

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

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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)
```

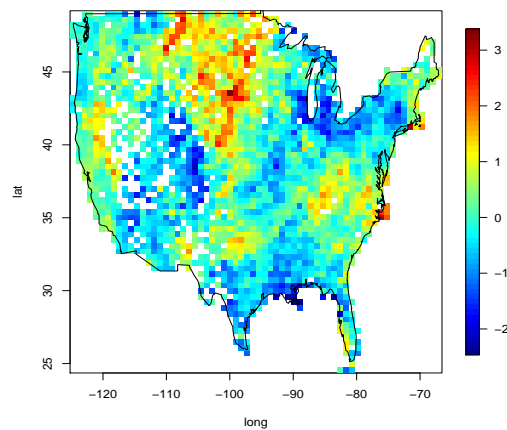


Figure 1: Coloured map of anomalies data.

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 asymmetry. 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)
```

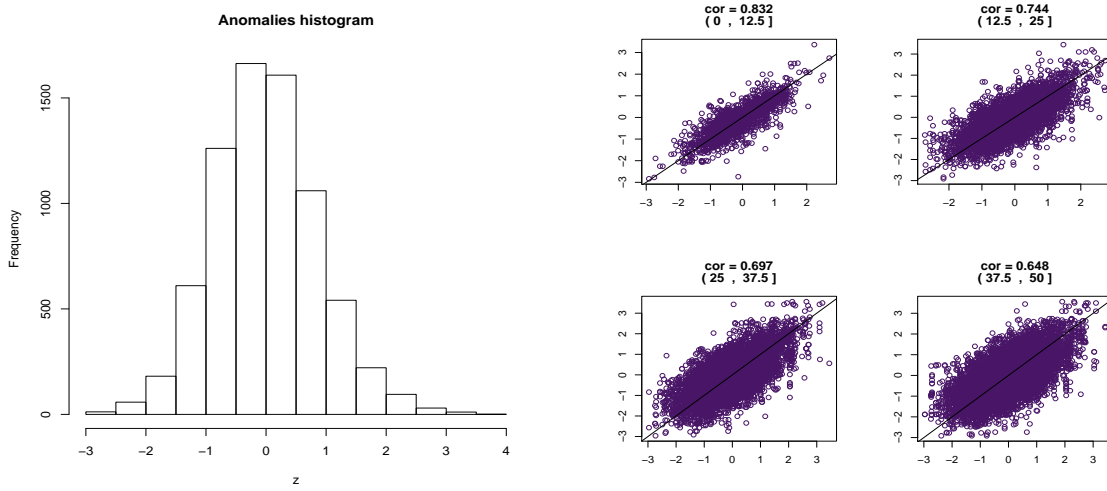


Figure 2: From left to right: histogram of anomalies data and associated h -scatterplot.

