# Package 'conformalInference.multi'

March 16, 2022

```
Type Package
Title Conformal Inference Tools for Regression with Multivariate
     Response
Version 1.1.1
Description It computes full conformal, split conformal and multi split
     conformal prediction regions when the response variable is
     multivariate (i.e. dimension is greater than one). Moreover, the
     package also contain plot functions to visualize the output of the
     full and split conformal functions.
     To guarantee consistency, the package structure mimics the univariate 'conformalInference'
     package of professor Ryan Tibshirani.
     The main references for the code are:
     Lei et al. (2016) <arXiv:1604.04173>,
     Diquigiovanni, Fontana, and Vantini (2021) <arXiv:2102.06746>,
     Diquigiovanni, Fontana, and Vantini (2021) <arXiv:2106.01792>,
     Solari, and Djordjilovic (2021) <arXiv:2103.00627>.
URL https://github.com/ryantibs/conformal,
     https://github.com/paolo-vergo/conformalInference.multi
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Author Jacopo Diquigiovanni [aut, ths],
     Matteo Fontana [aut, ths],
     Aldo Solari [aut, ths],
     Simone Vantini [aut, ths],
     Paolo Vergottini [aut, cre],
     Ryan Tibshirani [ctb]
```

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Maintainer Paolo Vergottini <paolo.vergottini@gmail.com>

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#### **Description**

A dataset containing the log of all the bike trips in Milan (using the BikeMi service), in the period from 25th of January to the 6th of March from Duomo to Duomo, as well as meteorological data.

# Usage

bikeMi

# **Format**

A data frame with 41 rows and 6 variables:

start number of trips started in Duomo a given day

end number of trips ended in Duomo a given day

we is weekend? If true, than we is 1

rain mean amount of rain during the day

dtemp difference between average temperature of the day and of the period

we\_rain interaction between weekend and rain

# Source

https://www.mate.polimi.it/biblioteca/add/qmox/19-2019.pdf

computing\_s\_regression

computing\_s\_regression

Computing modulation function for residuals.

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# **Description**

It computes values for local scoring.

# Usage

```
computing_s_regression(mat_residual, type, alpha, tau)
```

# **Arguments**

mat\_residual A vector of the residuals obtained via multivariate modeling.

type A string indicating the type of modulation function chosen. The alternatives are

"identity", "st-dev", "alpha-max".

alpha The value of the confidence interval.

tau A number between 0 and 1 used for the randomized version of the algorithm

#### **Details**

It is an helper function for conformal.multidim.split and conformal.multidim.msplit

#### Value

It returns local scoring values for the residuals.

# References

"Conformal Prediction Bands for Multivariate Functional Data" by Diquigiovanni, Fontana, Vantini (2021) <arXiv:2106.01792>.

conformal.multidim.full

Full Conformal Prediction Regions, Multivariate Response

#### Description

Compute prediction intervals using full conformal inference with multivariate response

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#### Usage

```
conformal.multidim.full(
 Х,
 у,
 x0,
  train.fun,
 predict.fun,
 alpha = 0.1,
 mad.train.fun = NULL,
 mad.predict.fun = NULL,
 score = "12",
  s.type = "st-dev",
  num.grid.pts.dim = 100,
  grid.factor = 1.25,
 verbose = FALSE
)
```

Matrix of features, of dimension (say) n x p.

Matrix of responses, of length (say) n X q. У

х0 Matrix of features, each row being a point at which we want to form a prediction

interval, of dimension (say) n0 x p.

train.fun A function to perform model training, i.e., to produce an estimator of E(Y|X),

the conditional expectation of the response variable Y given features X. Its input arguments should be x: matrix of features, y: vector of responses, and out: the output produced by a previous call to train.fun, at the same features x. The function train.fun may (optionally) leverage this returned output for efficiency

purposes. See details below.

predict.fun A function to perform prediction for the (mean of the) responses at new feature values. Its input arguments should be out: output produced by train.fun, and

newx: feature values at which we want to make predictions.

alpha Miscoverage level for the prediction intervals, i.e., intervals with coverage 1alpha are formed. Default for alpha is 0.1.

