# Package 'rminer'

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Version 1.4.8

**Title** Data Mining Classification and Regression Methods

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Description Facilitates the use of data mining algorithms in classification and regression (including time series forecasting) tasks by presenting a short and coherent set of functions. Versions: 1.4.8 improved help, several warning and error code fixes (more stable version, all examples run correctly); 1.4.7 improved Importance function and examples, minor error fixes; 1.4.6 / 1.4.5 / 1.4.4 new automated machine learning (AutoML) and ensembles, via improved fit(), mining() and mparheuristic() functions, and new categorical preprocessing, via improved delevels() function; 1.4.3 new metrics (e.g., macro precision, explained variance), new ``lssvm" model and improved mparheuristic() function; 1.4.2 new ``NMAE" metric, ``xgboost" and ``cv.glmnet" models (16 classification and 18 regression models); 1.4.1 new tutorial and more robust version; 1.4 - new classification and regression models, with a total of 14 classification and 15 regression methods, including: Decision Trees, Neural Networks, Support Vector Machines, Random Forests, Bagging and Boosting; 1.3 and 1.3.1 - new classification and regression metrics; 1.2 - new input importance methods via improved Importance() function; 1.0 - first version.

**Imports** methods, plotrix, lattice, nnet, kknn, pls, MASS, mda, rpart, randomForest, adabag, party, Cubist, kernlab, e1071, glmnet, xgboost

LazyLoad Yes

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2 CasesSeries

# **Contents**

CasesSeries		Create a training set (data.frame) from a time series using a sliding window.					
Index							72
	vecplot						69
	sin1reg						
	sa_fri1						
	savemining						66
	predict.fit						
	mparheuristic						
	mmetric						
	mining						
	lforecast mgraph						
	imputation						
	Importance						
							23
	fit						7
	delevels						5
	crossvaldata						
	CasesSeries						2

# Description

Create a training set (data.frame) from a time series using a sliding window.

# Usage

```
CasesSeries(t, W, start = 1, end = length(t))
```

# Arguments

t a time series (numeric vector).

W a sliding window (with time lags, numeric vector).

start starting period.

end ending period.

# **Details**

Check reference for details.

# Value

Returns a data.frame, where y is the output target and the inputs are the time lags.

crossvaldata 3

# Author(s)

Paulo Cortez http://www3.dsi.uminho.pt/pcortez/

#### References

• To check for more details:

P. Cortez.

Sensitivity Analysis for Time Lag Selection to Forecast Seasonal Time Series using Neural Networks and Support Vector Machines.

In Proceedings of the IEEE International Joint Conference on Neural Networks (IJCNN 2010), pp. 3694-3701, Barcelona, Spain, July, 2010. IEEE Computer Society, ISBN: 978-1-4244-6917-8 (DVD edition).

doi:10.1109/IJCNN.2010.5596890

• This tutorial shows additional code examples:

P. Cortez.

A tutorial on using the rminer R package for data mining tasks.

Teaching Report, Department of Information Systems, ALGORITMI Research Centre, Engineering School, University of Minho, Guimaraes, Portugal, July 2015.

```
http://hdl.handle.net/1822/36210
```

#### See Also

```
fit, lforecast, predict.fit.
```

# **Examples**

```
t=1:20
d=CasesSeries(1:10,c(1,3,4))
print(d)
d=CasesSeries(1:10,c(1,2,3))
print(d)
```

crossvaldata

Computes k-fold cross validation for rminer models.

# **Description**

Computes k-fold cross validation for rminer models.

# Usage

4 crossvaldata

### **Arguments**

x See fit for details.
 data See fit for details.
 theta.fit fitting function
 theta.predict prediction function
 ngroup number of folds

mode Possibilities are: "stratified", "random" or "order" (see holdout for details).

seed if NULL then no seed is used and the current R randomness is assumed; else

a fixed seed is adopted to generate local random sample sequences, returning always the same result for the same seed (local means that it does not affect the state of other random number generations called after this function, see holdout

example).

model See fit for details.
task See fit for details.
feature See fit for details.

... Additional parameters sent to theta.fit or theta.predic (e.g. search)

#### **Details**

Standard k-fold cross-validation adopted for rminer models. By default, for classification tasks ("class" or "prob") a stratified sampling is used (the class distributions are identical for each fold), unless mode is set to random or order (see holdout for details).

#### Value

Returns a list with:

- \$cv.fit all predictions (factor if task="class", matrix if task="prob" or numeric if task="reg");
- \$model vector list with the model for each fold.
- \$mpar vector list with the mpar for each fold;
- \$attributes the selected attributes for each fold if a feature selection algorithm was adopted;
- \$ngroup the number of folds;
- \$leave.out the computed size for each fold (=nrow(data)/ngroup);
- \$groups vector list with the indexes of each group;
- \$call the call of this function;

#### Note

A better control (e.g. use of several Runs) is achieved using the simpler mining function.

#### Author(s)

This function was adapted by Paulo Cortez from the crossval function of the bootstrap library (S original by R. Tibshirani and R port by F. Leisch).

delevels 5

#### References

Check the crossval function.

#### See Also

```
holdout, fit, mining and predict.fit.
```

#### **Examples**

delevels

Reduce, replace or transform levels of a data.frame or factor variable (useful for preprocessing datasets).

# Description

Reduce, replace or transform levels of a data.frame or factor variable (useful for preprocessing datasets).

## Usage

```
delevels(x, levels, label = NULL)
```

# **Arguments**

Χ

factor with several levels or a data.frame. If a data.frame, then all factor attributes are transformed.

levels

character vector with several options:

- idf factor is transformed into a numeric vector using IDF transform.
- pcp or c("pcp",perc) factor is transformed using PCP transform. If perc is not provided, the default 0.1 value is used.
- any other values all level values are merged into a single factor level according to label.

6 delevels

Another possibility is to define a vector list, with levels[[i]] values for each factor of the data.frame (see example).

label

the new label used for all levels examples (if NULL then "\_OTHER" is assumed).

#### **Details**

The Inverse Document Frequency (IDF) uses  $f(x) = \log(n/f_x)$ , where n is the length of x and  $f_x$  is the frequency of x.

The Percentage Categorical Pruned (PCP) merges all least frequent levels (summing up to perc percent) into a single level.

When other values are used for levels, this function replaces all levels values with the single label value.

# Value

Returns a transformed factor or data.frame.

#### Author(s)

```
Paulo Cortez http://www3.dsi.uminho.pt/pcortez/
```

#### References

• PCP transform:

L.M. Matos, P. Cortez, R. Mendes, A. Moreau.

Using Deep Learning for Mobile Marketing User Conversion Prediction. In Proceedings of the IEEE International Joint Conference on Neural Networks (IJCNN 2019), paper N-19327, Budapest, Hungary, July, 2019 (8 pages), IEEE, ISBN 978-1-7281-2009-6.

```
doi:10.1109/IJCNN.2019.8851888
http://hdl.handle.net/1822/62771
```

• IDF transform:

L.M. Matos, P. Cortez, R. Mendes and A. Moreau.

