Package ‘CARRoT’

October 13, 2023

Title Predicting Categorical and Continuous Outcomes Using One in Ten Rule

Version 3.0.2

Description Predicts categorical or continuous outcomes while concentrating on a number of key points. These are Cross-validation, Accuracy, Regression and Rule of Ten or``one in ten rule” (CARRoT), and, in addition to it R-squared statistics, prior knowledge on the dataset etc. It performs the cross-validation specified number of times by partitioning the input into training and test set and fitting linear/multinomial/binary regression models to the training set. All regression models satisfying chosen constraints are fitted and the ones with the best predictive power are given as an output. Best predictive power is understood as highest accuracy in case of binary/multinomial outcomes, smallest absolute and relative errors in case of continuous outcomes. For binary case there is also an option of finding a regression model which gives the highest AU-ROC (Area Under Receiver Operating Curve) value. The option of parallel toolbox is also available. Methods are described in Peduzzi et al. (1996) <doi:10.1016/S0895-4356(96)00236-3>, Rhemtulla et al. (2012) <doi:10.1037/a0029315>, Riley et al. (2018) <doi:10.1002/sim.7993>, Riley et al. (2019) <doi:10.1002/sim.7992>.

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**AUC**

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**Description**


**Usage**

```
AUC(probs, class)
```

**Arguments**

- `probs` probabilities
- `class` outcomes

**Value**

A value for AUC

**Examples**

```
AUC(runif(100,0,1),rbinom(100,1,0.3))
```
av_out

Averaging out the predictive power

Description

Function which averages out the predictive power over all cross-validations

Usage

av_out(preds, crv, k)

Arguments

preds An M x crvN matrix consisting of crv horizontally concatenated M x N matrices. These M x N matrices are the matrices of predictive powers for all feasible regressions (M is maximum feasible number of variables included in a regression, N is the maximum feasible number of regressions of the fixed size; the row index indicates the number of variables included in a regression)

crv number of cross-validations

k size of the test set for which the predictions are made

Value

Returns an M x N matrix of average predictive powers where M is maximum feasible number of variables included in a regression, N is the maximum feasible number of regressions of the fixed size; the row index indicates the number of variables included in a regression

Examples

#creating a matrix of predictive powers
preds<-cbind(matrix(runif(40,1,4),ncol=10), matrix(runif(40,1.5,4),ncol=10))
preds<-cbind(preds, matrix(runif(40,1,3.5),ncol=10))

#running the function
av_out(preds,3,5)
**comb**  
*Combining in a list*

**Description**
Function for combining outputs in a list

**Usage**
```
comb(...)
```

**Arguments**
- ... an argument of `mapply` used by this function

**See Also**
Function `mapply`

**Examples**
```
# array of numbers to be separated in a list
a<-1:4

# running the function
comb(a)
```

---

**compute_max_length**  
*Maximum number of the regressions*

**Description**
Function which computes the maximum number of regressions with fixed number of variables based on the rule of thumb

**Usage**
```
compute_max_length(vari_col,k,c,we,minx,maxx,st)
```
compute_max_weight

Arguments

- `vari_col` number of predictors
- `k` maximum weight of the predictors
- `c` array of all indices of the predictors
- `we` array of weights of the predictors. Continuous or categorical numerical variable with more than 5 categories has weight 1, otherwise it has weight \( n-1 \) where \( n \) is the number of categories
- `minx` minimum number of predictors, 1 by default
- `maxx` maximum number of predictors, total number of variables by default
- `st` a subset of predictors to be always included into a predictive model

Value

Integer corresponding to maximum number of regressions of the same size

References


See Also

Function uses `combn`

Examples

```r
compute_max_length(4,40,1:4,c(1,1,2,1))
```

---

compute_max_weight  Maximum feasible weight of the predictors

Description

Function which computes maximal weight (multiplied by the corresponding EPV rule) of a regression according to the rule of thumb applied to the outcome variable. Weight of a regression equals the sum of weights of its predictors.