A function to perform training on the absolute residuals i.e., to produce an estimad.train.fun

mator of E(R|X) where R is the absolute residual R = |Y - m(X)|, and m denotes the estimator produced by train.fun. This is used to scale the conformal score, to produce a prediction interval with varying local width. The input arguments to mad.train.fun should be x: matrix of features, y: vector of absolute residuals, and out: the output produced by a previous call to mad.train.fun, at the same features x. The function mad.train.fun may (optionally) leverage this returned output for efficiency purposes. See details below. The default for mad.train.fun is NULL, which means that no training is done on the absolute residuals, and the usual (unscaled) conformal score is used. Note that if mad.train.fun is non-NULL, then so must be mad.predict.fun (next).

**Arguments** 

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mad.predict.fun

A function to perform prediction for the (mean of the) absolute residuals at new feature values. Its input arguments should be out: output produced by mad.train.fun, and newx: feature values at which we want to make predictions. The default for mad.predict.fun is NULL, which means that no local scaling is done for the conformal score, i.e., the usual (unscaled) conformal score is used.

score

Method to compute nonconformity measure in the multivariate regime. The user can choose between squared l^2 norm of the residual, mahalanobis depth of the residual, the max norm of the residual.

s.type

The type of modulation function. Currently we have 3 options: "identity", "st-dev". Default is "st-dev"

num.grid.pts.dim

Number of grid points per dimension used when forming the conformal intervals (each num.grid.pts.dim^q points is a trial point). Default is 100.

grid.factor

Expansion factor used to define the grid for the conformal intervals, i.e., the grid points are taken to be equally spaced in between -grid.factor x max(abs(y)) and grid.factor x max(abs(y)). Default is 1.25. In this case (and with exchangeable data, thus unity weights) the restriction of the trial values to this range costs at most 1/(n+1) in coverage. See details below.

verbose

Should intermediate progress be printed out? Default is FALSE.

#### **Details**

Due to eventual computational overload the function is restricted to a bivariate y.

This function is based on the package future.apply to perform parallelisation.

If the data (training and test) are assumed to be exchangeable, the basic assumption underlying conformal prediction, then the probability that a new response value will lie outside of  $(-\max(abs(y)), \max(abs(y)))$ , where y is the vector of training responses, is 1/(n+1). Thus the restriction of the trials values to  $(-\text{grid.factor x} \max(abs(y)), \text{grid.factor x} \max(abs(y)))$ , for all choices grid.factor >= 1, will lead to a loss in coverage of at most 1/(n+1). This was also noted in "Trimmed Conformal Prediction for High-Dimensional Models" by Chen, Wang, Ha, Barber (2016) <arXiv:1611.09933> (who use this basic fact as motivation for proposing more refined trimming methods).

# Value

A list with the following components: pred, valid\_points. The first is a matrix of dimension n0 x q, while the second is a list of length n0, containing in each position a matrix of varying number of rows (depending on which points where accepted by the method) and with a number of columns equal to q + 1. Indeed, valid\_points contains the selected points on the y-grid as well as the p-values.

#### See Also

```
conformal.multidim.split
```

#### **Examples**

n=25

p=4

```
q=2
mu=rep(0,p)
x = mvtnorm::rmvnorm(n, mu)
beta<-sapply(1:q, function(k) c(mvtnorm::rmvnorm(1,mu)))</pre>
y = x\%*beta + t(mvtnorm::rmvnorm(q,1:n))
x0=x[ceiling(0.9*n):n,]
y0=y[ceiling(0.9*n):n,]
n0<-nrow(y0)
q<-ncol(y)
fun=mean_multi()
final.full=conformal.multidim.full(x, y, x0, fun$train.fun,
                             fun$predict.fun, score="12",
                             num.grid.pts.dim=5, grid.factor=1.25,
                             verbose=FALSE)
ppp<-plot_multidim(final.full)</pre>
```

conformal.multidim.jackplus

Multivariate Response Jackknife + Prediction Regions

# **Description**

Compute prediction regions using multivariate Jackknife + inference.