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")
```

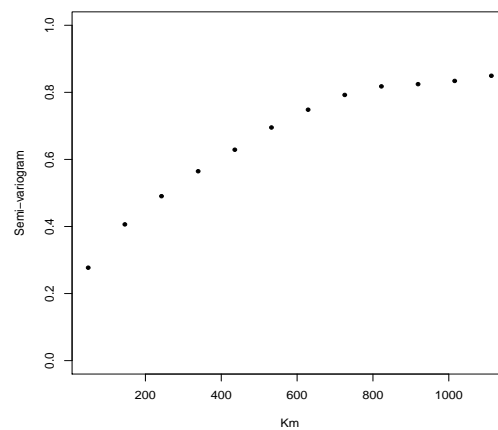


Figure 3: Empirical semi-variogram of anomalies data.

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 $G = \{G(\mathbf{s}), \mathbf{s} \in S\}$, where \mathbf{s} represents a location in the domain $S \subset \mathbb{R}^2$ with isotropic reparametrized (special case of) generalized Wendland function as proposed in Bevilacqua et al. (2020) with a nugget effect that is:

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

Here $\|\mathbf{h}\|$ is the Euclidean distance and $0 \leq \tau^2 < 1$ represents the nugget parameter. Additionally $\alpha > 0$ is a spatial dependence parameter and $\beta \geq 3/2$ is a parameter that allows to switch from compact support to global support dependence. In particular when $\beta \rightarrow \infty$ 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 random fields in our analysis. The first is a location-scale transformation of G that is a random field $Y = \{Y(\mathbf{s}), \mathbf{s} \in A\}$ defined as:

$$Y(\mathbf{s}) := \mu(\mathbf{s}) + \sigma G(\mathbf{s}) \quad (2)$$

with $\mathbb{E}(Y(\mathbf{s})) = \mu(\mathbf{s}) \in \mathbb{R}$ and $Var(Y(\mathbf{s})) = \sigma^2 > 0$.

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

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

with $\mathbb{E}(U_\eta(\mathbf{s})) = \mu(\mathbf{s}) + \eta\sqrt{2/\pi}$ and $Var(U_\eta(\mathbf{s})) = \sigma^2 + \eta^2(1 - 2/\pi)$ where $\eta \in \mathbb{R}$ is the asymmetry parameter, $\sigma > 0$ and G_i $i = 1, 2$ are two independent copies of a process G . More precisely, G_1 is a Gaussian random field with correlation (1) (assuming zero nugget) and G_2 is an independent Gaussian random field with correlation (1). Note that if $\eta = 0$ the Gaussian random field in (2) is obtained. As a consequence (3) is a generalization of

(2). The correlation function of the Skew-Gaussian random field is given by (Zhang and El-Shaarawi, 2010)

$$\rho_{U_\eta}(\mathbf{h}) = \frac{2\eta^2}{\pi\sigma^2 + \eta^2(\pi - 2)} \left((1 - \rho_1^2(\mathbf{h}))^{1/2} + \rho_1(\mathbf{h}) \arcsin(\rho_1(\mathbf{h})) - 1 \right) + \frac{\sigma^2 \rho(\mathbf{h})}{\sigma^2 + \eta^2(1 - 2/\pi)}. \quad (4)$$

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

For both random fields we assume a constant mean $\mu(\mathbf{s}) = \mu$, 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 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 $\mathbf{Y} = (y(\mathbf{s}_1), y(\mathbf{s}_2), \dots, y(\mathbf{s}_N))^T$ 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

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

with respect to $\boldsymbol{\theta}_Y = (\mu, \sigma^2, \alpha, \beta, \tau^2)^T$. Here $R = [\rho(\mathbf{s}_i - \mathbf{s}_j)]_{i,j=1}^N$ 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 $\mathbf{Y}_{ij} = (Y(\mathbf{s}_i), Y(\mathbf{s}_j))$ that is $f_{\mathbf{Y}_{ij}}(y_i, y_j; \boldsymbol{\theta}_Y)$

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

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

where $\boldsymbol{\theta}_{U_\eta} = (\mu, \sigma^2, \eta, \alpha, \beta, \tau^2)^T$, $\boldsymbol{\mu}_{ij} = (\mu, \mu)^T$ and \mathbf{A}_l , \mathbf{B}_l , \mathbf{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

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

and the pairwise likelihood function associated to U_η is given by

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

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

$$w_{ij} = \begin{cases} 1 & \mathbf{s}_i \in N_x(\mathbf{s}_j) \cup \mathbf{s}_j \in N_x(\mathbf{s}_i) \\ 0 & \text{otherwise} \end{cases} \quad (9)$$

where $N_x(\mathbf{s}_l)$ is the set of the neighbors of order x of the point \mathbf{s}_l . This kind of symmetric weights are computationally convenient since the distances involved can be computed efficiently using fast neighborhood algorithms. In particular the **GeoModels** package, exploits the functions implemented in the package **RANN**.

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 (**nllminb** 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)). The option `neighbs` set the order of neighbors in the weight function (9).

```
model="Gaussian"
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,
  neighb=10,optimizer="BFGS", start=start,fixed=fixed)
```

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: -85203.33
Estimated parameters:
      mean      nugget      scale      sill
-0.001864    0.102946   154.786753    0.762993
#####
```

Similarly, we use the following code to estimate the parameters θ_{U_η} of the skew-Gaussian random fields.

```
model="SkewGaussian"
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,neighb=10,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: -84932.40
Estimated parameters:
      mean      nugget      scale      sill      skew
      -0.6941      0.1471    216.8178      0.4868      0.8688
#####

```

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 random field is a special case of the skew Gaussian random field.

Checking model assumptions

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

$$\widehat{Y(s_i)} = \frac{y(s_i) - \hat{\mu}}{(\hat{\sigma}^2)^{\frac{1}{2}}} \quad i = 1, \dots, N \quad (10)$$

and

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

$\widehat{Y(s_i)}$, 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 $\rho(\mathbf{h})$. Similarly $\widehat{U_\eta(s_i)}$ 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 $\rho_{U_\eta}(\mathbf{h})$. 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 random fields. In the Gaussian case optimal linear prediction is equal to the optimal prediction (in the mean squared sense).

