\boldsymbol{s}_i)} = \frac{u(\boldsymbol{s}_i) - \widehat{\mu}}{(\widehat{\sigma}^2)^{\frac{1}{2}}} \quad i = 1, \dots N \tag{11}$$

$\widehat{Y(\boldsymbol{s}_i)}$, for $i = 1, \dots N$ can be viewed as a realization of a Gaussian random field with marginal distribution $N(0,1)$ and with correlation function $\rho(\boldsymbol{h})$. Similarly $\widehat{U_\eta(\boldsymbol{s}_i)}$ for $i = 1, \dots N$ can be viewed as a realization of a random field stationary of (3) with marginal distribution $SN(0, \omega, \delta)$ with $\delta = \eta/\sigma$, $\omega^2 = (\eta^2 + \sigma^2)/\sigma^2$ and with correlation function $\rho_{U_\eta}(\boldsymbol{h})$. The residuals can be computed using the `GeoResiduals` function:

```
resd1=GeoResiduals(pcl1); # residuals of Gaussian random field
```

```
resd2=GeoResiduals(pcl2); # residuals of skew-Gaussian random field
```

The marginal distribution assumption on the residuals can be graphically checked for instance with a qq-plot (see, Figure (4)) using the function `GeoQQ`:

```
### checking model  residuals assumptions: marginal distribution
GeoQQ(resd1);   #qq-plot residuals of Gaussian random field
GeoQQ(resd2);   #qq-plot residuals of skew-Gaussian random field
```

It can be appreciated that the skew Gaussian case shows a better agreement between the theoretical and estimated quantiles with respect to the Gaussian case. Additionally, the covariance model assumption can be checked comparing the empirical and the estimated semi-variogram of the residuals using the `GeoVariogram` and `GeoCovariogram` functions (see Figure (4)).

```
### checking model  residuals assumptions: covariance model

### semi-variogram residuals of Gaussian Random fields
vario1 <- GeoVariogram(data=resd2$data, coordx=loc,
          maxdist=maxdist/4);
GeoCovariogram(resd1,show.vario=TRUE,vario1=evariog,pch=20);

### semi-variogram residuals of skew-Gaussian Random fields
evariog2 <- GeoVariogram(data=resd2$data,coordx=loc,
            maxdist=maxdist/4);
GeoCovariogram(resd2,show.vario=TRUE,vario=evariog2,pch=20);
```

It can be appreciated that in both cases the estimated semivariogram exhibits a good agreement with the empirical semivariogram.

Prediction

The package `GeoModels` allows to perform optimal linear prediction for the Gaussian and skew-Gaussian RFs. In the Gaussian case optimal linear prediction is equal to the optimal prediction (in the mean squared sense).

For a given spatial location $\boldsymbol{s}_0$, the optimal linear prediction of a Gaussian or skew-Gaussian RFs is given by:

$$\widehat{L}(\boldsymbol{s}_0) = \mu + \boldsymbol{c}^T R^{-1}[\boldsymbol{l} - \mu], \tag{12}$$