# Usage

```
conformal.multidim.jackplus(x, y, x0, train.fun, predict.fun, alpha = 0.1)
```

# **Arguments**

Χ	The feature variables, a matrix n x p.
У	The matrix of multivariate responses (dimension n x q)
x0	The new points to evaluate, a matrix of dimension n0 x p.
train.fun	A function to perform model training, i.e., to produce an estimator of E(Y X), the conditional expectation of the response variable Y given features X. Its input arguments should be x: matrix of features, and y: matrix of responses.
predict.fun	A function to perform prediction for the (mean of the) responses at new feature values. Its input arguments should be out: output produced by train.fun, and newx: feature values at which we want to make predictions.

alpha

Miscoverage level for the prediction intervals, i.e., intervals with coverage 1-alpha are formed. Default for alpha is 0.1.

#### **Details**

The work is an extension of the univariate approach to jackknife + inference to a multivariate context, exploiting the concept of depth measures.

This function is based on the package future apply to perform parallelisation. If this package is not installed, then the function will abort.

# Value

A list with length n0, giving the lower and upper bounds for each observation.

#### **Examples**

```
{\tt conformal.multidim.msplit}
```

Multi Split Conformal Prediction Regions with Multivariate Response

#### **Description**

Compute prediction intervals using Multi Split conformal inference with multivariate response.

# Usage

```
conformal.multidim.msplit(
 у,
  χ0,
  train.fun,
  predict.fun,
  alpha = 0.1,
  split = NULL,
  seed = FALSE,
  randomized = FALSE,
  seed.rand = FALSE,
 verbose = FALSE,
  rho = NULL,
  score = "max",
  s.type = "st-dev",
 B = 100,
  lambda = 0,
  tau = 0.1,
 mad.train.fun = NULL,
 mad.predict.fun = NULL
)
```

# Arguments

x	The feature variables, a matrix nxp.
У	The matrix of multivariate responses (dimension nxq)
x0	The new points to evaluate, a matrix of dimension n0xp.
train.fun	A function to perform model training, i.e., to produce an estimator of $E(Y X)$ , the conditional expectation of the response variable Y given features X. Its input arguments should be x: matrix of features, and y: matrix of responses.
predict.fun	A function to perform prediction for the (mean of the) responses at new feature values. Its input arguments should be out: output produced by train.fun, and newx: feature values at which we want to make predictions.
alpha	Miscoverage level for the prediction intervals, i.e., intervals with coverage 1-alpha are formed. Default for alpha is 0.1.
split	Indices that define the data-split to be used (i.e., the indices define the first half of the data-split, on which the model is trained). Default is NULL, in which case the split is chosen randomly.
seed	Integer to be passed to set.seed before defining the random data-split to be used. Default is FALSE, which effectively sets no seed. If both split and seed are passed, the former takes priority and the latter is ignored.
randomized	Should the randomized approach be used? Default is FALSE.
seed.rand	The seed for the randomized version. Default is FALSE.
verbose	Should intermediate progress be printed out? Default is FALSE.

rho Split proportion between training and calibration set. Default is 0.5.

score The chosen score for the split conformal function.

s. type The type of modulation function. Currently we have 3 options: "identity", "st-

dev", "alpha-max". Default is "std-dev"

B Number of repetitions. Default is 100.

lambda Smoothing parameter. Default is 0.

tau It is a smoothing parameter: tau=1-1/B Bonferroni intersection method tau=0

unadjusted intersection Default is 1-(B+1)/(2\*B).

mad.train.fun A function to perform training on the absolute residuals i.e., to produce an esti-

mator of E(R|X) where R is the absolute residual R = |Y - m(X)|, and m denotes the estimator produced by train.fun. This is used to scale the conformal score, to produce a prediction interval with varying local width. The input arguments to mad.train.fun should be x: matrix of features, y: vector of absolute residuals, and out: the output produced by a previous call to mad.train.fun, at the *same* features x. The function mad.train.fun may (optionally) leverage this returned output for efficiency purposes. See details below. The default for mad.train.fun is NULL, which means that no training is done on the absolute residuals, and the usual (unscaled) conformal score is used. Note that if mad.train.fun is non-

NULL, then so must be mad.predict.fun (next).

mad.predict.fun

A function to perform prediction for the (mean of the) absolute residuals at new feature values. Its input arguments should be out: output produced by mad.train.fun, and newx: feature values at which we want to make predictions. The default for mad.predict.fun is NULL, which means that no local scaling is done for the conformal score, i.e., the usual (unscaled) conformal score is used.

