# Package 'Manifoldgstat'

July 13, 2019

Type Package

Title Kriging prediction for manifold-valued data.

Version 1.0.0
Description Predictive analysis for manifold-valued data. This package provides a C++ implementation of functions to create a model for spatial dependent manifold-valued data, in order to perform kriging.  In each location, specified by a vector of coordinates ([lat,long], [x,y] or [x,y,z]), the datum is supposed to be a symmetric positive definite matrix. The user is provided with three main functions: model_kriging, full_RDD, mixed_RDD, each designed to deliver kriging predictions following the corresponding algorithm (GlobalModel, FullRDD and MixedRDD), as presented in the reference dissertation. They exploit, to different extents, tangent space approximations, Random Domain Decomposition and advanced differential geometry concepts like parallel transport.
<b>Reference</b> Ilaria Sartori Luca Torriani (2019): Mixed Random Domain Decomposition: an innovative approach for kriging prediction of manifold valued data, Master Degree Thesis
<b>Depends</b> R (>= 3.2.0), Rcpp (>= 0.12.16), RcppEigen (>= 0.3.3.4.0), plyr(>= 1.8.4)
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R topics documented:  assign2center bootstrapVar create.rdd distance_manifold Eucldist full_RDD Geodist intrinsic_mean

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assign2center

Assign a point to the cell with the closest center

### Description

...

### Usage

assign2center(distance.vector)

### **Arguments**

distance.vector

vector of length K containing the distances between the point and the centers

### **Details**

..

### Value

it returns the index(es) of the cell(s) with the closest center(s). Returns 0 it the minimum does not exists

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bootstrapVar	Compute the bootstrap variance	

### **Description**

Compute the bootstrap variance

#### Usage

```
bootstrapVar(res.boot, res.aggr, K, metric_manifold)
```

### **Arguments**

res.boot A list of length B. Each field contains a list with the M predictions generated by

the corresponding iteration

res.aggr A list of lenght M. Each field a single prediction, computed aggregating the

corresponding data in res.boot

K number of cells the domain is subdivided in

metric\_manifold

metric used on the manifold. It must be chosen among "Frobenius", "LogEu-

clidean", "SquareRoot"

#### Value

It returns a vector of length M (i.e. the number of locations where we predict), containing the the prediction variance in the corresponding location

create.rdd	Divide the domain in K subregions	
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### Description

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### Usage

```
create.rdd(K, method.rdd = "Voronoi", data_coords, graph.distance,
  nk_min, grid, data.grid.distance, suppressMes = T)
```

### Arguments

K	number of regions the domain is divided in

method.rdd method used to define the subregions. So far only "Voronoi" has been imple-

mented

data\_coords N\*2 or N\*3 matrix of [lat,long], [x,y] or [x,y,z] coordinates of the locations where

data has been measured

 $\label{eq:continuous_problem} \textit{graph.distance} \quad \textit{N*N distance matrix (the [i,j] element is the length of the shortest path between the length of the length of the shortest path between the length of length of the length of the length of the leng$ 

points i and j)

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nk\_min minimum number of observations within a cell grid prediction grid, i.e. M\*2 or M\*3 matrix of coordinates where to predict data.grid.distance

N\*M distance matrix between locations where the datum has been observed and locations where the datum has to be predicted

suppressMes {TRUE, FALSE} controls the level of interaction and warnings given

#### **Details**

•••

### Value

it returns a list with the following fields

- assign vector of length N that indicates, for every known location, the cell it has been assigned to
- centers K\*3 matrix reporting the coordinates and the index of the locations drawn as centers
  of the K cells
- assigng vector of length M that indicates, for every new location, the cell it has been assigned to
- gridk list of K elements. The i-th element contains the coordinates of the grid points assigned to the i-th cell
- graph.distance.grid.centers K\*M matrix containing the distances between each grid points and the K centers

### Description

Compute the manifold distance between symmetric positive definite matrices

### Usage

```
distance_manifold(data1, data2, metric_manifold = "Frobenius")
```

### **Arguments**

data1 Either a list/array [p,p,B1] of B1 symmetric positive definite matrices of dimen-

sion p\*p, or a single p\*p matrix

data2 Either a list/array [p,p,B2] of B2 symmetric positive definite matrices of dimen-

sion p\*p, or a single p\*p matrix.

metric\_manifold

metric used on the manifold. It must be chosen among "Frobenius", "LogEu-

clidean", "SquareRoot", "Correlation"

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### **Details**

If B2=B1 then the result is a vector of length B1=B2 containing in position i the manifold distance beetween data1[,,i] and data2[,,i]. Instead if B2=1 and B1!=1 the result is a vector of length B1 containing in position i the manifold distance between data1[,,i] and data2[,,1]

### Value

A vector of distances, or a double if data1 and data2 are single matrices.

### **Examples**

```
data_manifold_model <- Manifoldgstat::rCov
distances <-distance_manifold(data_manifold_model, diag(2), metric_manifold = "Frobenius")
print(distances)</pre>
```

Eucldist

Compute the Euclidean distance between two points

### Description

...

### Usage

```
Eucldist(c1, c2)
```

### **Arguments**

- c1 coordinates of the first point.
- c2 coordinates of the second point.