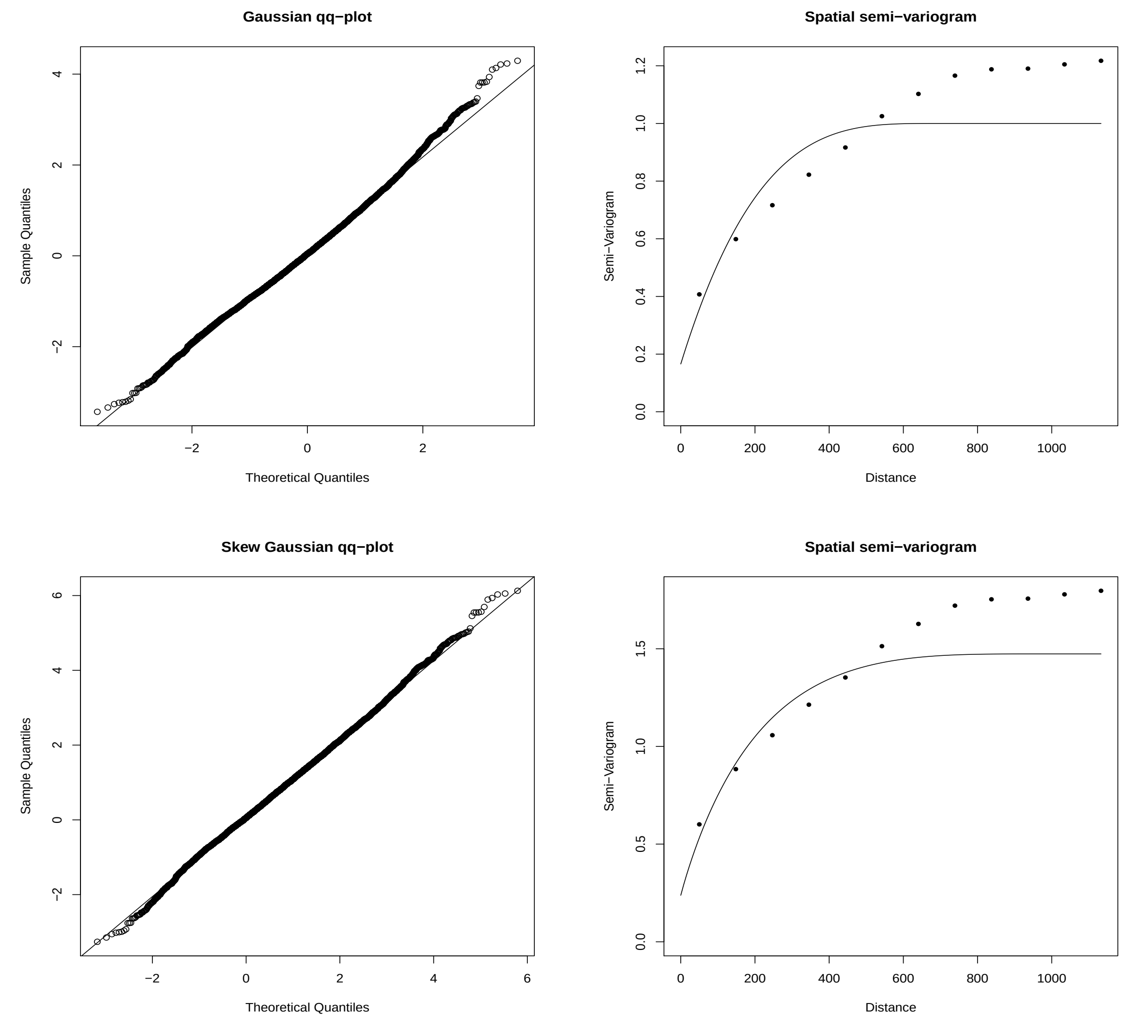

Figure 4: Upper part: qq-plot of the Gaussian residuals and empirical vs estimated semi-variogram of the residuals (from left to right). Bottom part: qq-plot of the skew Gaussian residuals and empirical vs estimated semi-variogram of the residuals (from left to right).

with $\widehat{L}(\boldsymbol{s}_0) = Y(\boldsymbol{s}_0)$, $\boldsymbol{l} = \boldsymbol{Y}$ or $\widehat{L}(\boldsymbol{s}_0) = U_\eta(\boldsymbol{s}_0)$, $\boldsymbol{l} = \boldsymbol{U}_\eta$ for the Gaussian and skew-Gaussian cases respectively. In addition:

- $\boldsymbol{c} = (cor(L(\boldsymbol{s}_0), L(\boldsymbol{s}_1)), \dots, cor(L(\boldsymbol{s}_0), L(\boldsymbol{s}_N)))^T$.
- $R = [\mathrm{cor}(L(\boldsymbol{s}_i), L(\boldsymbol{s}_j)]]_{i,j=1}^N$.

both R and $\boldsymbol{c}$ are computed by using $\rho(\boldsymbol{h})$ and $\rho_{U_\eta}(\boldsymbol{h})$ for the Gaussian and skew-Gaussian case respectively. Moreover the associated mean square error (MSE) is given by:

$$MSE(\widehat{L}(\boldsymbol{s}_0)) = Var(L(\boldsymbol{s}))(1 - \boldsymbol{c}^T R^{-1}\boldsymbol{c}). \tag{13}$$

where $Var(L(\boldsymbol{s}))$ is given by $Var(Y(\boldsymbol{s})) = \sigma^2$ and $Var(U_\eta(\boldsymbol{s})) = \sigma^2 + \eta^2(1 - 2/\pi)$ for the Gaussian and skew-Gaussian RF respectively. Both (12) and (13) can be computed replacing the parameters with the pairwise likelihood estimates.