Usage

```r
compute_max_weight(outi,mode)
```
compute_weights

Arguments

- **outi**: set of outcomes
- **mode**: indicates the mode: 'linear' (linear regression), 'binary' (logistic regression), 'multin' (multinomial regression)

Details

For continuous outcomes it equals sample size divided by 10, for multinomial it equals the size of the smallest category divided by 10

Value

returns an integer value of maximum allowed weight multiplied by 10

References


Examples

#continuous outcomes

    compute_max_weight(runif(100,0,1),'linear')

#binary outcomes

    compute_max_weight(rbinom(100,1,0.4),'binary')

<table>
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<th>compute_weights</th>
<th>Weights of predictors</th>
</tr>
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</table>

Description

Function which computes the weight of each predictor according to the rules of thumb and outputs it into corresponding array

Usage

    compute_weights(vari_col, vari)

Arguments

- **vari_col**: number of predictors
- **vari**: set of predictors
Details
Continuous or categorical numerical variable with more than 5 categories has weight 1, otherwise it has weight n-1 where n is the number of categories

Value
Returns an array of weights of the size vari_col

References


Examples
# creating data-set with for variables
a<-matrix(NA,nrow=100,ncol=4)

# binary variable
a[,1]=rbinom(100,1,0.3)

# continuous variable
a[,2]=runif(100,0,1)

# categorical numeric with less than 5 categories
a[,3]=t(rmultinom(100,1,c(0.2,0.3,0.5)))%*%c(1,2,3)

# categorical numeric with 5 categories
a[,4]=t(rmultinom(100,1,c(0.2,0.3,0.3,0.1,0.1)))%*%c(1,2,3,4,5)

# running the function
compute_weights(4,a)
cross_val  

Cross-validation run

Description

Function running a single cross-validation by partitioning the data into training and test set

Usage

cross_val(
  vari,  
  outi,  
  c,  
  rule,  
  part,  
  l,  
  we,  
  vari_col,  
  preds,  
  mode,  
  cmode,  
  predm,  
  cutoff,  
  objfun,  
  minx = 1,  
  maxx = NULL,  
  nr = NULL,  
  maxw = NULL,  
  st = NULL,  
  corr = 1,  
  Rsq = F,  
  marg = 0,  
  n_tr,  
  preds_tr  
)

Arguments

vari  set of predictors
outi  array of outcomes
c  set of all indices of the predictors
rule  an Events per Variable (EPV) rule, defaults to 10
part  indicates partition of the original data-set into training and test set in a proportion (part-1):1
l  number of observations
we  weights of the predictors
vari_col  overall number of predictors
preds  array to write predictions for the test split into, intially empty
mode  'binary' (logistic regression), 'multin' (multinomial regression)
cmode  'det' or ''; 'det' always predicts the more likely outcome as determined by the odds ratio; '' predicts certain outcome with probability corresponding to its odds ratio (more conservative). Option available for multinomial/logistic regression
predm  'exact' or ''; for logistic and multinomial regression; 'exact' computes how many times the exact outcome category was predicted, '' computes how many times either the exact outcome category or its nearest neighbour was predicted
cutoff  cut-off value for logistic regression
objfun  'roc' for maximising the predictive power with respect to AUC, 'acc' for maximising predictive power with respect to accuracy.
minx  minimum number of predictors to be included in a regression, defaults to 1
maxx  maximum number of predictors to be included in a regression, defaults to maximum feasible number according to one in ten rule
nr  a subset of the data-set, such that 1/part of it lies in the test set and 1-1/part is in the training set, defaults to empty set
maxw  maximum weight of predictors to be included in a regression, defaults to maximum weight according to one in ten rule
st  a subset of predictors to be always included into a predictive model, defaults to empty set
corr  maximum correlation between a pair of predictors in a model
Rsq  whether R-squared statistics constrained is introduced
marg  margin of error for R-squared statistics constraint
n_tr  size of the training set
preds_tr  array to write predictions for the training split into, intially empty