### **Details**

•••

#### Value

the Euclidean distance between c1 and c2

full\_RDD

full\_RDD

Perform full\_RDD

#### **Description**

Perform kriging prediction using FullRDD procedure

### Usage

```
full_RDD(data_coords, data_val, K, grid, nk_min = 1, B = 100,
    suppressMes = F, tol = 1e-12, max_it = 100, n_h = 15,
    tolerance_intrinsic = 10^(-6), X = NULL, X_new = NULL,
    ker.width.intrinsic = 0, ker.width.vario = 1.5,
    graph.distance.complete, data.grid.distance, aggregation_mean,
    aggregation_kriging, method.analysis = "Local mean", metric_manifold,
    metric_ts, model_ts, vario_model, distance = NULL)
```

### **Arguments**

data_coords	N*2 or N*3 matrix of [lat,long], [x,y] or [x,y,z] coordinates. [lat,long] are sup-
	posed to be provided in signed decimal degrees

data\_val array [p,p,N] of N symmetric positive definite matrices of dimension p\*p

K number of cells the domain is subdivided in

grid prediction grid, i.e. M\*2 or M\*3 matrix of coordinates where to predict

nk\_min minimum number of observations within a cell

B number of *divide* iterations to perform

suppressMes {TRUE, FALSE} controls the level of interaction and warnings given

tol tolerance for the main loop of model\_kriging

max\_it maximum number of iterations for the main loop of model\_kriging

n\_h number of bins in the empirical variogram

tolerance\_intrinsic

tolerance for the computation of the intrinsic mean

X matrix (N rows and unrestricted number of columns) of additional covariates for

the tangent space model, possibly NULL

X\_new matrix (with the same number of rows of new\_coords) of additional covariates

for the new locations, possibly NULL

ker.width.intrinsic

parameter controlling the width of the Gaussian kernel for the computation of the local mean (if 0, a "step kernel" is used, giving weight 1 to all the data within

the cell and 0 to those outside of it)

ker.width.vario

parameter controlling the width of the Gaussian kernel for the computation of the empirical variogram (if 0, a "step kernel" is used, giving weight 1 to all the data within the cell and 0 to those outside of it)

graph.distance.complete

N\*N distance matrix (the [i,j] element is the length of the shortest path between points i and j)

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data.grid.distance

N\*M distance matrix between locations where the datum has been observed and locations where the datum has to be predicted

aggregation\_mean

"Weighted" to aggregate the mean predictions using kernel-based weights, "Equal" to use equal weights

aggregation\_kriging

"Weighted" to aggregate the Kriging predictions using kernel-based weights, "Equal" to use equal weights

method.analysis

"Local mean" to predict just with the mean, "Kriging" to predict via Kriging procedure

metric\_manifold

metric used on the manifold. It must be chosen among "Frobenius", "LogEuclidean", "SquareRoot"

metric\_ts metric used on the tangent space. It must be chosen among "Frobenius", "Frobe-

niusScaled", "Correlation"

model\_ts type of model fitted on the tangent space. It must be chosen among "Intercept",

"Coord1", "Coord2", "Additive"

vario\_model type of variogram fitted. It must be chosen among "Gaussian", "Spherical",

"Exponential"

distance type of distance between coordinates. It must be either "Eucldist" or "Geodist"

### **Details**

It uses a repetition of local analyses, through a *divide* et *impera* strategy. In the *divide* step, the domain is randomly decomposed in subdomains where local tangent-space models are estimated in order to predict at new locations (in each subregion is performed exactly the analysis described in the model\_kriging function). This is repeated B times with different partitions of the domain. Then, in the *impera* step, the results of these iterations are aggregated, by means of the intrinsic mean, to provide a final prediction.

#### Value

According to the analysis chosen:

- If method. analysis = "Local mean" it returns a list with the following fields
  - resBootstrap A list consisting of
    - \* fmean list of length B. Each field contains the prediction (at iteration b) for each new location, obtained as the intrinsic mean of the data within the tile it belongs to
    - \* kervalues\_mean Weights used for aggregating fmean
  - resAggregated Predictions, for each new location, obtained aggregating fmean using kervalues\_mean as weights
- If method.analysis = "Kriging" it returns a list with the following fields
  - resBootstrap A list consisting of
    - \* fmean list of length B. Each field contains the prediction (at iteration b) for each new location, obtained as the intrinsic mean of the data within the tile it belongs to
    - \* fpred list of length B. Each field contains the prediction (at iteration b) for each new location, obtained through kriging
    - \* kervalues\_mean Weights used for aggregating fmean

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- \* kervalues\_krig Weights used for aggregating fpred
- \* variofit list of length B. Each field contains, for each datum, the parameters of the variogram fitted in the tile it belongs to
- resAggregated Predictions, for each new location, obtained aggregating fpred using kervalues\_krig as weights
- resLocalMean Predictions, for each new location, obtained aggregating fmean using kervalues\_mean as weights

Geodist

Compute the great-circle distance between two points

### Description

•••

### Usage

```
Geodist(c1, c2)
```

### **Arguments**

c1 coordinates [lat, long] of the first point.

c2 coordinates [lat, long] of the second point.

### **Details**

The distance is computed using the Haversine formula

### Value

the great-circle distance between c1 and c2

 $\verb"intrinsic_mean"$ 

Intrinsic mean

### **Description**

Evaluate the intrinsic mean of a given set of symmetric positive definite matrices

### Usage

```
intrinsic_mean(data, metric_manifold = "Frobenius",
  metric_ts = "Frobenius", tolerance = 1e-06,
  weight_intrinsic = NULL, weight_extrinsic = weight_intrinsic,
  tolerance_map_cor = 1e-06)
```

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### **Arguments**

data list or array [p,p,B] of B symmetric positive definite matrices of dimension p\*p metric\_manifold

> metric used on the manifold. It must be chosen among "Frobenius", "LogEuclidean", "SquareRoot", "Correlation"

metric\_ts metric used on the tangent space. It must be chosen among "Frobenius", "Frobe-

niusScaled", "Correlation"

tolerance for the computation of the intrinsic mean tolerance

weight\_intrinsic

vector of length B to weight the matrices in the computation of the intrinsic mean. If NULL a vector of ones is used

weight\_extrinsic

vector of length B to weight the matrices in the computation of the extrinsic mean. If NULL weight\_intrinsic is used

tolerance\_map\_cor

tolerance to use in the maps.