A Comparison of Data-Driven Approaches for Mobile Marketing User Conversion Prediction. In Proceedings of 9th IEEE International Conference on Intelligent Systems (IS 2018), pp. 140-146, Funchal, Madeira, Portugal, September, 2018, IEEE, ISBN 978-1-5386-7097-2. https://ieeexplore.ieee.org/document/8710472

```
http://hdl.handle.net/1822/61586
```

# See Also

```
fit and imputation.
```

# Examples

```
### simples examples:
f=factor(c("A","A","B","B","C","D","E"))
print(table(f))
# replace "A" with "a":
```

```
f1=delevels(f, "A", "a")
print(table(f1))
# merge c("C","D","E") into "CDE":
f2=delevels(f,c("C","D","E"),"CDE")
print(table(f2))
# merge c("B","C","D","E") into _OTHER:
f3=delevels(f,c("B","C","D","E"))
print(table(f3))
## Not run:
# larger factor:
x=factor(c(1,rep(2,2),rep(3,3),rep(4,4),rep(5,5),rep(10,10),rep(100,100)))
print(table(x))
# IDF: frequent values are close to zero and
# infrequent ones are more close to each other:
x1=delevels(x,"idf")
print(table(x1))
# PCP: infrequent values are merged
x2=delevels(x,c("pcp",0.1)) # around 10
print(table(x2))
# example with a data.frame:
y=factor(c(rep("a",100),rep("b",20),rep("c",5)))
z=1:125 # numeric
d=data.frame(x=x,y=y,z=z,x2=x)
print(summary(d))
# IDF:
d1=delevels(d,"idf")
print(summary(d1))
# PCP:
d2=delevels(d,"pcp")
print(summary(d2))
# delevels:
L=vector("list",ncol(d)) # one per attribute
L[[1]]=c("1","2","3","4","5")
L[[2]]=c("b","c")
L[[4]]=c("1","2","3") # different on purpose
d3=delevels(d,levels=L,label="other")
print(summary(d3))
## End(Not run) # end dontrun
```

fit

Fit a supervised data mining model (classification or regression) model

## **Description**

Fit a supervised data mining model (classification or regression) model. Wrapper function that allows to fit distinct data mining (16 classification and 18 regression) methods under the same

coherent function structure. Also, it tunes the hyperparameters of the models (e.g., kknn, mlpe and ksvm) and performs some feature selection methods.

#### **Usage**

```
fit(x, data = NULL, model = "default", task = "default",
    search = "heuristic", mpar = NULL, feature = "none",
    scale = "default", transform = "none",
    created = NULL, fdebug = FALSE, ...)
```

## Arguments

x a symbolic description (formula) of the model to be fit.

If data=NULL it is assumed that x contains a formula expression with known variables (see first example below).

data an optional data frame (

an optional data frame (columns denote attributes, rows show examples) containing the training data, when using a formula.

Typically this should be a character object with the model type name (data mining method, as explained in valid character options).

First usage: individual fit. Valid character options are the typical R base learning functions (individual models), namely one of:

- naive most common class (classification) or mean output value (regression)
- ctree conditional inference tree (classification and regression, uses ctree)
- cv.glmnet generalized linear model (GLM) with lasso or elasticnet regularization (classification and regression, uses cv.glmnet; note: cross-validation is used to automatically set the lambda parameter that is needed to compute the predictions)
- rpart or dt decision tree (classification and regression, uses rpart)
- kknn or knn k-nearest neighbor (classification and regression, uses kknn)
- ksvm or svm support vector machine (classification and regression, uses ksvm)
- lssvm least squares support vector machine (pure classification only, uses lssvm)
- mlp multilayer perceptron with one hidden layer (classification and regression, uses nnet (in this version, for both mlp and mlpe, the maximum number of weights was increased and fixed to MaxNWts=10000))
- mlpe multilayer perceptron ensemble (classification and regression, uses nnet)
- randomForest or randomforest random forest algorithm (classification and regression, uses randomForest)
- xgboost eXtreme Gradient Boosting (Tree) (classification and regression, uses xgboost; note: nrounds parameter is set by default to 2)
- bagging bagging from Breiman, 1996 (classification, uses bagging)
- boosting adaboost.M1 method from Freund and Schapire, 1996 (classification, uses boosting)

model

- 1da linear discriminant analysis (classification, uses 1da)
- multinom or lr logistic regression (classification, uses multinom)
- naiveBayes or naivebayes naive bayes (classification, uses naiveBayes)
- qda quadratic discriminant analysis (classification, uses qda)
- cubist M5 rule-based model (regression, uses cubist)
- 1m standard multiple/linear regression (uses 1m)
- mr multiple regression (regression, equivalent to 1m but uses nnet with zero hidden nodes and linear output function)
- mars multivariate adaptive regression splines (regression, uses mars)
- pcr principal component regression (regression, uses pcr)
- plsr partial least squares regression (regression, uses plsr)
- cppls canonical powered partial least squares (regression, uses cppls)
- rvm relevance vector machine (regression, uses rvm)

Second usage: multiple models. model can be used to perform Automated Machine Learning (AutoML) or ensembles of several individual models:

- auto first, the best model is automatically set by searching all models defined in search and selecting the one with the best "validation" metric on a validation set (depending on the method defined in search); then, the selected best model is fit to all training data. When auto is used, a ranked leaderboard of the models (and their selected hyperparameters) is returned as a new \$LB field of the @mpar returned slot (e.g., try: print(M@mpar\$LB), where M is an object returned by fit).
- AE, WE or SE all individual models are first fit to the data; then an ensemble is built by: AE Average Ensemble, majority (if task=="class") or average of the predictions; WE) Weighted Ensemble, similar to AE but each prediction is weighted according to the validation metric (for task=="class" it is equal to AE); SE Stacking Ensemble, applies a second-level GLM to weight the individual predictions. For any ensemble, when an individual model produces an error then it is excluded from the ensemble. After excluding invalid models, if there is just a single model then such model is returned (and no ensemble is produced).

Third usage: model can be a list with 2 possibilities of fields A) and B). A) if you have your one fit function, then you can embed it using:

- \$fit a fit function that accepts the arguments x, data and ..., the goal is to accept here any R classification or regression model, mainly for its use within the mining or Importance functions, or to use a hyperparameter search (via search).
- \$predict a predict function that accepts the arguments object, newdata, this function should behave as any rminer prediction, i.e., return: a factor when task=="class"; a matrix with *Probabilities x Instances* when task=="prob"; and a vector when task=="reg".
- \$name optional field with the name of the method.

B) automatically produced by some ensemble methods, for the sake of documentation the fields for the ensembles ("AE", "WE" or "SE") are listed here:

• \$m – a vector character with the fit object model names.

10

- \$f a vector list with several fit objects.
- \$w a vector with the "weighting" of the individual models.

Note: current rminer version emphasizes the use of native fitting functions from their respective packages, since these functions contain several specific hyperparameters that can now be searched or set using the search or . . . arguments. For compatibility with previous rminer versions, older model options are kept.

fit

data mining task. Valid options are:

- prob (or p) classification with output probabilities (i.e. the sum of all outputs equals 1).
- class (or c) classification with discrete outputs (factor)
- reg (or r) regression (numeric output)
- default tries to guess the best task (prob or reg) given the model and output variable type (if factor then prob else reg)

used to tune hyperparameter(s) of the model, such as: kknn – number of neighbors (k); mlp or mlpe – number of hidden nodes (*size*) or *decay*; ksvm – gaussian kernel parameter (*sigma*); randomForest – mtry parameter).

This is a very flexible argument that can be used under several options: simpler use, complex tuning of an individual model or multiple models. The simpler use is kept for compatibility issues but it is advised to define this argument via the easier mparheuristic function.