# Details

The work is an extension of the univariate approach to Multi Split conformal inference to a multivariate context, exploiting the concept of depth measure.

This function is based on the package future.apply to perform parallelization.

# Value

A list with length n0, giving the lower and upper bounds for each observation.

#### References

"Multi Split Conformal Prediction" by Solari, Djordjilovic (2021) <arXiv:2103.00627> is the baseline for the univariate case.

### **Examples**

```
set.seed(12345)
n=200
p=4
```

```
q=2
 mu=rep(0,p)
 x = mvtnorm::rmvnorm(n, mu)
 beta<-sapply(1:q, function(k) c(mvtnorm::rmvnorm(1,mu)))</pre>
 y = x%*%beta + t(mvtnorm::rmvnorm(q,1:n))
 x0=matrix(x[n,],nrow=1)
 y0=matrix(y[n,],nrow=1)
 n0<-nrow(y0)
 q<-ncol(y)
 B=100
 funs=lm_multi()
 sol < -conformal.multidim.msplit(x,y, x0, train.fun = funs$train.fun,
                                             predict.fun = funs$predict.fun, alpha=0.05,
                                             split=NULL, seed=FALSE, randomized=FALSE,
                                 seed.rand=FALSE,
                                             verbose=FALSE, rho=NULL,score = "max",
                                             s.type = "st-dev",B=B,lambda=0,
                                             tau = 0.1, mad.train.fun = NULL,
                                             mad.predict.fun = NULL)
sol
```

conformal.multidim.split

Split conformal prediction intervals with Multivariate Response

# **Description**

Compute prediction intervals using split conformal inference with multivariate response.

# Usage

```
conformal.multidim.split(
    x,
    y,
    x0,
    train.fun,
    predict.fun,
    alpha = 0.1,
    split = NULL,
    seed = FALSE,
    randomized = FALSE,
    seed.rand = FALSE,
    verbose = FALSE,
    rho = 0.5,
    score = "12",
    s.type = "st-dev",
```

```
mad.train.fun = NULL,
mad.predict.fun = NULL
)
```

#### **Arguments**

x The feature variables, a matrix n x p.

y The matrix of multivariate responses (dimension n x q) x0 The new points to evaluate, a matrix of dimension n0 x p.

train.fun A function to perform model training, i.e., to produce an estimator of E(Y|X),

the conditional expectation of the response variable Y given features X. Its input

arguments should be x: matrix of features, and y: matrix of responses.

predict.fun A function to perform prediction for the (mean of the) responses at new feature

values. Its input arguments should be out: output produced by train.fun, and

newx: feature values at which we want to make predictions.

alpha Miscoverage level for the prediction intervals, i.e., intervals with coverage 1-

alpha are formed. Default for alpha is 0.1.

split Indices that define the data-split to be used (i.e., the indices define the first half

of the data-split, on which the model is trained). Default is NULL, in which case

the split is chosen randomly.

seed Integer to be passed to set.seed before defining the random data-split to be used.

Default is FALSE, which effectively sets no seed. If both split and seed are

passed, the former takes priority and the latter is ignored.

randomized Should the randomized approach be used? Default is FALSE.

seed. rand The seed for the randomized version. Default is FALSE.

verbose Should intermediate progress be printed out? Default is FALSE.

rho Split proportion between training and calibration set. Default is 0.5.

score The non-conformity measure. It can either be "max", "l2", "mahalanobis". The

default is "12".