Required only if metric\_manifold== "Correlation"

#### Value

A matrix representing the intrinsic mean of the data

#### References

X. Pennec, P. Fillard, and N. Ayache. A riemannian framework for tensor computing. International Journal of computer vision, 66(1):41-66, 2006.

### **Examples**

```
data_manifold_tot <- Manifoldgstat::fieldCov</pre>
Sigma <-intrinsic_mean(data_manifold_tot, metric_manifold = "Frobenius",</pre>
              metric_ts = "Frobenius")
print(Sigma)
```

kerfn

Evaluate a gaussian kernel

### **Description**

### Usage

```
kerfn(newdata, center, ker.type = "Gau", param)
```

### **Arguments**

newdata coordinates of the locations where we want to compute the kernel values center coordinates of the reference center for the kernel type of kernel. So far only "Gau" (i.e gaussian kernel) has been implemented ker.type param

parameters that define the kernel. For the gaussian kernel it is the sigma param-

eter

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### **Details**

•••

### Value

the values of the kernel function corresponding to the vector of Euclidean distances between newdata and the center

kriging

Kriging prediction given the model

### Description

Given the GLS model, kriging prediction on new location(s) is performed.

### Usage

```
kriging(GLS_model, coords, new_coords, model_ts = "Additive",
  vario_model = "Gaussian", metric_manifold = "Frobenius",
  X_new = NULL, distance = "Geodist", tolerance_map_cor = 1e-06)
```

### **Arguments**

GLS_model	the object returned by model_GLS, or a list containing the fields: Sigma (tangent point), beta (vector of the beta matrices of the fitted model), gamma_matrix (N*N covariogram matrix), residuals (vector of the N residual matrices), fitted_par_vario (estimates of <i>nugget</i> , <i>sill-nugget</i> and <i>practical range</i> )
coords	N*2 or N*3 matrix of [lat,long], [x,y] or [x,y,z] coordinates. [lat,long] are supposed to be provided in signed decimal degrees
new_coords	matrix of coordinates for the M new locations where to perform kriging
model_ts	type of model fitted on the tangent space. It must be chosen among "Intercept", "Coord1", "Coord2", "Additive"
vario_model	type of variogram fitted. It must be chosen among "Gaussian", "Spherical", "Exponential"
metric_manifol	d
	metric used on the manifold. It must be chosen among "Frobenius", "LogEuclidean", "SquareRoot", "Correlation"
X_new	matrix (with the same number of rows of new_coords) of additional covariates for the new locations, possibly NULL
distance	type of distance between coordinates. It must be either "Eucldist" or "Geodist"
tolerance_map_	cor
	tolerance to use in the maps.  Required only if metric_manifold=="Correlation"
data_grid_dist	_mat
	Matrix of dimension N*M of distances between data points and grid points. If not

provided it is computed using distance

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#### **Details**

The model provided is used to perform simple kriging on the tangent space in correspondence of the new locations. The estimates are then mapped to the manifold to produce the actual prediction.

#### Value

A list with a single field:

prediction

vector of matrices predicted at the new locations

#### References

D. Pigoli, A. Menafoglio & P. Secchi (2016): Kriging prediction for manifold-valued random fields. Journal of Multivariate Analysis, 145, 117-131.

### **Examples**

```
data_manifold_tot <- Manifoldgstat::fieldCov</pre>
data_manifold_model <- Manifoldgstat::rCov</pre>
coords_model <- Manifoldgstat::rGrid</pre>
coords_tot <- Manifoldgstat::gridCov</pre>
Sigma <- matrix(c(2,1,1,1), 2,2)
model = model_GLS(data_manifold = data_manifold_model, coords = coords_model, Sigma = Sigma,
              metric_manifold = "Frobenius", metric_ts = "Frobenius", model_ts = "Coord1",
                 vario_model = "Spherical", n_h = 15, distance = "Eucldist", max_it = 100,
                    tolerance = 1e-7, plot = TRUE)
result = kriging (GLS_model = model, coords = coords_model, new_coords = coords_model,
              model_ts="Coord1", vario_model= "Spherical", metric_manifold = "Frobenius",
                  distance="Eucldist")
result_tot = kriging (GLS_model = model, coords = coords_model, new_coords = coords_tot,
               model_ts="Coord1", vario_model= "Spherical", metric_manifold = "Frobenius",
                      distance="Eucldist")
x.min=min(coords_tot[,1])
x.max=max(coords_tot[,1])
y.min=min(coords_tot[,2])
y.max=max(coords_tot[,2])
dimgrid=dim(coords_tot)[1]
radius = 0.02
par(cex=1.25)
plot(0,0, asp=1, col=fields::tim.colors(100), ylim=c(y.min,y.max), xlim=c(x.min, x.max),
     pch='', xlab='', ylab='', main = "Real Values")
for(i in 1:dimgrid){
  if(i %% 3 == 0)
     car::ellipse(c(coords_tot[i,1],coords_tot[i,2]), data_manifold_tot[,,i],
                    radius=radius, center.cex=.5, col='navyblue')
rect(x.min, y.min, x.max, y.max)
for(i in 1:250)
{ car::ellipse(c(coords_model[i,1],coords_model[i,2]), data_manifold_model[,,i],
               radius=radius, center.cex=.5, col='green')}
rect(x.min, y.min, x.max, y.max)
```

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mixed\_RDD

Perform mixed\_RDD

### **Description**

Perform kriging prediction using MixedRDD procedure

### Usage

```
mixed_RDD(data_coords, data_val, K, grid, nk_min = 1, B = 100,
    suppressMes = F, ker.width.intrinsic = 0, graph.distance.complete,
    data.grid.distance, N_samples, aggregation_mean, metric_ts,
    tol = 1e-12, max_it = 100, n_h = 15,
    tolerance_intrinsic = 10^(-6), max_sill = NULL, max_a = NULL,
    X = NULL, X_new = NULL, create_pdf_vario = FALSE,
    pdf_parameters = NULL, metric_manifold, model_ts, vario_model,
    distance)
```