Valid options for a simpler **character type** search use:

- heuristic simple heuristic, one search parameter (e.g., *size*=inputs/2 for mlp or *size*=10 if classification and inputs/2>10, *sigma* is set using kpar="automatic" and kernel="rbfdot" of ksvm). Important Note: instead of the "heuristic" options, it is advisable to use the explicit mparheuristic function that is designed for a wider option of models (all "heuristic" options were kept due to compatibility issues and work only for: kknn; mlp or mlpe; ksvm, with kernel="rbfdot"; and randomForest).
- heuristic5 heuristic with a 5 range grid-search (e.g., seq(1,9,2) for kknn, seq(0,8,2) for mlp or mlpe, 2^seq(-15,3,4) for ksvm, 1:5 for randomRorest)
- heuristic10 heuristic with a 10 range grid-search (e.g., seq(1,10,1) for kknn, seq(0,9,1) for mlp or mlpe, 2^seq(-15,3,2) for ksvm, 1:10 for randomRorest)
- UD, UD1 or UD2 uniform design 2-Level with 13 (UD or UD2) or 21 (UD1) searches (only works for ksvm and kernel="rbfdot").

Another simpler use of the search argument is a **numeric type**:

 a-vector – numeric vector with all hyperparameter values that will be searched within an internal grid-search (the number of searches is length(search) when convex=0)

A more complex but advised use of search is to use a list. Non expert users should create this list via the mparheuristic function, which is very easy to use. Nevertheless, the fields of the list for a single fit (individual model) are shown here:

• \$smethod – type of search method. Valid options are:

task

search

- none no search is executed, one single fit is performed.
- matrix matrix search (tests only n searches, all search parameters are
  of size n).
- grid normal grid search (tests all combinations of search parameters).
- 2L nested 2-Level grid search. First level range is set by \$search and then the 2nd level performs a fine tuning, with length(\$search) searches around (original range/2) best value in first level (2nd level is only performed on numeric searches).
- UD, UD1 or UD2 uniform design 2-Level with 13 (UD or UD2) or 21 (UD1) searches (note: only works for model="ksvm" and kernel="rbfdot"). Under this option, \$search should contain the first level ranges, such as c(-15,3,-5,15) for classification (gamma min and max, C min and max, after which a 2^ transform is applied) or c(-8,0,-1,6,-8,-1) for regression (last two values are epsilon min and max, after which a 2^ transform is applied).
- \$search a-list with all hyperparameter values to be searched or character with previous described options (e.g., "heuristic", "heuristic5", "UD"). If a character, then \$smethod equal to "none" or "grid" or "UD" is automatically assumed.
- \$convex number that defines how many searches are performed after a local minimum/maximum is found (if >0, the search can be stopped without testing all grid-search values)
- \$method type of internal (validation) estimation method used during the search (see method argument of mining for details)
- \$metric used to compute a metric value during internal estimation. Can be a single character such as "SAD" or a list with all the arguments used by the mmetric function except y and x, such as: search\$metric=list(metric="AUC",TC=3,D=0.7). See mmetric for more details.

A more sophisticated definition of search involves the tuning of several models (used by the model= auto, AE, WE or SE). Again, this sophisticated definition should be automatically set using the mparheuristic function. The list of fields for the multiple tuning mode are:

- \$models a vector character with LM individual model values. This field can also include ensembles ("AE", "WE", "SE") provided they appear at the end of this vector. They will work if more than one valid individual model is included.
- \$1s a vector list with LM search values (for each individual model, the values are the same as in individual search \$search field).
- \$smethod must have the auto value.
- \$smethod must have the auto value.
- \$method internal (validation) estimation method (equal to the individual search \$method field).
- \$metric internal (validation) estimation metric (equal to the individual search \$metric field).

• \$convex - equal to the individual search \$convex field.

Note: the mpar argument only appears due to compatibility issues. If used, then the mpar values are automatically fed into search. However, a direct use of the search argument is advised instead of mpar, since search is more flexible and powerful.

(important note: this argument only is kept in this version due to compatibility with previous rminer versions. Instead of mpar, you should use the more flexible and powerful search argument.)

vector with extra default (fixed) model parameters (used for modeling, search and feature selection) with:

- c(vmethod,vpar,metric) generic use of mpar (including most models);
- c(C,epsilon,vmethod,vpar,metric) if ksvm and C and epsilon are explicitly set;
- c(nr,maxit,vmethod,vpar,metric) if mlp or mlpe and nr and maxit are explicitly set;

C and *epsilon* are default values for svm (if any of these is =NA then heuristics are used to set the value).

*nr* is the number of mlp runs or mlpe individual models, while *maxit* is the maximum number of epochs (if any of these is =NA then heuristics are used to set the value).

For help on *vmethod* and *vpar* see mining.

metric is the internal error function (e.g., used by search to select the best model), valid options are explained in mmetric. When mpar=NULL then default values are used. If there are NA values (e.g., mpar=c(NA,NA)) then default values are used.

feature

mpar

feature selection and sensitivity analysis control. Valid fit function options are:

- none no feature selection;
- a *fmethod* character value, such as sabs (see below);
- a-vector vector with c(fmethod,deletions,Runs,vmethod,vpar,defaultsearch)
- a-vector vector with c(fmethod,deletions,Runs,vmethod,vpar)

fmethod sets the type. Valid options are:

- sbs standard backward selection;
- sabs sensitivity analysis backward selection (faster);
- sabsv equal to sabs but uses variance for sensitivity importance measure;
- sabsr equal to sabs but uses range for sensitivity importance measure;
- sabsg equal to sabs (uses gradient for sensitivity importance measure);

*deletions* is the maximum number of feature deletions (if -1 not used).

*Runs* is the number of runs for each feature set evaluation (e.g., 1).

For help on *vmethod* and *vpar* see mining.

*defaultsearch* is one hyperparameter used during the feature selection search, after selecting the best feature set then search is used (faster). If not defined, then search is used during feature selection (may be slow).

When feature is a vector then default values are used to fill missing values or NA values. Note: feature selection capabilities are expected to be enhanced in next rminer versions.

scale

if data needs to be scaled (i.e. for mlp or mlpe). Valid options are:

- default uses scaling when needed (i.e. for mlp or mlpe)
- none no scaling;
- inputs standardizes (0 mean, 1 st. deviation) input attributes;
- all standardizes (0 mean, 1 st. deviation) input and output attributes;

If needed, the predict function of rminer performs the inverse scaling.

transform

if the output data needs to be transformed (e.g., log transform). Valid options are:

- none no transform;
- log y=(log(y+1)) (the inverse function is applied in the predict function);
- positive all predictions are positive (negative values are turned into zero);
- logpositive both log and logpositive;

created

time stamp for the model. By default, the system time is used. Else, you can specify another time.

fdebug

if TRUE show some search details.

. . .

additional and specific parameters send to each fit function model (e.g., dt, rpart, randomforest, kernlab). A few examples:

- the rpart function is used for decision trees, thus you can have: control=rpart.control(cp=.05) (see crossvaldata example).

- the ksvm function is used for support vector machines, thus you can change the kernel type: kernel="polydot" (see examples below).

Important note: if you use package functions and get an error, then try to explicitly define the package. For instance, you might need to use fit(several-arguments, control=Cubist::cubistControl()) instead of fit(several-arguments, control=cubistControl()).

#### **Details**

Fits a classification or regression model given a data.frame (see [Cortez, 2010] for more details). The ... optional arguments should be used to fix values used by specific model functions (see examples). Notes:

- if there is an error in the fit, then a warning is issued (see example).
- the new search argument is very flexible and allows a powerful design of supervised learning models
- the search correct use is very dependent on the R learning base functions. For example, if you are tuning model="rpart" then read carefully the help of function rpart.
- mpar argument is only kept due to compatibility issues and should be avoided; instead, use the more flexible search.

