# GeoModels Tutorial: analysis of spatial precipitation anomalies

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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(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)
```

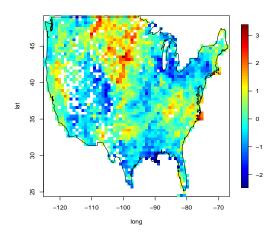


Figure 1: Coloured map of anomalies data.

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

```
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 suggests 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)
```

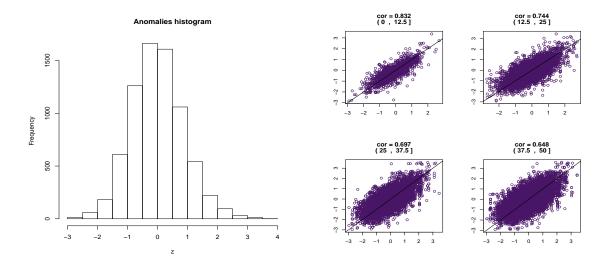


Figure 2: From left to right: histrogram of anomalies data and associated h-scatterlylot.

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,ylim=c(0,1), pch=20,xlab="Km",ylab="Semi-variogram")
```

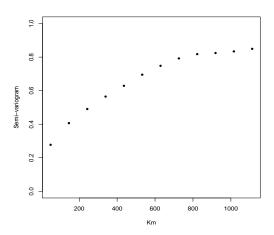


Figure 3: Empirical semi-variogram of anomalies data.

This preliminary graphical analysis suggest the a Gaussian or a skew-Gaussian random field with a covariance model including a nugget effect can be suitable models for the anomalies data.

#### 2 Gaussian and skew-Gaussian random fields

We first consider a zero mean, unit variance and weakly stationary standard Gaussian random field  $G = \{G(s), s \in S\}$ , where s represents a location in the domain  $S \subset \mathbb{R}^2$  with isotropic exponential correlation model with a nugget effect that is:

$$\rho(\mathbf{h}) = \begin{cases} 1 & ||\mathbf{h}|| = 0\\ (1 - \tau^2)e^{-||\mathbf{h}|/\alpha} & ||\mathbf{h}|| > 0 \end{cases}$$
 (1)

Here  $||\boldsymbol{h}||$  is the Euclidean distance and  $0 \le \tau^2 < 1$  represents the nugget parameter. Additionally  $\alpha > 0$  is a spatial dependence parameter.

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

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

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

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

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

with  $\mathbb{E}(U_{\eta}(s)) = \mu(s) + \eta \sqrt{2/\pi}$  and  $Var(U_{\eta}(s)) = \sigma^2 + \eta^2(1 - 2/\pi)$  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 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)

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

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

For both random fields we assume a constant mean  $\mu(s) = \mu$ . However, the GeoModels package allows to specify a model regression for the spatial mean.

To obtain the names of the correlation parameters of the correlation model (1) and the names of the nuisance parameters of the Gaussian and Skew-Gaussian models, two useful functions are CorrParam and NuisParam:

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

For the exponential model we consider a Matern model where scale is the  $\alpha$  parameter in equation (1) and smooth is a smoothness parameter that will be fixed equal to 0.5. Finally nugget is the  $\tau^2$  parameter, sill is the  $\sigma^2$  parameter, skew is the  $\eta$  parameter and mean is the constant mean parameter  $\mu$ .

#### 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

$$f_{\mathbf{Y}}(y_1, \dots, y_N; \boldsymbol{\theta}_Y) = (2\pi)^{-N/2} |\sigma^2 R|^{-1/2} \exp\left\{-\frac{(\mathbf{Y} - \mu \mathbf{1}_N)^T R^{-1} (\mathbf{Y} - \mu \mathbf{1}_N)}{2\sigma^2}\right\}$$
 (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 composite likelihood estimation method based on pairs. Specifically we focus on the conditional pairwise likelihood method as described in Bevilacqua and Gaetan (2015). This method involve only the bivariate and marginal pdfs associated with the bivariate random vector  $\mathbf{Y}_{ij} = (Y(\mathbf{s}_i), Y(\mathbf{s}_j))^T$ .

Similarly, given a realization  $U_{\eta} = (u_{\eta}(s_1), u_{\eta}(s_2), \dots, u_{\eta}(s_N))^T$ , from a skew-Gaussian random field the conditional pairwise likelihood method involves the bivariate and marginal pdfs of the bivariate random vector  $U_{\eta;ij} = (U_{\eta}(s_i), U_{\eta}(s_j))^T$ . In particular the bivariate pdf is given by (Alegria et al., 2017):

$$f_{U_{\eta;ij}}(u_i, u_j; \boldsymbol{\theta}_{U_{\eta}}) = 2\sum_{l=1}^{2} \phi_2(\boldsymbol{u}_{ij} - \boldsymbol{\mu}_{ij}; \boldsymbol{A}_l) \Phi_n(\boldsymbol{c}_l; \boldsymbol{0}, \boldsymbol{B}_l)$$
(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 conditional pairwise likelihood function associated to Y is given by

$$pl(\boldsymbol{\theta}_Y) = \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} [log(f_{\boldsymbol{Y}_{ij}}(y_i, y_j)) - log(f_{\boldsymbol{Y}_j}(y_j))] w_{ij}$$

$$(7)$$

and the conditional pairwise likelihood function associated to  $U_{\eta}$  is given by