### Arguments

data_coords	N*2 or $N*3$ matrix of [lat,long], [x,y] or [x,y,z] coordinates. [lat,long] are supposed to be provided in signed decimal degrees
data_val	array [p,p,N] of N symmetric positive definite matrices of dimension p*p
K	number of cells the domain is subdivided in
grid	prediction grid, i.e. M*2 or M*3 matrix of coordinates where to predict
nk_min	minimum number of observations within a cell
В	number of divide iterations to perform
suppressMes	{TRUE, FALSE} controls the level of interaction and warnings given
ker.width.intri	nsic
	parameter controlling the width of the Gaussian kernel for the computation of the local mean (if $0$ , a "step kernel" is used, giving weight 1 to all the data within the cell and $0$ to those outside of it)
graph.distance.	complete

N\*N distance matrix (the [i,j] element is the length of the shortest path between points i and j)

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data.grid.distance

N\*M distance matrix between locations where the datum has been observed and

locations where the datum has to be predicted

N\_samples number of data N

aggregation\_mean

"Weighted" to aggregate the mean predictions using kernel-based weights, "Equal"

to use equal weights

metric\_ts metric used on the tangent space. It must be chosen among "Frobenius", "Frobe-

niusScaled", "Correlation"

tol tolerance for the main loop of model\_kriging

max\_it maximum number of iterations for the main loop of model\_kriging

n\_h number of bins in the empirical variogram

tolerance\_intrinsic

tolerance for the computation of the intrinsic mean

max\_sill max value allowed for sill in the fitted variogram. If NULL it is defined as

1.15\*max(emp\_vario\_values)

max\_a maximum value for a in the fitted variogram. If NULL it is defined as 1.15\*h\_max

X matrix (N rows and unrestricted number of columns) of additional covariates for

the tangent space model, possibly NULL

X\_new matrix (with the same number of rows of new\_coords) of additional covariates

for the new locations, possibly NULL

create\_pdf\_vario

boolean. If TRUE the empirical and fitted variograms are plotted in a pdf file

pdf\_parameters list with the fields test\_nr and sample\_draw. Additional parameters to name

the pdf

metric\_manifold

metric used on the manifold. It must be chosen among "Frobenius", "LogEu-

clidean", "SquareRoot"

model\_ts type of model fitted on the tangent space. It must be chosen among "Intercept",

"Coord1", "Coord2", "Additive"

vario\_model type of variogram fitted. It must be chosen among "Gaussian", "Spherical",

"Exponential"

distance type of distance between coordinates. It must be either "Eucldist" or "Geodist"

### **Details**

It employs a *divide* et *impera* strategy to provide an estimate of a "fictional" field of tangent points, used to encode the information regarding the drift of the field. To this end in the *divide* step, the domain is randomly decomposed and in each subdomain a tangent point (assigned to each location in that subregion) is estimated as the intrinsic mean of the data belonging to it. This is repeated B times with different partitions of the domain and the results are then aggregated in the *impera* stage by means of the intrinsic mean. Eventually, exploiting this "fictional" field of tangent points and the concept of parallel transport, a kriging analysis over the whole domain is performed to predict the field values at new locations.

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#### Value

it returns a list with the following fields

• resBootstrap list of length B. Each field contains a tangent point estimate (at iteration b) for each new location, obtained as the intrinsic mean of the data within the tile it belongs to

- resAggregated field of tangent points computed, for each location (both those where data are measured and where they must be predicted), aggregating the corresponding resBootstrap
- model\_pred list with the details of the global model fitted on the common Hibert space and the resulting kriging predictions. Namely it contains the following fields: beta vector of the beta matrices of the fitted model gamma\_matrix N\*N covariogram matrix residuals vector of the N residual matrices emp\_vario\_values vector of empircal variogram values in correspondence of h\_vec h\_vec vector of positions at which the empirical variogram is computed fitted\_par\_vario estimates of nugget, sill-nugget and practical range iterations number of iterations of the main loop prediction vector of matrices predicted at the new locations

model\_GLS

Create a GLS model

### Description

Given the coordinates and corresponding manifold values, this function creates a GLS model on the tangent space.

#### Usage

```
model_GLS(data_manifold, coords, X = NULL, Sigma = NULL,
  metric_manifold = "Frobenius", metric_ts = "Frobenius",
  model_ts = "Additive", vario_model = "Gaussian", n_h = 15,
  distance = "Geodist", max_it = 100, tolerance = 1e-06,
  weight_intrinsic = NULL, tolerance_intrinsic = 1e-06,
  max_sill = NULL, max_a = NULL, param_weighted_vario = NULL,
  plot = FALSE, suppressMes = FALSE, weight_extrinsic = NULL,
  tolerance_map_cor = 1e-06)
```

### **Arguments**

data_manifold	list or array [p,p,N] of N symmetric positive definite matrices of dimension p*p
coords	N*2 or $N*3$ matrix of [lat,long], [x,y] or [x,y,z] coordinates. [lat,long] are supposed to be provided in signed decimal degrees
X	matrix (N rows and unrestricted number of columns) of additional covariates for the tangent space model, possibly NULL
Sigma	$p*p$ matrix representing the tangent point. If NULL the tangent point is computed as the intrinsic mean of data_manifold
metric_manifold	
	metric used on the manifold. It must be chosen among "Frobenius", "LogEuclidean", "SquareRoot", "Correlation"
metric_ts	metric used on the tangent space. It must be chosen among "Frobenius", "FrobeniusScaled", "Correlation"

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model\_ts type of model fitted on the tangent space. It must be chosen among "Intercept",

"Coord1", "Coord2", "Additive"

vario\_model type of variogram fitted. It must be chosen among "Gaussian", "Spherical",