# Details about some models:

Neural Network: mlp trains nr multilayer perceptrons (with maxit epochs, size hidden nodes
and decay value according to the nnet function) and selects the best network according to
minimum penalized error (\$value). mlpe uses an ensemble of nr networks and the final

prediction is given by the average of all outputs. To tune mlp or mlpe you can use the search parameter, which performs a grid search for *size* or *decay*.

- Support Vector Machine: svm adopts by default the gaussian (rbfdot) kernel. For classification tasks, you can use search to tune *sigma* (gaussian kernel parameter) and *C* (complexity parameter). For regression, the epsilon insensitive function is adopted and there is an additional hyperparameter *epsilon*.
- Other methods: Random Forest if needed, you can tune several parameters, including the default mtry parameter adopted by search heuristics; k-nearest neighbor search by default tunes k. The remaining models can also be tunned but a full definition of search is required (e.g., with \$smethod, \$search and other fields); please check mparheuristic function for further tuning examples (e.g., rpart).

#### Value

Returns a model object. You can check all model elements with str(M), where M is a model object. The slots are:

- @formula the x:
- @model the model:
- @task the task:
- @mpar data.frame with the best model parameters (interpretation depends on model);
- @attributes the attributes used by the model;
- @scale the scale;
- @transform the transform;
- @created the date when the model was created;
- @time computation effort to fit the model;
- @object the R object model (e.g., rpart, nnet, ...);
- @outindex the output index (of @attributes);
- @levels if task=="prob" | | task=="class" stores the output levels;
- @error similarly to mining this is the "validation" error for some search options;

### Note

```
See also http://hdl.handle.net/1822/36210 and http://www3.dsi.uminho.pt/pcortez/rminer.html
```

# Author(s)

```
Paulo Cortez https://pcortez.dsi.uminho.pt
```

#### References

• To check for more details about rminer and for citation purposes: P. Cortez.

Data Mining with Neural Networks and Support Vector Machines Using the R/rminer Tool. In P. Perner (Ed.), Advances in Data Mining - Applications and Theoretical Aspects 10th Industrial Conference on Data Mining (ICDM 2010), Lecture Notes in Artificial Intelligence 6171, pp. 572-583, Berlin, Germany, July, 2010. Springer. ISBN: 978-3-642-14399-1. @Springer: https://link.springer.com/chapter/10.1007/978-3-642-14400-4\_44 http://www3.dsi.uminho.pt/pcortez/2010-rminer.pdf

• This tutorial shows additional code examples:

P. Cortez.

A tutorial on using the rminer R package for data mining tasks.

Teaching Report, Department of Information Systems, ALGORITMI Research Centre, Engineering School, University of Minho, Guimaraes, Portugal, July 2015.

http://hdl.handle.net/1822/36210

• For the grid search and other optimization methods:

P. Cortez.

Modern Optimization with R.

Use R! series, Springer, 2nd edition, July 2021, ISBN 978-3-030-72818-2.

https://link.springer.com/book/10.1007/978-3-030-72819-9

• The automl is inspired in this work:

L. Ferreira, A. Pilastri, C. Martins, P. Santos, P. Cortez.

An Automated and Distributed Machine Learning Framework for Telecommunications Risk Management. In J. van den Herik et al. (Eds.), Proceedings of 12th International Conference on Agents and Artificial Intelligence – ICAART 2020, Volume 2, pp. 99-107, Valletta, Malta, February, 2020, SCITEPRESS, ISBN 978-989-758-395-7.

@INSTICC: http://hdl.handle.net/1822/66818

• For the sabs feature selection:

P. Cortez, A. Cerdeira, F. Almeida, T. Matos and J. Reis.

Modeling wine preferences by data mining from physicochemical properties.

In Decision Support Systems, Elsevier, 47(4):547-553, 2009.

doi:10.1016/j.dss.2009.05.016

• For the uniform design details:

C.M. Huang, Y.J. Lee, D.K.J. Lin and S.Y. Huang.

Model selection for support vector machines via uniform design,

In Computational Statistics & Data Analysis, 52(1):335-346, 2007.

## See Also

mparheuristic,mining, predict.fit, mgraph, mmetric, savemining, CasesSeries, lforecast, holdout and Importance. Check all rminer functions using: help(package=rminer).