Kriging computation involve the (inverse of) the correlation matrix. If the correlation model is compactly supported as the model in (1) then the package `GeoModels` allows the use of sparse matrix algorithms implemented in `spam` package (Furrer and Sain (2010)). The estimated covariance matrices in the Gaussian and skew-Gaussian cases can be obtained with the following code:

```
matrix1 = GeoCovmatrix(coordx=loc,corrmodel=corrmodel,sparse=TRUE,
 model="Gaussian",param=as.list(c(pcl1$param,pcl1$fixed)))
matrix2 = GeoCovmatrix(coordx=loc,corrmodel=corrmodel,sparse=TRUE,
 model="SkewGaussian",param=as.list(c(pcl2$param,pcl2$fixed)))
```

Note that the option `sparse=TRUE` means that the covariances matrices are computed as `spam` object. For instance we can compute the nonsparsity (i.e.the percentage of nonzero in the covariance matrices) with the following code:

```
matrix1$nozero; matrix2$nozero
[1] 0.1595542
[1] 0.2668984
```

This means that approximatively 85% and 74% of the elements of the covariance matrices are zeros.

We further evaluate the predictive performances of the Gaussian and skew Gaussian RFs using cross validation, with the function `GeoCV`.

```
a1=GeoCV(pcl1, K=50, n.fold=0.25,seed=9,sparse=TRUE)
[1] ‘Cross-validation  kriging can be time consuming ...‘
[1] ‘Starting iteration from 1 to 50  ...‘
a2=GeoCV(pcl2, K=50, n.fold=0.25,seed=9,sparse=TRUE)
[1] ‘Cross-validation  kriging can be time consuming ...
[1] ‘Starting iteration from 1 to 50  ...
```

The function basically randomly choose 75% of the spatial locations and use the remaining 25% as data for the predictions, where the (optimal linear) predictions are internally obtained using GeoKrig function. Then some prediction scores as RMSE and MAE (Gneiting and Raftery, 2007) are constructed by comparing the predictions with the (known) values. This is iterated 50 times (it can computationally intensive for large datasets as in this example).

We can compare the two RFs from prediction viewpoint, using the empirical mean of the 50 RMSEs and MAEs

```
> mean(a1$rmse);
[1] 0.4779008
> mean(a2$rmse);
[1] 0.4774589
> mean(a1$mae);
[1] 0.3634575
> mean(a2$mae);
[1] 0.3630654
```

It can be appreciated that the estimated skew Gaussian RF perform slightly better from prediction viewpoint even if, in the skew-Gaussian case, the optimal linear prediction is used.

A kriging map with associated MSE can be obtained using the GeoKrig function. For the given location sites, we first need to specify the border of the region and then to construct a fine grid inside the border. The following code perform this task:

```
Sr1 = Polygon(loc)
Srs1 = Polygons(list(Sr1), "s1")
SpP = SpatialPolygons(list(Srs1))
long1=min(loc[,1])-10;long2=max(loc[,1])+10
lat1=min(loc[,2])-10;lat2=max(loc[,2])+10
lat_seq=seq(lat1,lat2,24)
lon_seq=seq(long1,long2,24)
coords_tot=as.matrix(expand.grid(lon_seq,lat_seq))
gr.in <- locations.inside(coords_tot, SpP)
```