"Exponential"

n\_h number of bins in the emprical variogram

distance type of distance between coordinates. It must be either "Eucldist" or "Geodist"

max\_it max number of iterations for the main loop

tolerance tolerance for the main loop

weight\_intrinsic

vector of length N to weight the locations in the computation of the intrinsic mean. If NULL a vector of ones is used. Not needed if Sigma is provided

tolerance\_intrinsic

tolerance for the computation of the intrinsic mean. Not needed if Sigma is

provided

max\_sill max value allowed for sill in the fitted variogram. If NULL it is defined as

1.15\*max(emp\_vario\_values)

max\_a maximum value for *a* in the fitted variogram. If NULL it is defined as 1.15\*h\_max param\_weighted\_vario

List of 7 elements to be provided to consider Kernel weights for the variogram (significant only within an RDD procedure). Indeed in this case the N\_tot data regarding the whole domain must be provided to the algorithm, not only the N in the cell under consideration. Therefore the list must contain the following fields: weight\_vario (vector of length N\_tot to weight the locations in the computation of the empirical variogram), distance\_matrix\_tot (N\_tot\*N\_tot matrix of distances between the locations), data\_manifold\_tot (list or array

[p,p,N\_tot] of N\_tot symmetric positive definite matrices of dimension p\*p), coords\_tot (N\_tot\*2 or N\_tot\*3 matrix of [lat,long], [x,y] or [x,y,z] coordinates), X\_tot (matrix with N\_tot rows and unrestricted number of columns of additional covariates for the tangent space model, possibly NULL), h\_max (maximum value of distance for which the variogram is computed), indexes\_model (indexes of the N\_tot data corresponding to the N data in the cell).

plot boolean. If TRUE the empirical and fitted variograms are plotted

suppressMes boolean. If TRUE warning messagges are not printed

weight\_extrinsic

vector of length N to weight the locations in the computation of the extrinsic mean. If NULL weight\_intrinsic are used. Needed only if Sigma is not provided and metric\_manifold== "Correlation"

tolerance\_map\_cor

tolerance to use in the maps.

Required only if metric\_manifold== "Correlation"

data\_dist\_mat Matrix of dimension N\*N of distances between data points. If not provided it is computed using distance

#### **Details**

The manifold values are mapped on the tangent space and then a GLS model is fitted to them. A first estimate of the beta coefficients is obtained assuming spatially uncorrelated errors. Then, in the main the loop, new estimates of the beta are obtained as a result of a weighted least square problem where the weight matrix is the inverse of gamma\_matrix. The residuals

(residuals = data\_ts - fitted) are updated accordingly. The parameters of the variogram fitted to the residuals (and used in the evaluation of the gamma\_matrix) are computed using Gauss-Newton with backtrack method to solve the associated non-linear least square problem. The stopping criteria is based on the absolute value of the variogram residuals' norm if ker.width.vario=0, while it is based on its increment otherwise.

#### Value

A list with the following fields:

beta vector of the beta matrices of the fitted model

gamma\_matrix N\*N covariogram matrix

residuals vector of the N residual matrices

emp\_vario\_values

vector of empircal variogram values in correspondence of h\_vec

h\_vec vector of positions at which the empirical variogram is computed

fitted\_par\_vario

estimates of nugget, sill-nugget and practical range

iterations number of iterations of the main loop

Sigma tangent point

### References

D. Pigoli, A. Menafoglio & P. Secchi (2016): Kriging prediction for manifold-valued random fields. Journal of Multivariate Analysis, 145, 117-131.

### **Examples**

model\_kriging

Create a GLS model and directly perform kriging

### Description

Given the coordinates and corresponding manifold values, this function firstly creates a GLS model on the tangent space, and then performs kriging on the new locations.

#### Usage

```
model_kriging(data_manifold, coords, X = NULL, Sigma = NULL,
 metric_manifold = "Frobenius", metric_ts = "Frobenius",
 model_ts = "Additive", vario_model = "Gaussian", n_h = 15,
 distance = NULL, data_dist_mat = NULL, data_grid_dist_mat = NULL,
 max_it = 100, tolerance = 1e-06, weight_intrinsic = NULL,
  tolerance_intrinsic = 1e-06, max_sill = NULL, max_a = NULL,
 param_weighted_vario = NULL, new_coords, X_new = NULL,
 create_pdf_vario = TRUE, pdf_parameters = NULL,
  suppressMes = FALSE, weight_extrinsic = NULL,
  tolerance_map_cor = 1e-06)
```

#### **Arguments**

list or array [p,p,N] of N symmetric positive definite matrices of dimension p\*p data\_manifold coords N\*2 or N\*3 matrix of [lat,long], [x,y] or [x,y,z] coordinates. [lat,long] are supposed to be provided in signed decimal degrees Χ matrix (N rows and unrestricted number of columns) of additional covariates for the tangent space model, possibly NULL Sigma p\*p matrix representing the tangent point. If NULL the tangent point is computed as the intrinsic mean of data\_manifold metric\_manifold metric used on the manifold. It must be chosen among "Frobenius", "LogEuclidean", "SquareRoot", "Correlation" metric\_ts metric used on the tangent space. It must be chosen among "Frobenius", "FrobeniusScaled", "Correlation" model\_ts type of model fitted on the tangent space. It must be chosen among "Intercept", "Coord1", "Coord2", "Additive" type of variogram fitted. It must be chosen among "Gaussian", "Spherical", vario\_model "Exponential" n\_h number of bins in the emprical variogram distance type of distance between coordinates. It must be either "Eucldist" or "Geodist" data\_dist\_mat Matrix of dimension N\*N of distances between data points. If not provided it is computed using distance data\_grid\_dist\_mat Matrix of dimension N\*M of distances between data points and grid points. If not provided it is computed using distance