Value
regr  An M x N matrix of sums of the absolute errors for each element of the test set for each feasible regression. M is maximum feasible number of variables included in a regression, N is the maximum feasible number of regressions of the fixed size; the row index indicates the number of variables included in a regression. Therefore each row corresponds to results obtained from running regressions with the same number of variables and columns correspond to different subsets of predictors used.
regr  An M x N matrix of sums of the relative errors for each element of the test set (only for mode = 'linear') for each feasible regression. M is maximum feasible number of variables included in a regression, N is the maximum feasible number of regressions of the fixed size; the row index indicates the number of variables included in a regression. Therefore each row corresponds to results obtained from running regressions with the same number of variables and columns correspond to different subsets of predictors used.
nvar Maximum feasible number of variables in the regression
emp An accuracy of always predicting the more likely outcome as suggested by the training set (only for mode = 'binary' and objfun = 'acc')

In regr and regrr NA values are possible since for some numbers of variables there are fewer feasible regressions than for the others.

See Also
Uses compute_max_weight, sum_weights_sub, make_numeric_sets, get_predictions_lin, get_predictions, get_probabilities, AUC, combn

Examples
#creating variables
vari<-matrix(c(1:100,seq(1,300,3)),ncol=2)
#creating outcomes
out<-rbinom(100,1,0.3)
#creating array for predictions
pr<-array(NA,c(2,2))
pr_tr<-array(NA,c(2,2))
#passing set of the inxes of the predictors
c<-c(1:2)
#passing the weights of the predictors
we<-c(1,1)
#setting the mode
m<- 'binary'
#running the function
cross_val(vari,out,c,10,10,100,we,2,pr,m,'det','exact',0.5,'acc',nr=c(1,4),n_tr=90,preds_tr=pr_tr)

cub Three-way interactions and squares

Description
Function transforms a set of predictors into a set of predictors, their squares, pairwise interactions, cubes and three-way interactions.
find_int

Usage

cub(A, n = 1000)

Arguments

A set of predictors
n first n predictors, whose interactions with the rest should be taken into account, defaults to all of the predictors

Value

Returns the predictors including their squares, pairwise interactions, cubes and three-way interactions

Examples

cub(cbind(1:100,rnorm(100),runif(100),rnorm(100,0,2)))

find_int Finding the interacting terms based on the index

Description

Function transforms an index of an array of two- or three-way interactions into two or three indices corresponding to the interacting variables

Usage

find_int(ind,N)

Arguments

ind index to transform
N number of interacting variables

Value

Returns two or three indices corresponding to a combination of variables written under the given index

Examples

find_int(28,9)
find_sub

Finds certain subsets of predictors

Description
Reorders the columns of matrix \( a \) according to the ordered elements of array \( s \)

Usage
\[
\text{find_sub}(a, s, j, c, st)
\]

Arguments
- \( a \): A \( j \times N \) matrix, containing all possible subsets (\( N \) overall) of the size \( j \) of predictors’ indices.
- \( s \): array of numbers of the size \( N \)
- \( j \): number of rows in \( a \)
- \( c \): array of all indices of the predictors
- \( st \): a subset of predictors to be always included into a predictive model

Value
Returns a submatrix of matrix \( a \) which consists of columns determined by the input array \( s \)

Examples
\[
\begin{align*}
\text{#all two-element subsets of 1:3} \\
a &<-\text{combn}(3, 2) \\
s &<-\text{c}(3, 2, 3) \\
\text{find_sub}(a, s, 2, 1:3)
\end{align*}
\]

get_indices

Best regression

Description
Function which identifies regressions with the highest predictive power

Usage
\[
\text{get_indices}(\text{predsp}, \text{nvar}, c, \text{we}, \text{st}, \text{minx})
\]
get_predictions

get_predictions  Predictions for multinomial regression

Arguments

predsp  An M x N matrix of averaged out predictive power values. M is maximum feasible number of variables included in a regression, N is the maximum feasible number of regressions of the fixed size; the row index indicates the number of variables included in a regression.

nvar  array of maximal number of variables for each cross-validation

c  array of all indices of the prediction variables

we  array of all weights of the prediction variables

st  a subset of predictors to be always included into a predictive model

minx  minimum number of predictors, defaults to 1

Value

A list of arrays which contain indices of the predictors corresponding to the best regressions