# **Examples**

```
### dontrun is used when the execution of the example requires some computational effort.
### simple regression (with a formula) example.
x1=rnorm(200,100,20); x2=rnorm(200,100,20)
y=0.7*sin(x1/(25*pi))+0.3*sin(x2/(25*pi))
M=fit(y~x1+x2,model="mlpe")
new1=rnorm(100,100,20); new2=rnorm(100,100,20)
ynew=0.7*sin(new1/(25*pi))+0.3*sin(new2/(25*pi))
P=predict(M,data.frame(x1=new1,x2=new2,y=rep(NA,100)))
print(mmetric(ynew,P,"MAE"))
### simple classification example.
## Not run:
data(iris)
M=fit(Species~.,iris,model="rpart")
plot(M@object); text(M@object) # show model
P=predict(M,iris)
print(mmetric(iris$Species,P,"CONF"))
print(mmetric(iris$Species,P,"ALL"))
mgraph(iris$Species,P,graph="ROC",TC=2,main="versicolor ROC",
baseline=TRUE,leg="Versicolor",Grid=10)
M2=fit(Species~.,iris,model="ctree")
plot(M2@object) # show model
P2=predict(M2,iris)
print(mmetric(iris$Species,P2,"CONF"))
# ctree with different setup:
# (ctree_control is from the party package)
M3=fit(Species~.,iris,model="ctree",controls = party::ctree_control(testtype="MonteCarlo"))
plot(M3@object) # show model
## End(Not run)
### simple binary classification example with cv.glmnet and xgboost
## Not run:
data(sa_ssin_2)
H=holdout(sa_ssin_2$y,ratio=2/3)
# cv.glmnet:
M=fit(y~.,sa_ssin_2[H$tr,],model="cv.glmnet",task="cla") # pure classes
P=predict(M,sa_ssin_2[H$ts,])
cat("1st prediction, class:",as.character(P[1]),"\n")
cat("Confusion matrix:\n")
print(mmetric(sa_ssin_2[H$ts,]$y,P,"CONF")$conf)
M2=fit(y~.,sa_ssin_2[H$tr,],model="cv.glmnet") # probabilities
P2=predict(M2,sa_ssin_2[H$ts,])
L=M2@levels
cat("1st prediction, prob:",L[1],"=",P2[1,1],",",L[2],"=",P2[1,2],"\n")
cat("Confusion matrix:\n")
print(mmetric(sa_ssin_2[H$ts,]$y,P2,"CONF")$conf)
```

```
cat("AUC of ROC curve:\n")
print(mmetric(sa_ssin_2[H$ts,]$y,P2,"AUC"))
M3=fit(y~.,sa_ssin_2[H$tr,],model="cv.glmnet",nfolds=3) # use 3 folds instead of 10
plot(M3@object) # show cv.glmnet object
P3=predict(M3,sa_ssin_2[H$ts,])
# xgboost:
M4=fit(y^{-},sa_ssin_2[H$tr,],model="xgboost",verbose=1) # nrounds=2, show rounds:
P4=predict(M4,sa_ssin_2[H$ts,])
print(mmetric(sa_ssin_2[H$ts,]$y,P4,"AUC"))
\label{local-model} M5=fit(y^-.,sa\_ssin\_2[H$tr,],model="xgboost",nrounds=3,verbose=1) \ \# \ nrounds=3, \ show \ rounds=3,verbose=1) \ \# \ nrounds=3,verbose=1) \ \# \ nrounds=3,verbos
P5=predict(M5,sa_ssin_2[H$ts,])
print(mmetric(sa_ssin_2[H$ts,]$y,P5,"AUC"))
## End(Not run)
### classification example with discrete classes, probabilities and holdout
## Not run:
data(iris)
H=holdout(iris$Species,ratio=2/3)
M=fit(Species~.,iris[H$tr,],model="ksvm",task="class")
M1=fit(Species~.,iris[H$tr,],model="lssvm") # default task="class" is assumed
M2=fit(Species~.,iris[H$tr,],model="ksvm",task="prob")
P=predict(M,iris[H$ts,]) # classes
P1=predict(M1,iris[H$ts,]) # classes
P2=predict(M2,iris[H$ts,]) # probabilities
print(mmetric(iris$Species[H$ts],P,"CONF"))
print(mmetric(iris$Species[H$ts],P1,"CONF"))
print(mmetric(iris$Species[H$ts],P2,"CONF"))
print(mmetric(iris$Species[H$ts],P,"CONF",TC=1))
print(mmetric(iris$Species[H$ts],P2,"CONF",TC=1))
print(mmetric(iris$Species[H$ts],P2,"AUC"))
### exploration of some rminer classification models:
models=c("lda","naiveBayes","kknn","randomForest","cv.glmnet","xgboost")
for(m in models)
 { cat("model:",m,"\n")
     M=fit(Species~.,iris[H$tr,],model=m)
     P=predict(M,iris[H$ts,])
     print(mmetric(iris$Species[H$ts],P,"AUC")[[1]])
  }
## End(Not run)
### classification example with hyperparameter selection
              note: for regression, similar code can be used
### SVM
## Not run:
data(iris)
# large list of SVM configurations:
# SVM with kpar="automatic" sigma rbfdot kernel estimation and default C=1:
# note: each execution can lead to different M@mpar due to sigest stochastic nature:
```

```
M=fit(Species~.,iris,model="ksvm")
print(M@mpar) # model hyperparameters/arguments
# same thing, explicit use of mparheuristic:
M=fit(Species~.,iris,model="ksvm",search=list(search=mparheuristic("ksvm")))
print(M@mpar) # model hyperparameters
# SVM with C=3, sigma=2^-7
M=fit(Species~.,iris,model="ksvm",C=3,kpar=list(sigma=2^-7))
print(M@mpar)
# SVM with different kernels:
M=fit(Species~.,iris,model="ksvm",kernel="polydot",kpar="automatic")
print(M@mpar)
# fit already has a scale argument, thus the only way to fix scale of "tanhdot"
# is to use the special search argument with the "none" method:
s=list(smethod="none",search=list(scale=2,offset=2))
M=fit(Species~.,iris,model="ksvm",kernel="tanhdot",search=s)
print(M@mpar)
# heuristic: 10 grid search values for sigma, rbfdot kernel (fdebug is used only for more verbose):
s=list(search=mparheuristic("ksvm",10)) # advised "heuristic10" usage
M=fit(Species~.,iris,model="ksvm",search=s,fdebug=TRUE)
print(M@mpar)
# same thing, uses older search="heuristic10"
M=fit(Species~.,iris,model="ksvm",search="heuristic10",fdebug=TRUE)
print(M@mpar)
# identical search under a different and explicit code:
s=list(search=2^seq(-15,3,2))
M=fit(Species~.,iris,model="ksvm",search=2^seq(-15,3,2),fdebug=TRUE)
print(M@mpar)
# uniform design "UD" for sigma and C, rbfdot kernel, two level of grid searches,
# under exponential (2^x) search scale:
M=fit(Species~.,iris,model="ksvm",search="UD",fdebug=TRUE)
print(M@mpar)
M=fit(Species~.,iris,model="ksvm",search="UD1",fdebug=TRUE)
print(M@mpar)
# now the more powerful search argument is used for modeling SVM:
# grid 3 x 3 search:
s=list(smethod="grid", search=list(sigma=2^c(-15, -5, 3), C=2^c(-5, 0, 15)), convex=0,
            metric="AUC",method=c("kfold",3,12345))
print(s)
M=fit(Species~.,iris,model="ksvm",search=s,fdebug=TRUE)
print(M@mpar)
# identical search with different argument smethod="matrix"
s$smethod="matrix"
ssearch=list(sigma=rep(2^{c}(-15,-5,3),times=3),C=rep(2^{c}(-5,0,15),each=3))
M=fit(Species~.,iris,model="ksvm",search=s,fdebug=TRUE)
print(M@mpar)
# search for best kernel (only works for kpar="automatic"):
s=list(smethod="grid",search=list(kernel=c("rbfdot","laplacedot","polydot","vanilladot")),
       convex=0,metric="AUC",method=c("kfold",3,12345))
print(s)
M=fit(Species~.,iris,model="ksvm",search=s,fdebug=TRUE)
```

```
print(M@mpar)
# search for best parameters of "rbfdot" or "laplacedot" (which use same kpar):
s$search=list(kernel=c("rbfdot","laplacedot"),sigma=2^seq(-15,3,5))
M=fit(Species~.,iris,model="ksvm",search=s,fdebug=TRUE)
print(M@mpar)
### randomForest
# search for mtry and ntree
s=list(smethod="grid",search=list(mtry=c(1,2,3),ntree=c(100,200,500)),
            convex=0,metric="AUC",method=c("kfold",3,12345))
print(s)
M=fit(Species~.,iris,model="randomForest",search=s,fdebug=TRUE)
print(M@mpar)
### rpart
# simpler way to tune cp in 0.01 to 0.9 (10 searches):
s=list(search=mparheuristic("rpart",n=10,lower=0.01,upper=0.9),method=c("kfold",3,12345))
M=fit(Species~.,iris,model="rpart",search=s,fdebug=TRUE)
print(M@mpar)
# same thing but with more lines of code
# note: this code can be adapted to tune other rpart parameters,
       while mparheuristic only tunes cp
# a vector list needs to be used for the search$search parameter
lcp=vector("list",10) # 10 grid values for the complexity cp
names(lcp)=rep("cp",10) # same cp name
scp=seq(0.01,0.9,length.out=10) # 10 values from 0.01 to 0.18
for(i in 1:10) lcp[[i]]=scp[i] # cycle needed due to [[]] notation
s=list(smethod="grid",search=list(control=lcp),
            convex=0,metric="AUC",method=c("kfold",3,12345))
M=fit(Species~.,iris,model="rpart",search=s,fdebug=TRUE)
print(M@mpar)
### ctree
# simpler way to tune mincriterion in 0.1 to 0.98 (9 searches):
mint=c("kfold",3,123) # internal validation method
s=list(search=mparheuristic("ctree", n=8, lower=0.1, upper=0.99), method=mint)
M=fit(Species~.,iris,model="ctree",search=s,fdebug=TRUE)
print(M@mpar)
# same thing but with more lines of code
# note: this code can be adapted to tune other ctree parameters,
        while mparheuristic only tunes mincriterion
# a vector list needs to be used for the search$search parameter
lmc=vector("list",9) # 9 grid values for the mincriterion
smc=seq(0.1,0.99,length.out=9)
for(i in 1:9) lmc[[i]]=party::ctree_control(mincriterion=smc[i])
s=list(smethod="grid",search=list(controls=lmc),method=mint,convex=0)
M=fit(Species~.,iris,model="ctree",search=s,fdebug=TRUE)
print(M@mpar)
### some MLP fitting examples:
# simplest use:
```

```
M=fit(Species~.,iris,model="mlpe")
print(M@mpar)
# same thing, with explicit use of mparheuristic:
M=fit(Species~.,iris,model="mlpe",search=list(search=mparheuristic("mlpe")))
print(M@mpar) # hidden nodes and number of ensemble mlps
# setting some nnet parameters:
M=fit(Species~.,iris,model="mlpe",size=3,decay=0.1,maxit=100,rang=0.9)
print(M@mpar) # mlpe hyperparameters
# MLP, 5 grid search fdebug is only used to put some verbose in the console:
s=list(search=mparheuristic("mlpe",n=5)) # 5 searches for size
print(s) # show search
M=fit(Species~.,iris,model="mlpe",search=s,fdebug=TRUE)
print(M@mpar)
# previous searches used a random holdout (seed=NULL), now a fixed seed (123) is used:
s=list(smethod="grid", search=mparheuristic("mlpe", n=5), convex=0, metric="AUC",
            method=c("holdout",2/3,123))
print(s)
M=fit(Species~.,iris,model="mlpe",search=s,fdebug=TRUE)
print(M@mpar)
# faster and greedy grid search:
s$convex=1;s$search=list(size=0:9)
print(s)
M=fit(Species~.,iris,model="mlpe",search=s,fdebug=TRUE)
print(M@mpar)
# 2 level grid with total of 5 searches
# note of caution: some "2L" ranges may lead to non integer (e.g., 1.3) values at
# the 2nd level search. And some R functions crash if non integer values are used for
# integer parameters.
s$smethod="2L";s$convex=0;s$search=list(size=c(4,8,12))
M=fit(Species~.,iris,model="mlpe",search=s,fdebug=TRUE)
print(M@mpar)
# testing of all 17 rminer classification methods:
model=c("naive","ctree","cv.glmnet","rpart","kknn","ksvm","lssvm","mlp","mlpe",
 "randomForest", "xgboost", "bagging", "boosting", "lda", "multinom", "naiveBayes", "qda")
inputs=ncol(iris)-1
ho=holdout(iris$Species,2/3,seed=123) # 2/3 for training and 1/3 for testing
Y=iris[ho$ts,ncol(iris)]
for(i in 1:length(model))
 {
  cat("i:",i,"model:",model[i],"\n")
  search=list(search=mparheuristic(model[i])) # rminer default values
  M=fit(Species~.,data=iris[ho$tr,],model=model[i],search=search,fdebug=TRUE)
  P=predict(M,iris[ho$ts,])
  cat("predicted ACC:",round(mmetric(Y,P,metric="ACC"),1),"\n")
 }
## End(Not run)
### example of an error (warning) generated using fit:
## Not run:
```

```
data(iris)
# size needs to be a positive integer, thus 0.1 leads to an error:
M=fit(Species~.,iris,model="mlp",size=0.1)
print(M@object)
## End(Not run)
### exploration of some rminer regression models:
## Not run:
data(sa_ssin)
H=holdout(sa_ssin$y,ratio=2/3,seed=12345)
models=c("lm","mr","ctree","mars","cubist","cv.glmnet","xgboost","rvm")
for(m in models)
 { cat("model:",m,"\n")
   M=fit(y~.,sa_ssin[H$tr,],model=m)
   P=predict(M,sa_ssin[H$ts,])
   print(mmetric(sa_ssin$y[H$ts],P,"MAE"))
## End(Not run)
# testing of all 18 rminer regression methods:
## Not run:
model=c("naive","ctree","cv.glmnet","rpart","kknn","ksvm","mlp","mlpe",
 "randomForest", "xgboost", "cubist", "lm", "mr", "mars", "pcr", "plsr", "cppls", "rvm")
# note: in this example, default values are considered for the hyperparameters.
# better results can be achieved by tuning hyperparameters via improved usage
# of the search argument (via mparheuristic function or written code)
data(iris)
ir2=iris[,1:4] # predict iris "Petal.Width"
names(ir2)[ncol(ir2)]="y" # change output name
inputs=ncol(ir2)-1
ho=holdout(ir2$y,2/3,seed=123) # 2/3 for training and 1/3 for testing
Y=ir2[ho$ts,ncol(ir2)]
for(i in 1:length(model))
 {
  cat("i:",i,"model:",model[i],"\n")
  search=list(search=mparheuristic(model[i])) # rminer default values
  M=fit(y^{-}, data=ir2[ho$tr,], model=model[i], search=search, fdebug=TRUE)
  P=predict(M,ir2[ho$ts,])
  cat("predicted MAE:",round(mmetric(Y,P,metric="MAE"),1),"\n")
 }
## End(Not run)
### regression example with hyperparameter selection:
## Not run:
data(sa_ssin)
# some SVM experiments:
# default SVM:
M=fit(y~.,data=sa_ssin,model="svm")
print(M@mpar)
# SVM with (Cherkassy and Ma, 2004) heuristics to set C and epsilon:
```

```
M=fit(y~.,data=sa_ssin,model="svm",C=NA,epsilon=NA)
print(M@mpar)
# SVM with Uniform Design set sigma, C and epsilon:
M=fit(y~.,data=sa_ssin,model="ksvm",search="UD",fdebug=TRUE)
print(M@mpar)
# sensitivity analysis feature selection
M=fit(y~.,data=sa_ssin,model="ksvm",search=list(search=mparheuristic("ksvm",n=5)),feature="sabs")
print(M@mpar)
print(M@attributes) # selected attributes (1, 2 and 3 are the relevant inputs)
# example that shows how transform works:
M=fit(y~.,data=sa_ssin,model="mr") # linear regression
P=predict(M, data.frame(x1=-1000, x2=0, x3=0, x4=0, y=NA)) # P should be negative
print(P)
M=fit(y~.,data=sa_ssin,model="mr",transform="positive")
P=predict(M, data.frame(x1=-1000, x2=0, x3=0, x4=0, y=NA)) # P is not negative
print(P)
## End(Not run)
### pure classification example with a generic R (not rminer default) model ###
## Not run:
### nnet is adopted here but virtually ANY fitting function/package could be used:
# since the default nnet prediction is to provide probabilities, there is
# a need to create this "wrapping" function:
predictprob=function(object,newdata)
{ predict(object, newdata, type="class") }
# list with a fit and predict function:
# nnet::nnet (package::function)
model=list(fit=nnet::nnet,predict=predictprob,name="nnet")
# note that size is not a fit parameter and it is sent directly to nnet:
M=fit(Species~.,iris,model=model,size=3,task="class")
P=predict(M,iris)
print(P)
## End(Not run)
### multiple models: automl and ensembles
## Not run:
data(iris)
d=iris
names(d)[ncol(d)]="y" # change output name
inputs=ncol(d)-1
metric="AUC"
# consult the help of mparheuristic for more automl and ensemble examples:
# automatic machine learining (automl) with 5 distinct models and "SE" ensemble.
# the single models are tuned with 10 internal hyperparameter searches,
# except ksvm that uses 13 searches via "UD".
```