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

where  $w_{ij}$  are non-negative non-symmetric weights specified as:

$$w_{ij}(k) = \begin{cases} 1 & \mathbf{s}_i \in N_k(\mathbf{s}_j) \\ 0 & \text{otherwise.} \end{cases}$$
 (9)

Here  $N_k(\mathbf{s}_l)$  is the set of the neighbors of order k of the point  $\mathbf{s}_l$ . This kind of weights are computationally convenient since kd-tree type algorithms can be used to find exact or approximate nearest neighbors of order k for each location sites, that is  $N_k(\mathbf{s}_l)$  for  $l = 1, \ldots, n$  with a computational complexity of order Nlog(N) and associated storage of order N.

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

In the GeoModels package we can choose the fixed parameters and the parameters that must be estimated. Conditional pairwise likelihood estimation is performed with the function GeoFit2. This function performs a preliminary estimation of the marginal parameters under the assumption of independence (the so-called independence composite likelihood) and then compute conditional pairwise likelihood estimation optimization using the estimates at first step as starting value.

In this example, we perform optimization of (7) and (8) using the function nlminb that allows for box-constrained optimization. We use the following code to estimate the parameters  $\theta_Y$  of the Gaussian random field (the option neighbs set the order of neighbors k in the weight function (9) and the lower and lower objects define the upper and lower bounds of the parametric space).

```
I=Inf
lower=list(mean=-I,sill=0,nugget=0,scale=0)
upper=list(mean=I,sill=I,nugget=1,scale=I)
start=list(mean=mean(z),sill=var(z),nugget=0.10,scale=140)
```

```
fixed=list(smooth=0.5)
## estimation
pcl1=GeoFit2(coordx=loc,corrmodel=corrmodel,data=z,
likelihood="Conditional",type="Pairwise",model="Gaussian",
    optimizer="nlminb",lower=lower,upper=upper, neighb=3,
    start=start,fixed=fixed,sensitivity=TRUE)
```

The object pcl1 include information about the pairwise likelihood estimation:

```
pcl1
Maximum Composite-Likelihood Fitting of Gaussian Random Fields
Setting: Conditional Composite-Likelihood
Model: Gaussian
Type of the likelihood objects: Pairwise
Covariance model: Matern
Optimizer: nlminb
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: -19189.38
Estimated parameters:
                    scale
                              sill
   mean
           nugget
 0.03651
          0.07004 112.69057
                            0.79248
```

We now estimate the skew-Gaussian random field.

```
start=list(nugget=0, scale=100, mean=mean(z), sill=var(z), skew=0.4)
fixed=list(smooth=.5)
lower2=list(mean=-I, sill=0, skew=-I, scale=0, nugget=0)
upper2=list(mean=I, sill=I, skew=I, scale=I, nugget=1)
pcl2=GeoFit2(coordx=loc, corrmodel=corrmodel, data=z,
    likelihood="Conditional", type="Pairwise", model="SkewGaussian",
optimizer="nlminb", lower=lower2, upper=upper2,
    neighb=3, start=start, fixed=fixed, sensitivity=TRUE)
pcl2
```

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

```
pcl2
Maximum Composite-Likelihood Fitting of Skew Gaussian Random Fields
Setting: Conditional Composite-Likelihood
Model: SkewGaussian
Type of the likelihood objects: Pairwise
Covariance model: Matern
Optimizer: nlminb
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: -19145.47
Estimated parameters:
    mean
          nugget
                     scale
                              sill
                                        skew
-0.63582
          0.09506 156.00527
                            0.53085
                                     0.84761
```

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 higher maximum log-conditional pairwise likelihood value, as expected, since the Gaussian random field is a special case of the skew Gaussian random field.

In both cases standard error estimation can be performed using parametric bootstrap. To speed up the computation an approximate simulation method based on Vecchia's method and implemented in the package GpGp, is used

Standard error estimates and interval confidence can be obtained as:

```
pcl1_est$stderr;pcl2_est$stderr;
                 nugget
                               scale
                                             sill
       mean
0.100441564 0.008147183 9.537681942 0.058867922
                 nugget
                               scale
                                             sill
                                                          skew
 0.15168541
             0.01865673 20.13690531
                                       0.07947798
                                                   0.11490896
 pcl1_est$conf.int;pcl2_est$conf.int
                   nugget
                                           sill
low -0.1603493 0.05406781
                            93.99706 0.6770985
     0.2333744 0.08600418 131.38409 0.9078566
                  nugget
                             scale
                                         sill
                                                   skew
          mean
low -0.9331178 0.0584939 116.5377 0.3750713 0.6223956
upp -0.3385219 0.1316270 195.4729 0.6866193 1.0728305
```

Finally model selection can be performed using the AIC criteria for composite likelihood

```
pcl1_est$claic;pcl2_est$claic
[1] 38507.35
[1] 38495.07
```

It turns out that the information criteria selects the skew-Gaussian random field.