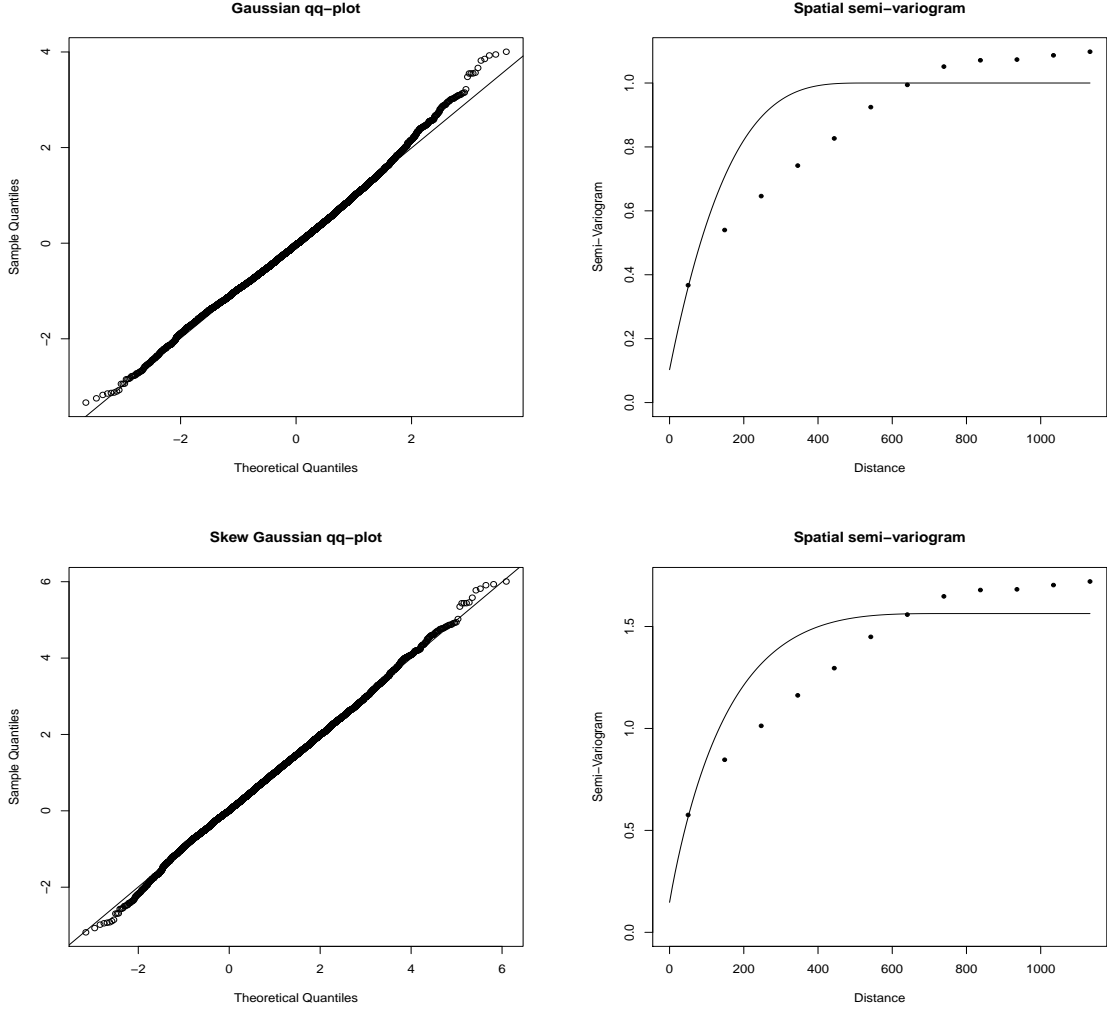


Figure 4: Upper part: qq-plot of the Gaussian residuals and empirical vs estimated semi-variogram of the residuals (from left to right). Bottom part: qq-plot of the skew Gaussian residuals and empirical vs estimated semi-variogram of the residuals (from left to right).

For a given spatial location \mathbf{s}_0 , the optimal linear prediction of a Gaussian or skew-Gaussian random fields is given by:

$$\hat{L}(\mathbf{s}_0) = \mu + \mathbf{c}^T R^{-1}[\mathbf{l} - \mu], \quad (12)$$

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

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

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

$$MSE(\hat{L}(\mathbf{s}_0)) = Var(L(\mathbf{s}))(1 - \mathbf{c}^T R^{-1} \mathbf{c}). \quad (13)$$

where $Var(L(\mathbf{s}))$ is given by $Var(Y(\mathbf{s})) = \sigma^2$ and $Var(U_\eta(\mathbf{s})) = \sigma^2 + \eta^2(1 - 2/\pi)$ for the Gaussian and skew-Gaussian random field 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] 0.1007367
[1] 0.1738654
```

This means that approximatively 90% and 83% of the elements of the covariance matrices are zeros.

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