holdout 23

```
# fit performs an internal validation
sm=mparheuristic(model="automl3",n=NA,task="prob", inputs= inputs )
method=c("kfold",3,123)
search=list(search=sm,smethod="auto",method=method,metric=metric,convex=0)
M=fit(y~.,data=d,model="auto",search=search,fdebug=TRUE)
P=predict(M,d)
# show leaderboard:
cat("> leaderboard models:",M@mpar$LB$model,"\n")
cat("> validation values:",round(M@mpar$LB$eval,4),"\n")
cat("best model is:",M@model,"\n")
cat(metric, "=", round(mmetric(d$y,P,metric=metric),2),"\n")
# average ensemble of 5 distinct models
# the single models are tuned with 1 (heuristic) hyperparameter search
sm2=mparheuristic(model="automl",n=NA,task="prob", inputs= inputs )
method=c("kfold",3,123)
search2=list(search=sm2, smethod="auto", method=method, metric=metric, convex=0)
M2=fit(y~.,data=d,model="AE",search=search2,fdebug=TRUE)
P2=predict(M,d)
cat("best model is:",M2@model,"\n")
cat(metric,"=",round(mmetric(d$y,P2,metric=metric),2),"\n")
# example with an invalid model exclusion:
# in this case, randomForest produces an error and warning
# thus it is excluded from the leaderboard
sm=mparheuristic(model="automl3",n=NA,task="prob", inputs= inputs )
method=c("holdout",2/3,123)
search=list(search=sm, smethod="auto", method=method, metric=metric, convex=0)
d2=d
d2[,2]=as.factor(1:150) # force randomForest error
M=fit(y~.,data=d2,model="auto",search=search,fdebug=TRUE)
P=predict(M,d2)
# show leaderboard:
cat("> leaderboard models:",M@mpar$LB$model,"\n")
cat("> validation values:",round(M@mpar$LB$eval,4),"\n")
cat("best model is:",M@model,"\n")
cat(metric, "=", round(mmetric(d$y,P,metric=metric),2),"\n")
## End(Not run)
```