 $max_it$ max number of iterations for the main loop

tolerance tolerance for the main loop

weight\_intrinsic

vector of length N to weight the locations in the computation of the intrinsic mean. If NULL a vector of ones is used. Not needed if Sigma is provided

tolerance\_intrinsic

tolerance for the computation of the intrinsic mean. Not needed if Sigma is provided

max\_sill max value allowed for sill in the fitted variogram. If NULL it is defined as 1.15\*max(emp\_vario\_values)

max\_a maximum value for a in the fitted variogram. If NULL it is defined as 1.15\*h\_max param\_weighted\_vario

List of 7 elements to be provided to consider Kernel weights for the variogram (significant only within an RDD procedure). Indeed in this case the N\_tot data regarding the whole domain must be provided to the algorithm, not only the N in the cell under consideration. Therefore the list must contain the following fields: weight\_vario (vector of length N\_tot to weight the locations in the computation of the empirical variogram), distance\_matrix\_tot (N\_tot\*N\_tot matrix of distances between the locations), data\_manifold\_tot (list or array

[p,p,N\_tot] of N\_tot symmetric positive definite matrices of dimension p\*p), coords\_tot (N\_tot\*2 or N\_tot\*3 matrix of [lat,long], [x,y] or [x,y,z] coordinates), X\_tot (matrix with N\_tot rows and unrestricted number of columns of additional covariates for the tangent space model, possibly NULL), h\_max (maximum value of distance for which the variogram is computed), indexes\_model (indexes of the N\_tot data corresponding to the N\_data in the cell).

(indexes of the N\_tot data corresponding to the N data in the cell).

X\_new matrix (with the same number of rows of new\_coords) of additional covariates for the new locations, possibly NULL

create\_pdf\_vario

new coords

boolean. If TRUE the empirical and fitted variograms are plotted in a pdf file

matrix of coordinates for the M new locations where to perform kriging

pdf\_parameters list with the fields test\_nr and sample\_draw. Additional parameters to name

the pdf

suppressMes boolean. If TRUE warning messagges are not printed

weight\_extrinsic

vector of length N to weight the locations in the computation of the extrinsic mean. If NULL weight\_intrinsic are used. Needed only if Sigma is not provided and metric\_manifold== "Correlation"

tolerance\_map\_cor

tolerance to use in the maps.

Required only if metric\_manifold== "Correlation"

### **Details**

The manifold values are mapped on the tangent space and then a GLS model is fitted to them. A first estimate of the beta coefficients is obtained assuming spatially uncorrelated errors. Then, in the main the loop, new estimates of the beta are obtained as a result of a weighted least square problem where the weight matrix is the inverse of gamma\_matrix. The residuals

(residuals = data\_ts - fitted) are updated accordingly. The parameters of the variogram fitted to the residuals (and used in the evaluation of the gamma\_matrix) are computed using Gauss-Newton with backtrack method to solve the associated non-linear least square problem. The stopping criteria is based on the absolute value of the variogram residuals' norm if ker.width.vario=0, while it is based on its increment otherwise. Once the model is computed, simple kriging on the tangent space is performed in correspondence of the new locations and eventually the estimates are mapped to the manifold.

#### Value

list with the following fields:

beta vector of the beta matrices of the fitted model

gamma\_matrix N\*N covariogram matrix

```
residuals vector of the N residual matrices
emp_vario_values
vector of empircal variogram values in correspondence of h_vec
h_vec vector of positions at which the empirical variogram is computed
fitted_par_vario
estimates of nugget, sill-nugget and practical range
iterations number of iterations of the main loop
Sigma tangent point
prediction vector of matrices predicted at the new locations
```

### References

D. Pigoli, A. Menafoglio & P. Secchi (2016): Kriging prediction for manifold-valued random fields. Journal of Multivariate Analysis, 145, 117-131.

#### **Examples**

```
data_manifold_tot <- Manifoldgstat::fieldCov</pre>
data_manifold_model <- Manifoldgstat::rCov</pre>
coords_model <- Manifoldgstat::rGrid</pre>
coords_tot <- Manifoldgstat::gridCov</pre>
Sigma <- matrix(c(2,1,1,1), 2,2)
result = model_kriging (data_manifold = data_manifold_model, coords = coords_model,
                        Sigma = Sigma, metric_manifold = "Frobenius"
                        metric_ts = "Frobenius", model_ts = "Coord1",
                        vario_model = "Spherical", n_h = 15, distance = "Eucldist",
                        max_it = 100, tolerance = 10e-7, new_coords = coords_model)
result_tot = model_kriging (data_manifold = data_manifold_model, coords = coords_model,
                            metric_ts = "Frobenius", Sigma = Sigma,
                            metric_manifold = "Frobenius", model_ts = "Coord1",
                            vario_model = "Spherical", n_h = 15, distance = "Eucldist",
                            max_it = 100, tolerance = 10e-7, new_coords = coords_tot,
                            create_pdf_vario = FALSE)
x.min=min(coords_tot[,1])
x.max=max(coords_tot[,1])
y.min=min(coords_tot[,2])
y.max=max(coords_tot[,2])
dimgrid=dim(coords_tot)[1]
radius = 0.02
par(cex=1.25)
plot(0,0, asp=1, col=fields::tim.colors(100), ylim=c(y.min,y.max), xlim=c(x.min, x.max),
      pch='', xlab='', ylab='', main = "Real Values")
for(i in 1:dimgrid){
 if(i %% 3 == 0)
    car::ellipse(c(coords_tot[i,1],coords_tot[i,2]) , data_manifold_tot[,,i],
                                  radius=radius, center.cex=.5, col='navyblue')
rect(x.min, y.min, x.max, y.max)
for(i in 1:250)
{ car::ellipse(c(coords_model[i,1],coords_model[i,2]) , data_manifold_model[,,i],
               radius=radius, center.cex=.5, col='green')}
rect(x.min, y.min, x.max, y.max)
```