s.type The type of modulation function. Currently we have 3 options: "identity", "st-

dev", "alpha-max". Default is "st-dev"

mad.train.fun A function to perform training on the absolute residuals i.e., to produce an esti-

mator of E(R|X) where R is the absolute residual R = |Y - m(X)|, and m denotes the estimator produced by train.fun. This is used to scale the conformal score, to produce a prediction interval with varying local width. The input arguments to mad.train.fun should be x: matrix of features, y: vector of absolute residuals, and out: the output produced by a previous call to mad.train.fun, at the *same* features x. The function mad.train.fun may (optionally) leverage this returned output for efficiency purposes. See details below. The default for mad.train.fun is NULL, which means that no training is done on the absolute residuals, and the usual (unscaled) conformal score is used. Note that if mad.train.fun is non-

NULL, then so must be mad.predict.fun (next).

```
mad.predict.fun
```

A function to perform prediction for the (mean of the) absolute residuals at new feature values. Its input arguments should be out: output produced by mad.train.fun, and newx: feature values at which we want to make predictions. The default for mad.predict.fun is NULL, which means that no local scaling is done for the conformal score, i.e., the usual (unscaled) conformal score is used.

#### **Details**

If the two mad functions are provided they take precedence over the s.type parameter, and they force a local scoring via the mad function predicted values.

#### Value

A list with the following components: x0,pred,k\_s,s.type,s,alpha,randomized,tau, average\_width,lo,up. In particular pred, lo, up are the matrices of dimension n0 x q, k\_s is a scalar, s.type is a string, s is a vector of length q, alpha is a scalar between 0 and 1, randomized is a logical value, tau is a scalar between 0 and 1,and average\_width is a positive scalar.

#### References

The s\_regression and the "max" score are taken from "Conformal Prediction Bands for Multivariate Functional Data" by Diquigiovanni, Fontana, Vantini (2021).

#### See Also

```
conformal.multidim.full
```

# **Examples**

```
n=50
p=4
q=2
mu=rep(0,p)
x = mvtnorm::rmvnorm(n, mu)
beta<-sapply(1:q, function(k) c(mvtnorm::rmvnorm(1,mu)))</pre>
y = x\%*\%beta + t(mvtnorm::rmvnorm(q,1:n))
x0=x[ceiling(0.9*n):n,]
y0=y[ceiling(0.9*n):n,]
n0 < -nrow(y0)
q<-ncol(y)
fun=mean_multi()
final.point = conformal.multidim.split(x,y,x0, fun$train.fun, fun$predict.fun,
                              alpha=0.1,
                                split=NULL, seed=FALSE, randomized=FALSE, seed.rand=FALSE,
                                 verbose=FALSE, rho=0.5,score ="12",s.type="st-dev")
ppp2<-plot_multidim(final.point)
```

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elastic.funs

Elastic Net, Lasso, Ridge Regression Training and Prediction Functions

# **Description**

Construct training and prediction functions for the elastic net, the lasso, or ridge regression, based on the glmnet package, over a sequence of (given or internally computed) lambda values.

# Usage

```
elastic.funs(
  gamma = 0.5,
  standardize = TRUE,
  intercept = TRUE,
  lambda = NULL,
  nlambda = 50,
  lambda.min.ratio = 1e-04,
  cv.rule = c("min", "1se")
)
lasso.funs(
  standardize = TRUE,
  intercept = TRUE,
  lambda = NULL,
  nlambda = 50,
  lambda.min.ratio = 1e-04,
  cv.rule = c("min", "1se")
)
ridge.funs(
  standardize = TRUE,
  intercept = TRUE,
  lambda = NULL,
  nlambda = 50,
  lambda.min.ratio = 1e-04,
  cv.rule = c("min", "1se")
)
```

#### **Arguments**

gamma

Mixing parameter (between 0 and 1) for the elastic net, where 0 corresponds to ridge regression, and 1 to the lasso. Default is 0.5.

standardize, intercept

Should the data be standardized, and should an intercept be included? Default for both is TRUE.