## Checking model assumptions

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

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

and

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

 $\widehat{Y(s_i)}$ , for  $i=1,\ldots N$  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  $i=1,\ldots N$  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)).

It can be seen that in the skew-Gaussian model the estimated semivariogram presents a better 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).

For a given spatial location  $s_0$ , the optimal linear prediction of a Gaussian or skew-Gaussian random fields is given by:

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

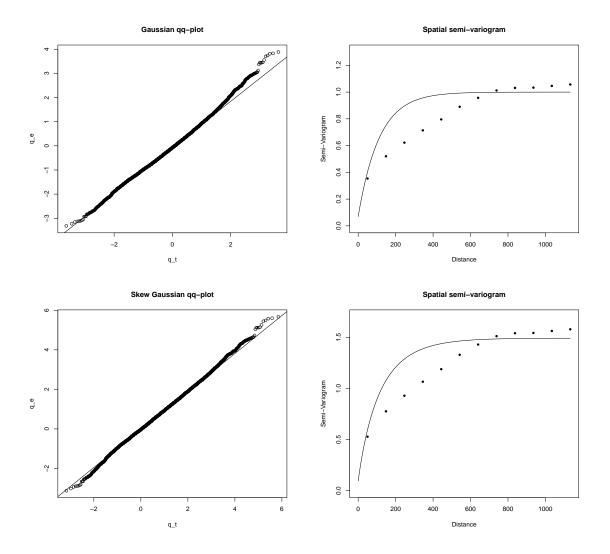


Figure 4: Upper part: qq-plot of the Gaussian residuals and empirical vs estimated semi-variogram of the residuals (from left to right). Bottom part: qq-plot of the skew Gaussian residuals and empirical vs estimated semi-variogram of the residuals (from left to right).

with  $\widehat{L}(s_0) = Y(s_0)$ , l = Y or  $\widehat{L}(s_0) = U_{\eta}(s_0)$ ,  $l = U_{\eta}$  for the Gaussian and skew-Gaussian cases respectively. In addition:

- $c = (cor(L(s_0), L(s_1)), \dots, cor(L(s_0), L(s_N)))^T$ .
- $R = [\operatorname{cor}(L(s_i), L(s_j))]_{i,j=1}^N$ .

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

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

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

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

The function basically randomly choose 75% of the data for estimation and prediction and use the remaining 25% as validation dataset. To speed-up the computation, the (optimal linear) predictions are internally obtained using the GeoKrigloc function that perform local kriging using a fixed set of neighbors specified in the neighb option. Then some prediction scores as RMSE (root mean squared error) and MAE (mean absolute value) are constructed by comparing the predictions with the (known) values in the validation dataset. This is iterated 100 times (it can be computationally intensive for large datasets, as in this example). We can compare the two models from prediction performance viewpoint, using the empirical mean of the 100 RMSEs and MAEs

```
mean(a1$rmse); mean(a2$rmse);
[1] 0.4819512
[1] 0.4813987
> mean(a1$mae); mean(a2$mae);
[1] 0.364884
[1] 0.3645455
```

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)</pre>
```

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)</pre>
```

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

Alegria, A., S. Caro, M. Bevilacqua, E. Porcu, and J. Clarke (2017). Estimating covariance functions of multivariate skew-gaussian random fields on the sphere. *Spatial Statistics* 22, 388 – 402. Spatio-temporal Statistical Methods in Environmental and Biometrical Problems.

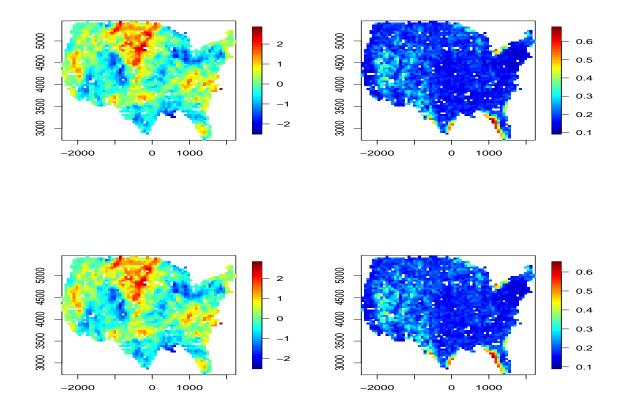


Figure 5: Kriging map and mean squared error map for the estimated. Gaussian (first row) and SkewGaussian (second row) random fields.

Bevilacqua, M. and C. Gaetan (2015). Comparing composite likelihood methods based on pairs for spatial Gaussian random fields. *Statistics and Computing* 25, 877–892.

Furrer, R. and S. R. Sain (2010). spam: A sparse matrix R package with emphasis on MCMC methods for Gaussian Markov random fields. *Journal of Statistical Software* 36(10), 1–25.

Kaufman, C. G., M. J. Schervish, and D. W. Nychka (2008). Covariance tapering for likelihood-based estimation in large spatial data sets. *Journal of the American Statistical* Association 103, 1545–1555.

Zhang, H. and A. El-Shaarawi (2010). On spatial skew-Gaussian processes and applications. Environmetrics 21(1), 33–47.