See Also

Uses sum_weights_sub, find_sub, combn

Examples

# creating a set of averaged out predictive powers

predsp<-matrix(NA,ncol=3,nrow=3)
predsp[1,]=runif(3,0.7,0.8)
predsp[2,]=runif(3,0.65,0.85)
predsp[3,1]=runif(1,0.4,0.5)

# running the function

get_indices(predsp,c(3,3,3),1:3,c(1,1,1))

Description

Function which makes a prediction for multinomial/logistic regression based on the given cut-off value and probabilities.

Usage

get_predictions(p,k,cutoff,cmode,mode)
get_predictions_lin

Arguments

- **p**: probabilities of the outcomes for the test set given either by an array (logistic regression) or by a matrix (multinomial regression)
- **k**: size of the test set
- **cutoff**: cut-off value of the probability
- **cmode**: 'det' or ''; 'det' always predicts the more likely outcome as determined by the odds ratio; '' predicts certain outcome with probability corresponding to its odds ratio (more conservative). Option available for multinomial/logistic regression
- **mode**: 'binary' (logistic regression), 'multin' (multinomial regression)

Value

Outputs the array of the predictions of the size of p.

See Also

Uses `rbinom`, `rmultinom`

Examples

```r
#binary mode
get_predictions(runif(20,0.4,0.6),20,0.5,'det','binary')

#creating a data-set for multinomial mode
p1<-runif(20,0.4,0.6)
p2<-runif(20,0.1,0.2)
p3<-1-p1-p2

#running the function
get_predictions(matrix(c(p1,p2,p3),ncol=3),20,0.5,'det','multin')
```

get_predictions_lin  Predictions for linear regression

Description

Function which runs a linear regression on a training set, computes predictions for the test set

Usage

`get_predictions_lin(trset,testset,outc,k,n_tr,p,Rsq,Rsq_v,marg)`
get_probabilities

Arguments

- **trset**: values of predictors on the training set
- **testset**: values of predictors on the test set
- **outc**: values of predictors on the training set
- **k**: length of the test set
- **n_tr**: size of the training set
- **p**: weight of the model
- **Rsq**: whether the R-squared statistics constraint is introduced
- **Rsq_v**: value of R-squared statistics on the training split of the data
- **marg**: margin of error for R-squared statistics constraint

Value

An array of continuous variables of the length equal to the size of a testset

See Also

Function uses function `lsfit` and `coef`

Examples

```r
trset<-matrix(c(rnorm(90,2,4),runif(90,0,0.5),rbinom(90,1,0.5)),ncol=3)

testset<-matrix(c(rnorm(10,2,4),runif(10,0,0.5),rbinom(10,1,0.5)),ncol=3)

generate_predictions_lin(trset,testset,runif(90,0,1),10)
```

get_probabilities

**Probabilities for multinomial regression**

Description

Function which computes probabilities of outcomes on the test set by applying regression parameters inferred by a run on the training set. Works for logistic or multinomial regression.

Usage

```r
generate_probabilities(trset,testset,outc,mode,Rsq,p,n_tr)
```
make_numeric

Arguments

- **trset**: values of predictors on the training set
- **testset**: values of predictors on the test set
- **outc**: values of outcomes on the training set
- **mode**: `'binary'` (logistic regression) or `'multin'` (multinomial regression)
- **Rsq**: whether R-squared statistics constrained is introduced
- **p**: weight of the model
- **n_tr**: size of the training set

Details

In binary mode this function computes the probabilities of the event '0'. In multinomial mode computes the probabilities of the events '0','1',...,'N-1'.

Value

Probabilities of the outcomes. In 'binary' mode returns an array of the size of the number of observations in a testset. In 'multin' returns an M x N matrix where M is the size of the number of observations in a testset and N is the number of unique outcomes minus 1.