20 model\_kriging\_mixed

model\_kriging\_mixed

Perform main routine for mixed\_RDD

### **Description**

•••

### Usage

```
model_kriging_mixed(data_manifold, coords, X = NULL, Sigma_data,
  metric_manifold = "Frobenius", model_ts = "Additive",
  vario_model = "Gaussian", n_h = 15, distance = NULL,
  data_dist_mat = NULL, data_grid_dist_mat = NULL, max_it = 100,
  tolerance = 1e-06, max_sill = NULL, max_a = NULL, new_coords,
  Sigma_new, X_new = NULL, create_pdf_vario = TRUE,
  pdf_parameters = NULL, suppressMes = FALSE)
```

### **Arguments**

data_manifold	array [p,p,N] of N symmetric positive definite matrices of dimension p*p
coords	N*2 or N*3 matrix of [lat,long], [x,y] or [x,y,z] coordinates.
X	matrix (N rows and unrestricted number of columns) of additional covariates for the tangent space model, possibly NULL
Sigma_data	List of the N fictional tangent points in correspondence with the data used to build the model
metric_manifold	
	metric used on the manifold. It must be chosen among "Frobenius", "LogEuclidean", "SquareRoot"
model_ts	type of model fitted on the tangent space. It must be chosen among "Intercept", "Coord1", "Coord2", "Additive"
vario_model	type of variogram fitted. It must be chosen among "Gaussian", "Spherical", "Exponential" $\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$
n_h	number of bins in the empirical variogram

distance type of distance between coordinates. It must be either "Eucldist" or "Geodist"

data\_dist\_mat N\*N distance matrix (the [i,j] element is the length of the shortest path between

points i and j)

data\_grid\_dist\_mat

N\*M distance matrix between locations where the datum has been observed and

locations where the datum has to be predicted

max\_it maximum number of iterations for the main loop of model\_kriging

tolerance tolerance for the main loop of model\_kriging

max\_sill max value allowed for sill in the fitted variogram. If NULL it is defined as

1.15\*max(emp\_vario\_values)

max\_a maximum value for a in the fitted variogram. If NULL it is defined as 1.15\*h\_max

new\_coords prediction grid, i.e. M\*2 or M\*3 matrix of coordinates where to predict

Sigma\_new List of the M fictional tangent points in correspondence with the locations where

we want to predict

X\_new matrix (with the same number of rows of new\_coords) of additional covariates

for the new locations, possibly NULL

create\_pdf\_vario

boolean. If TRUE the empirical and fitted variograms are plotted in a pdf file

pdf\_parameters list with the fields test\_nr and sample\_draw. Additional parameters to name

the pdf

suppressMes {TRUE, FALSE} controls the level of interaction and warnings given

### **Details**

•••

### Value

it returns a list with the following fields

beta vector of the beta matrices of the fitted model

gamma\_matrix N\*N covariogram matrix

residuals vector of the N residual matrices

emp\_vario\_values

vector of empircal variogram values in correspondence of h\_vec

h\_vec vector of positions at which the empirical variogram is computed

fitted\_par\_vario

estimates of nugget, sill-nugget and practical range

iterations number of iterations of the main loop

prediction vector of matrices predicted at the new locations

22 plot\_variogram

|--|

### Description

Plot kernel

### Usage

```
plot_ker_rect(data_coords, id, xmax, ymax, m, n, ker.width)
```

### **Arguments**

data_coords	coordinates of the data
id	the index of the row of data_coords that will be used as center
xmax	the maximum value for the x-coordinate (the minimum is 0)
ymax	the maximum value for the y-coordinate (the minimum is 0)
m	number of points on the grid in horizontal direction
n	number of points on the grid in vertical direction
ker.width	kernel width
plot_variogram	Plot empirical and fitted variogram

### **Description**

Plot empirical and fitted variogram

### Usage

```
plot_variogram(empirical_variogram, fitted_variogram, model, distance)
```

### **Arguments**

mode1

empirical\_variogram

A list containing the two following fields: - h\_vec: vector of positions at which the empirical variogram is computed - emp\_vario\_values: vector of empircal variogram values in correspondence of h\_vec

fitted\_variogram

A list containing the two following fields: - hh: dense vector of positions at which fit\_vario\_values is computed - fit\_vario\_values: Vector of fitted variogram values in correspondence of hh

Type of variogram used for fitting (it will be reported on the y-axis). It can be

"Gaussian", "Spherical" or "Exponential"

distance Type of distance used to compute h\_vec (it will be reported on the x-axis). It

must be either "Eucldist" or "Geodist"

RDD\_OOK\_aggr\_man

Aggregate the results of the bootrap iterations

### **Description**

•••

### Usage

```
RDD_OOK_aggr_man(fOKBV, weights_intrinsic, ker.width.intrinsic)
```

### **Arguments**

**fOKBV** 

list of length B, containing the results obtained, for each location, at the B bootstrap iterations (Usually it is the fmean or fpred returned by RDD\_OOK\_boot\_man or RDD\_OOK\_boot\_man\_mixed)

weights\_intrinsic

weights to use to aggregate the results

ker.width.intrinsic

width of the kernel used to compute weights\_intrinsic. 0 if we use equal weights

### **Details**

If ker.width.intrinsic!=0 the data are aggregated using the normalized weights\_intrinsic. Otherwise equal weights are used

### Value

the aggregated result, obtained as the intrinsic\_mean of fOKBV

RDD\_OOK\_boot\_man

Main routine for full\_RDD

### **Description**

...