```
a1=GeoCV(pcl1, K=50, n.fold=0.25,seed=9,local=TRUE,neighb=100)
[1] 'Cross-validation kriging can be time consuming ...'
[1] 'Starting iteration from 1 to 100 ...'
a2=GeoCV(pcl2, K=50, n.fold=0.25,seed=9,local=TRUE,neighb=100)
[1] 'Cross-validation kriging can be time consuming ...'
[1] 'Starting iteration from 1 to 100 ...'
```

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 the `GeoKrigloc` function. This function perform local kriging using a fixed set of neighbors specified in the `neighb` option. 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 100 times (it can computationally intensive for large datasets, as in this example). We can compare the two models from prediction viewpoint, using the empirical mean of the 100 RMSEs and MAEs

```
> mean(a1$rmse);
[1] 0.4793319
> mean(a2$rmse);
[1] 0.4789699
> mean(a1$mae);
[1] 0.3634462
> mean(a2$mae);
[1] 0.363221
```

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

A kriging map with associated MSE can be obtained using the `GeoKrig` or the `GeoKrigloc` 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 (local) 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:

```
pr1<-GeoKrigloc(loc=gr.in,coordx=loc,corrmodel=corrmodel,mse=TRUE,  
  model="Gaussian",neighb=100,  
  param=as.list(c(pcl1$param,pcl1$fixed)),data=z)  
pr2<-GeoKrigloc(loc=gr.in,coordx=loc,corrmodel=corrmodel,mse=TRUE,  
  model="SkewGaussian",neighb=100,  
  param=as.list(c(pcl2$param,pcl2$fixed)),data=z)
```

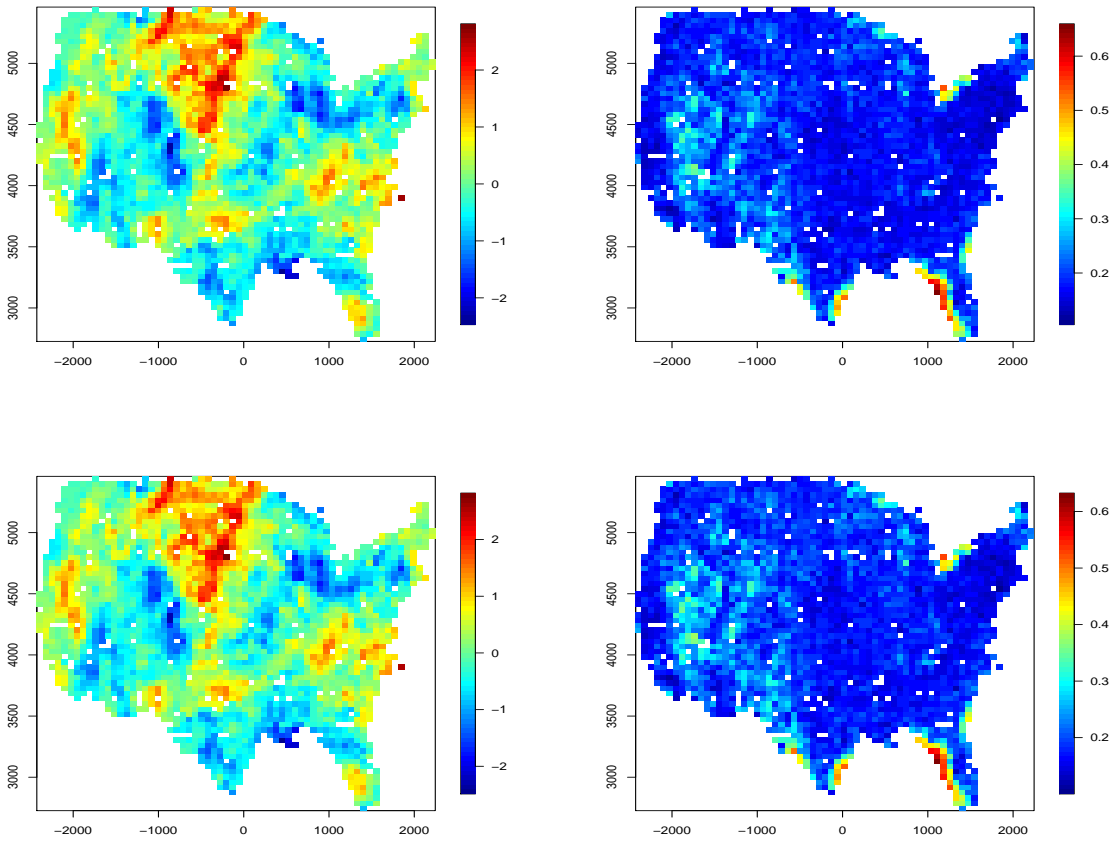


Figure 5: Kriging map and mean squared error map for the estimated. Gaussian (first row) and SkewGaussian (second row) random fields.

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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- Bevilacqua, M., C. Caamaño-Carrillo, and E. Porcu (2020). Unifying compactly supported and matérn covariance functions in spatial statistics. *ArXiv e-prints*.
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