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lambda Sequence of lambda values over which training is performed. This must be in

decreasing order, and — this argument should be used with caution! When used, it is usually best to grab the sequence constructed by one initial call to glmnet (see examples). Default is NULL, which means that the nlambda,

lambda.min.ratio arguments will define the lambda sequence (see next).

nlambda Number of lambda values over which training is performed. In particular, the

lambda sequence is defined by nlambda log-spaced values between lambda.max and lambda.min.ratio \* lambda.max, where lambda.max is the smallest value of lambda at which the solution has all zero components, and lambda.min.ratio is

a small fraction (see next). Default is 50.

lambda.min.ratio

Small fraction that gets used in conjunction with nlambda to specify a lambda

sequence (see above). Default is 1e-4.

cv.rule If the cv argument is TRUE, then cv.rule determines which rule should be used

for the predict function, either "min" (the usual rule) or "1se" (the one-standard-

error rule). See the glmnet help files for details. Default is "min".

#### **Details**

This function is based on the packages glmnet. Notice that Cross Validation to select the best lambda value is compulsory! The functions lasso funs and ridge funs are convenience functions, they simply call elastic funs with gamma = 1 and gamma = 0, respectively.

# Value

A list with three components: train.fun, predict.fun, active.fun. The third function is designed to take the output of train.fun, and reports which features are active for each fitted model contained in this output.

lm multi

Linear Modeling of Multivariate Response

# **Description**

This model is fed to conformal.multidim.full, conformal.multidim.split, and conformal.multidim.msplit. It outputs a training function and a prediction function.

#### Usage

lm\_multi()

#### **Details**

The training function takes as input:

x The feature matrix (dim n x p) y The response matrix (dim n x q)

The predict function, instead, takes as input:

out The output of a previous call to train.fun newx The new features to evaluate (i.e. an  $n0 \times p$  matrix) Here I defined an lm model for every dimension of the responses (q).

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#### Value

A list with the training function and the prediction function.

mean\_multi

Mean of Multivariate Response

# **Description**

This model is fed to conformal.multidim.full, conformal.multidim.split, and conformal.multidim.msplit. It outputs a training function and a prediction function.

#### Usage

```
mean_multi()
```

#### **Details**

The training function takes as input:

x The feature matrix (dim n x p) y The response matrix (dim n x q)

The predict function, instead, takes as input:

out The output of a previous call to train.fun newx The new features to evaluate (i.e. an  $n0 \times p$  matrix)

#### Value

A list with the training function and the prediction function.

plot\_multidim

Plot Confidence Regions obtained with Split Conformal

# Description

Plot Confidence Regions obtained with Split Conformal

# Usage

```
plot_multidim(out, same.scale = FALSE)
```

#### **Arguments**

out The output of a prediction function.

same.scale Should I force the same scale for all the y-axis? Default is FALSE.

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# **Details**

It exploits the package ggplot2, gridExtra and hrbrthemes to better visualize the results.

#### Value

g\_list A list of ggplots (output[[i]] is the i-th observation confidence region).

# **Examples**

```
n=50
p=4
q=2
mu=rep(0,p)
x = mvtnorm::rmvnorm(n, mu)
beta<-sapply(1:q, function(k) c(mvtnorm::rmvnorm(1,mu)))</pre>
y = x\%*\%beta + t(mvtnorm::rmvnorm(q,1:n))
x0=x[ceiling(0.9*n):n,]
y0=y[ceiling(0.9*n):n,]
n0 < -nrow(y0)
q<-ncol(y)
fun=mean_multi()
final.point = conformal.multidim.split(x,y,x0, fun$train.fun, fun$predict.fun,
                            alpha=0.1,
                              split=NULL, seed=FALSE, randomized=FALSE, seed.rand=FALSE,
                               verbose=FALSE, rho=0.5,score ="12",s.type="st-dev")
ppp2<-plot_multidim(final.point)</pre>
n=25
p=4
q=2
mu=rep(0,p)
x = mvtnorm::rmvnorm(n, mu)
beta<-sapply(1:q, function(k) c(mvtnorm::rmvnorm(1,mu)))</pre>
y = x\%*\%beta + t(mvtnorm::rmvnorm(q,1:n))
x0=x[ceiling(0.9*n):n,]
y0=y[ceiling(0.9*n):n,]
n0<-nrow(y0)
q<-ncol(y)
fun=mean_multi()
```

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ppp<-plot\_multidim(final.full)</pre>

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