### Usage

```
RDD_OOK_boot_man(data_coords, data_val, K, grid, nk_min, B, suppressMes, tol, max_it, n_h, tolerance_intrinsic, X, X_new, ker.width.intrinsic, ker.width.vario, graph.distance.complete, data.grid.distance, method.analysis, metric_manifold, metric_ts, model_ts, vario_model, distance)
```

#### **Arguments**

data\_coords N\*2 or N\*3 matrix of [lat,long], [x,y] or [x,y,z] coordinates.

data\_val list of N symmetric positive definite matrices of dimension p\*p

K Number of neighborhood (i.e., centers) to sample at each iteration

grid M\*2 or M\*3 matrix of [lat,long], [x,y] or [x,y,z] coordinates of the new locations

where to predict

nk\_min Minimum number of observations within a neighborhood

B Number of bootstap iterations

suppressMes boolean. If TRUE warning messagges are not printed

tol tolerance for each main loop

max\_it max number of iterations for each main loop n\_h number of bins in the emprical variogram

tolerance\_intrinsic

tolerance for the computation of the intrinsic mean

X Additional covariates for the locations used to create the modelX\_new Additional covariates for the M locations where to perform kriging

ker.width.intrinsic

Parameter controlling the width of the Gaussian kernel for the computation of the local mean (if 0, no kernel is used)

ker.width.vario

Parameter controlling the width of the Gaussian kernel for the computation of the empirical variogram (if 0, no kernel is used)

graph.distance.complete

N\*N distance matrix (the [i,j] element is the length of the shortest path between points i and j)

data.grid.distance

N\*M distance matrix between locations where the datum has been observed and locations where the datum has to be predicted

method.analysis

"Local mean" to predict just with the mean, "Kriging" to predict via Kriging procedure

metric\_manifold

Metric used on the manifold. It must be chosen among "Frobenius", "LogEuclidean", "SquareRoot" and "Correlation"

metric\_ts Metric used on the tangent space. It must be chosen among "Frobenius", "Frobe-

niusScaled", "Correlation"

model\_ts Type of model fitted on the tangent space. It must be chosen among "Intercept",

"Coord1", "Coord2", "Additive"

vario\_model Type of variogram fitted. It must be chosen among "Gaussian", "Spherical",

"Exponential"

distance Type of distance between coordinates. It must be either "Eucldist" or "Geodist"

### Details

...

#### Value

According to the analysis chosen:

- If method.analysis = "Local mean" it returns a list with the following fields
  - fmean list of length B. Each field contains the prediction (at iteration b) for each new location, obtained as the intrinsic mean of the data within the tile it belongs to
  - kervalues\_mean Weights used for aggregating fmean
- If method.analysis = "Kriging" it returns a list with the following fields
  - fmean list of length B. Each field contains the prediction (at iteration b) for each new location, obtained as the intrinsic mean of the data within the tile it belongs to
  - fpred list of length B. Each field contains the prediction (at iteration b) for each new location, obtained through kriging
  - kervalues\_mean Weights used for aggregating fmean
  - kervalues\_krig Weights used for aggregating fpred
  - variofit list of length B. Each field contains, for each datum, the parameters of the variogram fitted in the tile it belongs to

RDD\_OOK\_boot\_man\_mixed

Main routine for mixed\_RDD

### **Description**

•••

### Usage

```
RDD_OOK_boot_man_mixed(data_coords, data_val, K, grid, nk_min, B, suppressMes, ker.width.intrinsic, graph.distance.complete, data.grid.distance, metric_ts, vario_model, tol, max_it, n_h, tolerance_intrinsic, X, X_new, metric_manifold, model_ts, distance)
```

### **Arguments**

data_coords	N*2 or $N*3$ matrix of [lat,long], [x,y] or [x,y,z] coordinates. [lat,long] are supposed to be provided in signed decimal degrees	
data_val	array [p,p,N] of N symmetric positive definite matrices of dimension $p*p$	
K	number of cells the domain is subdivided in	
grid	prediction grid, i.e. M*2 or M*3 matrix of coordinates where to predict	
nk_min	minimum number of observations within a cell	
В	number of divide iterations to perform	
suppressMes	{TRUE, FALSE} controls the level of interaction and warnings given	
ker.width.intrinsic		

parameter controlling the width of the Gaussian kernel for the computation of the local mean (if 0, a "step kernel" is used, giving weight 1 to all the data within the cell and 0 to those outside of it)

graph.distance.complete

N\*N distance matrix (the [i,j] element is the length of the shortest path between points i and j)

data.grid.distance

N\*M distance matrix between locations where the datum has been observed and locations where the datum has to be predicted

metric\_ts metric used on the tangent space. It must be chosen among "Frobenius", "Frobe-

niusScaled", "Correlation"

vario\_model type of variogram fitted. It must be chosen among "Gaussian", "Spherical",

"Exponential"

tol tolerance for the main loop of model\_kriging

max\_it maximum number of iterations for the main loop of model\_kriging

n\_h number of bins in the empirical variogram

tolerance\_intrinsic

tolerance for the computation of the intrinsic mean

X matrix (N rows and unrestricted number of columns) of additional covariates for

the tangent space model, possibly NULL

X\_new matrix (with the same number of rows of new\_coords) of additional covariates

for the new locations, possibly NULL

metric\_manifold

metric used on the manifold. It must be chosen among "Frobenius", "LogEu-

clidean", "SquareRoot"

model\_ts type of model fitted on the tangent space. It must be chosen among "Intercept",

"Coord1", "Coord2", "Additive"

distance type of distance between coordinates. It must be either "Eucldist" or "Geodist"

### **Details**

•••

### Value

it returns a list with the following fields

- fmean list of length B. Each field contains the prediction (at iteration b) for each location, obtained as the intrinsic mean of the data within the tile it belongs to
- kervalues\_mean Weights used for aggregating fmean

return\_ith\_list\_element

Return a given element of a list

### **Description**

Return a given element of a list

### Usage

```
return_ith_list_element(lista, i)
```

return\_ith\_row 27

### Arguments

lista A list

i The index of the element to extract

### Value

It returns the i-th element of lista

return\_ith\_row

Return a given row of a matrix

### Description

Return a given row of a matrix

### Usage

```
return_ith_row(mat, i)
```

### Arguments

mat A matrix

i The index of the row to extract

### Value

It returns the i-th row of mat

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