holdout

Computes indexes for holdout data split into training and test sets.

# **Description**

Computes indexes for holdout data split into training and test sets.

24 holdout

#### **Usage**

```
holdout(y, ratio = 2/3, internalsplit = FALSE, mode = "stratified", iter = 1,
               seed = NULL, window=10, increment=1)
```

#### **Arguments**

desired target: numeric vector; or factor - then a stratified holdout is applied У (i.e. the proportions of the classes are the same for each set).

split ratio (in percentage – sets the training set size; or in total number of examratio ples – sets the test set size).

> if TRUE then the training data is further split into training and validation sets. The same ratio parameter is used for the internal split.

sampling mode. Options are:

- stratified stratified randomized holdout if y is a factor; else it behaves as standard randomized holdout;
- random standard randomized holdout;
- order static mode, where the first examples are used for training and the later ones for testing (useful for time series data);
- rolling rolling window, also known as sliding window (e.g. useful for stock market prediction), similar to order except that window is the window size, iter is the rolling iteration and increment is the number of samples slided at each iteration. In each iteration, the training set size is fixed to window, while the test set size is equal to ratio except for the last iteration (where it may be smaller).
- incremental incremental retraining mode, also known as growing windows, similar to order except that window is the initial window size, iter is the incremental iteration and increment is the number of samples added at each iteration. In each iteration, the training set size grows (+increment), while the test set size is equal to ratio except for the last iteration (where it may be smaller).

iteration of the incremental retraining mode (only used when mode="rolling" or "incremental", typically iter is set within a cycle, see the example below).

if NULL then no seed is used and the current R randomness is assumed; else a fixed seed is adopted to generate local random sample sequences, returning always the same result for the same seed (local means that it does not affect the

state of other random number generations called after this function, see exam-

ple).

training window size (if mode="rolling") or initial training window size (if window

mode="incremental").

number of samples added to the training window at each iteration (if mode="incremental" increment

or mode="rolling").

# **Details**

Computes indexes for holdout data split into training and test sets.

internalsplit

mode

iter

seed

holdout 25

# Value

A list with the components:

- \$tr numeric vector with the training examples indexes;
- \$ts numeric vector with the test examples indexes;
- \$itr numeric vector with the internal training examples indexes;
- \$val numeric vector with the internal validation examples indexes;

# Author(s)

```
Paulo Cortez http://www3.dsi.uminho.pt/pcortez/
```

#### References

See fit.

#### See Also

```
fit, predict.fit, mining, mgraph, mmetric, savemining, Importance.
```

# **Examples**

```
### simple examples:
# preserves order, last two elements go into test set
H=holdout(1:10,ratio=2,internal=TRUE,mode="order")
print(H)
# no seed or NULL returns different splits:
H=holdout(1:10,ratio=2/3,mode="random")
print(H)
H=holdout(1:10,ratio=2/3,mode="random",seed=NULL)
print(H)
# same seed returns identical split:
H=holdout(1:10,ratio=2/3,mode="random",seed=12345)
print(H)
H=holdout(1:10, ratio=2/3, mode="random", seed=12345)
print(H)
### classification example
## Not run:
data(iris)
# random stratified holdout
H=holdout(iris$Species,ratio=2/3,mode="stratified")
print(table(iris[H$tr,]$Species))
print(table(iris[H$ts,]$Species))
M=fit(Species~.,iris[H$tr,],model="rpart") # training data only
P=predict(M,iris[H$ts,]) # test data
print(mmetric(iris$Species[H$ts],P,"CONF"))
## End(Not run)
### regression example with incremental and rolling window holdout:
```

```
## Not run:
ts=c(1,4,7,2,5,8,3,6,9,4,7,10,5,8,11,6,9)
d=CasesSeries(ts,c(1,2,3))
print(d) # with 14 examples
# incremental holdout example (growing window)
for(b in 1:4) # iterations
   H=holdout(d$y,ratio=4,mode="incremental",iter=b,window=5,increment=2)
   M=fit(y~.,d[H$tr,],model="mlpe",search=2)
   P=predict(M,d[H$ts,])
   cat("batch :",b,"TR from:",H$tr[1],"to:",H$tr[length(H$tr)],"size:",length(H$tr),
       "TS from:", H$ts[1], "to:", H$ts[length(H$ts)], "size:", length(H$ts),
       "mae:",mmetric(d$y[H$ts],P,"MAE"),"\n")
# rolling holdout example (sliding window)
for(b in 1:4) # iterations
  {
  H=holdout(d$y,ratio=4,mode="rolling",iter=b,window=5,increment=2)
   M=fit(y~.,d[H$tr,],model="mlpe",search=2)
   P=predict(M,d[H$ts,])
   cat("batch :",b,"TR from:",H$tr[1],"to:",H$tr[length(H$tr)],"size:",length(H$tr),
       "TS from: ",H$ts[1], "to: ",H$ts[length(H$ts)], "size: ",length(H$ts),
       "mae:",mmetric(d$y[H$ts],P,"MAE"),"\n")
  }
## End(Not run)
### local seed simple example
## Not run:
# seed is defined, same sequence for N1 and N2:
# s2 generation sequence is not affected by the holdout call
set.seed(1); s1=sample(1:10,3)
set.seed(1);
N1=holdout(1:10, seed=123) # local seed
N2=holdout(1:10, seed=123) # local seed
print(N1$tr)
print(N2$tr)
s2=sample(1:10,3)
cat("s1:",s1,"\n")
cat("s2:",s2,"\n") # s2 is equal to s1
## End(Not run)
```

**Importance** 

Measure input importance (including sensitivity analysis) given a supervised data mining model.

# **Description**

Measure input importance (including sensitivity analysis) given a supervised data mining model.

# Usage

# **Arguments**

Μ

fitted model, typically is the object returned by fit. Can also be any fitted model (i.e. not from rminer), provided that the predict function PRED is defined (see examples for details).

data

training data (the same data.frame that was used to fit the model, currently only used to add data histogram to VEC curve).