See Also

Function uses *multinom* and *coef*

Examples

```r
trset<-matrix(c(rbinom(70,1,0.5),runif(70,0.1)),ncol=2)
testset<-matrix(c(rbinom(10,1,0.5),runif(10,0.1)),ncol=2)
generate_probabilities(trset,testset,rbinom(70,1,0.6),'binary')
```

Description

Function which turns a single categorical (non-numeric) variable into a numeric one (or several) by introducing dummy '0'/1' variables.

Usage

```r
make_numeric(vari, outcome, ra, mode)
```
Arguments

vari        array of values to be transformed
outcome     TRUE/FALSE indicates whether the variable vari is an outcome (TRUE) or a predictor (FALSE)
ra          indices of the input array vari which indicate which values will be transformed
mode        'binary' (logistic regression), 'multin' (multinomial regression)

Details

This function is essentially a standard way to turn categorical non-numeric variables into numeric ones in order to run a regression.

Value

Returned value is an M x N matrix where M is the length of the input array of indices ra and N is length(vari) - 1.

Examples

# creating a non-numeric set

a<-t(rmultinom(100,1,c(0.2,0.3,0.5)))%*%c(1,2,3)
a[a==1]='red'
a[a==2]='green'
a[a==3]='blue'

# running the function

make_numeric(a,FALSE,sample(1:100,50),"linear")
make_numeric(a,TRUE,sample(1:100,50))

Description

Function which turns a set of predictors containing non-numeric variables into a fully numeric set.

Usage

make_numeric_sets(a,ai,k,vari,ra,l,mode)
Arguments

- `a`: An M x N matrix, containing all possible subsets (N overall) of the size M of predictors' indices; therefore each column of `a` defines a unique subset of the predictors.
- `ai`: array of indices of the array `a`.
- `k`: index of the array `ai`.
- `vari`: set of all predictors.
- `ra`: array of sample indices of `vari`.
- `l`: size of the sample.
- `mode`: 'binary' (logistic regression), 'multin' (multinomial regression).

Details

Function transforms the whole set of predictors into a numeric set by consecutively calling function `make_numeric` for each predictor.

Value

Returns a list containing two objects: `tr` and `test`.

- `tr`: training set transformed into a numeric one.
- `test`: test set transformed into a numeric one.

See Also

- `make_numeric`

Examples

```r
# creating a categorical numeric variable
a <- t(rmultinom(100, 1, c(0.2, 0.3, 0.5))) %*% c(1, 2, 3)

# creating an analogous non-numeric variable
b <- array(NA, 100)
c[a == 1] <- 'red'
c[a == 2] <- 'green'
c[a == 3] <- 'blue'

# creating a data-set
b <- data.frame(matrix(c(a, rbinom(100, 1, 0.3), runif(100, 0, 1)), ncol = 3))

# making the first column of the data-set non-numeric
b[, 1] <- data.frame(c)
```
#running the function
make_numeric_sets(combn(3,2),1:3,1,b,sample(1:100,60),100,"binary")

---

**quadr**

*Pairwise interactions and squares*

---

**Description**

Function transforms a set of predictors into a set of predictors, their squares and pairwise interactions.

**Usage**

```r
quadr(A, n = 1000)
```

**Arguments**

- `A`: set of predictors
- `n`: first n predictors, whose interactions with the rest should be taken into account, defaults to all of the predictors.

**Value**

Returns the predictors including their squares and pairwise interactions.

**Examples**

```r
quadr(cbind(1:100,rnorm(100),runif(100),rnorm(100,0,2)))
```

---

**regr_ind**

*Indices of the best regressions*

---

**Description**

One of the two main functions of the package. Identifies the predictors included into regressions with the highest average predictive power.
Usage

regr_ind(
  vari,
  outi,
  crv,
  cutoff = NULL,
  part = 10,
  mode,
  cmode = "det",
  predm = "exact",
  objfun = "acc",
  parallel = FALSE,
  cores,
  minx = 1,
  maxx = NULL,
  nr = NULL,
  maxw = NULL,
  st = NULL,
  rule = 10,
  corr = 1,
  Rsq = F,
  marg = 0
)