Then optimal linear prediction (12) and associated MSE (13) can be computed (using the estimated parameters) for the Gaussian and skew Gaussian cases, with the following code (the procedure are computationally intensive for this example)

```
pr1<-GeoKrig(loc=gr.in,coordx=loc,corrmodel=corrmodel,mse=TRUE,
```

```
  model="Gaussian",sparse=TRUE,
  param=as.list(c(pcl1$param,pcl1$fixed)),data=z)
pr2<-GeoKrig(loc=gr.in,coordx=loc,corrmodel=corrmodel,mse=TRUE,
  model="SkewGaussian",sparse=TRUE,
  param=as.list(c(pcl2$param,pcl2$fixed)),data=z)
```

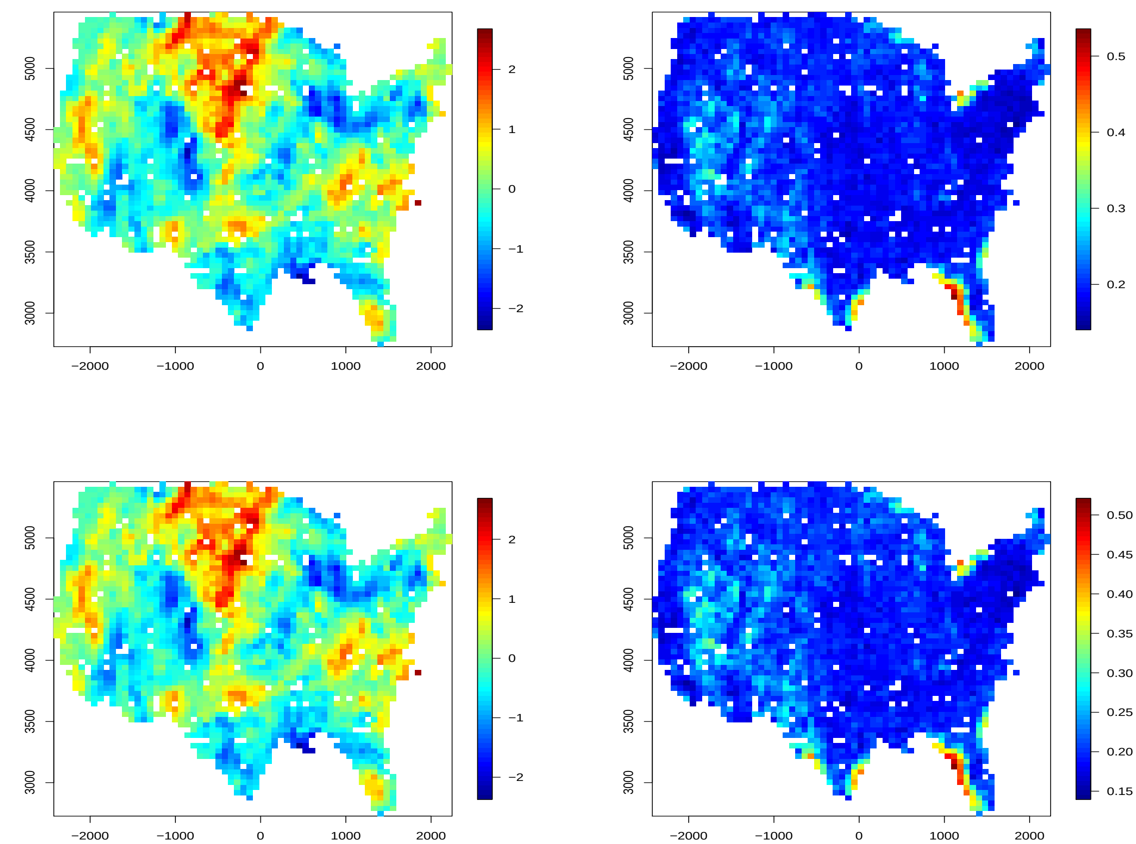

Figure 5: Kriging map and mean squared error map for the Gaussian (first row) and SkewGaussian (second row) RFs.

Finally a kriging map with associated mean square error (Figure 5) can be obtained with the following code:

```
quilt.plot(gr.in,pr1$pred)
quilt.plot(gr.in,pr1$mse)
quilt.plot(gr.in,pr2$pred)
quilt.plot(gr.in,pr2$mse)
```

References

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