Arguments

vari set of predictors
outi array of outcomes
crv number of cross-validations
cutoff cut-off value for mode 'binary'
part for each cross-validation partitions the dataset into training and test set in a proportion (part-1):part
mode 'binary' (logistic regression), 'multin' (multinomial regression)
cmode 'det' or ''; 'det' always predicts the more likely outcome as determined by the odds ratio; '' predicts certain outcome with probability corresponding to its odds ratio (more conservative). Option available for multinomial/logistic regression
predm 'exact' or ''; for logistic and multinomial regression; 'exact' computes how many times the exact outcome category was predicted, '' computes how many times either the exact outcome category or its nearest neighbour was predicted
objfun 'roc' for maximising the predictive power with respect to AUC, available only for mode='binary'; 'acc' for maximising predictive power with respect to accuracy.
parallel TRUE if using parallel toolbox, FALSE if not. Defaults to FALSE
cores number of cores to use in case of parallel=TRUE
**regr_ind**

- **minx**: minimum number of predictors to be included in a regression, defaults to 1
- **maxx**: maximum number of predictors to be included in a regression, defaults to maximum feasible number according to one in ten rule
- **nr**: a subset of the data-set, such that 1/part of it lies in the test set and 1-1/part is in the training set, defaults to empty set. This is to ensure that elements of this subset are included both in the training and in the test set.
- **maxw**: maximum weight of predictors to be included in a regression, defaults to maximum weight according to one in ten rule
- **st**: a subset of predictors to be always included into a predictive model, defaults to empty set
- **rule**: an Events per Variable (EPV) rule, defaults to 10'
- **corr**: maximum correlation between a pair of predictors in a model
- **Rsq**: whether the R-squared statistics constraint is introduced
- **marg**: margin of error for R-squared statistics constraint

**Value**

Prints the best predictive power provided by a regression, predictive accuracy of the empirical prediction (value of emp computed by cross_val for logistic and linear regression). Returns indices of the predictors included into regressions with the highest predictive power written in a list. For mode='linear' outputs a list of two lists. First list corresponds to the smallest absolute error, second corresponds to the smallest relative error

**See Also**

Uses compute_weights, make_numeric, compute_max_weight, compute_weights, compute_max_length, cross_val, av_out, get_indices

**Examples**

```r
#creating variables for linear regression mode
variables_lin<-matrix(c(rnorm(56,0,1),rnorm(56,1,2)),ncol=2)
#creating outcomes for linear regression mode
outcomes_lin<-rnorm(56,2,1)
#running the function
regr_ind(variables_lin,outcomes_lin,100,mode='linear',parallel=TRUE,cores=2)
```

#creating variables for binary mode
```r
vari<-matrix(c(1:100,seq(1,300,3)),ncol=2)
```

#creating outcomes for binary mode
out<-rbinom(100,1,0.3)

#running the function

regr_ind(vari,out,20,cutoff=0.5,part=10,mode='binary',parallel=TRUE,cores=2,nr=c(1,10,20),maxx=1)

---

**sum_weights_sub**

*Cumulative weights of the predictors' subsets*

**Description**

Function which computes the sum of predictors' weights for each subset containing a fixed number of predictors.

**Usage**

```
sum_weights_sub(a,m,we,st)
```

**Arguments**

<table>
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<tr>
<th>Argument</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td><code>a</code></td>
<td>an m x N matrix, containing all possible subsets (N overall) of the size m of predictors' indices; therefore each column of <code>a</code> defines a unique subset of the predictors</td>
</tr>
<tr>
<td><code>m</code></td>
<td>number of elements in each subset of indices</td>
</tr>
<tr>
<td><code>we</code></td>
<td>array of weights of the predictors</td>
</tr>
<tr>
<td><code>st</code></td>
<td>a subset of predictors to be always included into a predictive model</td>
</tr>
</tbody>
</table>

**Value**

Returns an array of weights for predictors defined by each column of the matrix `a`.

**Examples**

```
#all two-element subsets of the set 1:3
a<-combn(3,2)
sum_weights_sub(a,2,c(1,2,1))
```
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