RealL method the number of sensitivity analysis levels (e.g. 7). Note: you need to use RealL>=2.

input importance method. Options are:

- 1D-SA 1 dimensional sensitivity analysis, very fast, sets interactions to NULL.
- sens or SA sensitivity analysis. There are some extra variants: sensa equal to sens but also sets measure="AAD"; sensy sets measure="variance"; sensg sets measure="gradient"; sensr sets measure="range". if interactions is not null, then GSA is assumed, else 1D-SA is assumed.
- DSA Data-based SA (good option if input interactions need to be detected).
- MSA Monte-Carlo SA.
- CSA Cluster-based SA.
- GSA Global SA (very slow method, particularly if the number of inputs is large, should be avoided).
- randomForest uses method of Leo Breiman (type=1), only makes sense when M is a randomRorest.

measure

sensitivity analysis measure (used to measure input importance). Options are:

- AAD average absolute deviation from the median.
- gradient average absolute gradient (y\_i+1-y\_i) of the responses.
- variance variance of the responses.
- range maximum minimum of the responses.

sampling

for numeric inputs, the sampling scan function. Options are:

• regular – regular sequence (uniform distribution), do not change this value, kept here only due to compatibility issues.

baseline

baseline vector used during the sensitivity analysis. Options are:

- mean uses a vector with the mean values of each attribute from data.
- median uses a vector with the median values of each attribute from data.
- a data.frame with the baseline example (should have the same attribute names as data).

responses if TRUE then all sensitivity analysis responses are stored and returned.

outindex the output index (column) of data if M is not a model object (returned by fit).

the task as defined in fit if M is not a model object (returned by fit). task

**PRED** the prediction function of M, if M is not a model object (returned by fit). Note: this function should behave like the rminer predict-methods, i.e. return a nu-

meric vector in case of regression; a matrix of examples (rows) vs probabilities (columns) (task="prob") or a factor (task="class") in case of classification.

numeric vector with the attributes (columns) used by Ith-D sensitivity analysis interactions (2-D or higher, "GSA" method):

• if NULL then only a 1-D sensitivity analysis is performed.

- if length(interactions)==1 then a "special" 2-D sensitivity analysis is performed using the index of interactions versus all remaining inputs. Note: the \$sresponses[[interactions]] will be empty (in vecplot do not use xval =interactions).
- if length(interactions)>1 then a full Ith-D sensitivity analysis is performed, where I=length(interactions). Note: Computational effort can highly increase if I is too large, i.e. O(RealL^I). Also, you need to preprocess the returned list (e.g. using avg\_imp) to use the vecplot function (see the examples).

Aggregation numeric value that sets the number of multi-metric aggregation function (used only for "DSA", ""). Options are:

- -1 the default value that should work in most cases (if regression, sets Aggregation=3, else if classification then sets Aggregation=1).
- 1 value that should work for classification (only use the average of all sensitivity values).
- 3 value that should work for regression (use 3 metrics, the minimum, average and maximum of all sensitivity values).

number of samples used by DSA and MSA methods. The default value is -1,

which means: use a number equal to training set size. If a different value is used (1<= value <= number of training samples), then LRandom samples are

randomly selected.

sampling type used by MSA: "discrete" (default discrete uniform distribution)

or "continuous" (from continuous uniform distribution).

sets the maximum number of sensitivity levels for discrete inputs. if FALSE then

a maximum of up to RealL levels are used (most frequent ones), else (TRUE)

then all levels of the input are used in the SA analysis.

#### **Details**

This function provides several algorithms for measuring input importance of supervised data mining models and the average effect of a given input (or pair of inputs) in the model. A particular emphasis is given on sensitivity analysis (SA), which is a simple method that measures the effects on the output of a given model when the inputs are varied through their range of values. Check the references for more details.

I Random

**MRandom** 

Lfactor

#### Value

A list with the components:

- \$value numeric vector with the computed sensitivity analysis measure for each attribute.
- \$imp numeric vector with the relative importance for each attribute (only makes sense for 1-D analysis).
- \$sresponses vector list as described in the Value documentation of mining.
- \$data if DSA or MSA, store the used data samples, needed for visualizations made by vecplot.
- \$method SA method
- \$measure SA measure
- \$agg Aggregation value
- \$nclasses if task="prob" or "class", the number of output classes, else nclasses=1
- \$inputs indexes of the input attributes
- \$Llevels sensitivity levels used for each attribute (NA means output attribute)
- \$interactions which attributes were interacted when method=GSA.

# Note

```
See also http://www3.dsi.uminho.pt/pcortez/rminer.html
```

## Author(s)

```
Paulo Cortez http://www3.dsi.uminho.pt/pcortez/
```

## References

• To cite the Importance function, sensitivity analysis methods or synthetic datasets, please use: P. Cortez and M.J. Embrechts.

Using Sensitivity Analysis and Visualization Techniques to Open Black Box Data Mining Models.

```
In Information Sciences, Elsevier, 225:1-17, March 2013. doi:10.1016/j.ins.2012.10.039
```

# See Also

```
vecplot, fit, mining, mgraph, mmetric, savemining.
```

# **Examples**

```
### dontrun is used when the execution of the example requires some computational effort.
### 1st example, regression, 1-D sensitivity analysis
## Not run:
data(sa_ssin) # x1 should account for 55
M=fit(y~.,sa_ssin,model="ksvm")
```

```
I=Importance(M,sa_ssin,method="1D-SA") # 1-D SA, AAD
print(round(I$imp,digits=2))
L=list(runs=1,sen=t(I$imp),sresponses=I$sresponses)
mgraph(L,graph="IMP",leg=names(sa_ssin),col="gray",Grid=10)
mgraph(L,graph="VEC",xval=1,Grid=10,data=sa_ssin,
  main="VEC curve for x1 influence on y") # or:
vecplot(I,xval=1,Grid=10,data=sa_ssin,datacol="gray",
  main="VEC curve for x1 influence on y") # same graph
vecplot(I, xval=c(1,2,3), pch=c(1,2,3), Grid=10,
leg=list(pos="bottomright",leg=c("x1","x2","x3"))) # all x1, x2 and x3 VEC curves
## End(Not run)
### 2nd example, regression, DSA sensitivity analysis:
## Not run:
I2=Importance(M,sa_ssin,method="DSA")
print(I2)
# influence of x1 and x2 over y
vecplot(I2,graph="VEC",xval=1) # VEC curve
vecplot(I2,graph="VECB",xval=1) # VEC curve with boxplots
vecplot(I2,graph="VEC3",xval=c(1,2)) # VEC surface
vecplot(I2,graph="VECC",xval=c(1,2)) # VEC contour
## End(Not run)
### 3th example, classification (pure class labels, task="cla"), DSA:
## Not run:
data(sa_int2_3c) # pair (x1,x2) is more relevant than x3, all x1,x2,x3 affect y,
                 # x4 has a null effect.
M2=fit(y~.,sa_int2_3c,model="mlpe",task="class")
I4=Importance(M2, sa_int2_3c, method="DSA")
# VEC curve (should present a kind of "saw" shape curve) for class B (TC=2):
vecplot(I4,graph="VEC",xval=2,cex=1.2,TC=2,
main="VEC curve for x2 influence on y (class B)",xlab="x2")
# same VEC curve but with boxplots:
vecplot(I4,graph="VECB",xval=2,cex=1.2,TC=2,
main="VEC curve with box plots for x2 influence on y (class B)",xlab="x2")
## End(Not run)
### 4th example, regression, DSA and GSA:
## Not run:
data(sa_psin)
# same model from Table 1 of the reference:
M3=fit(y^{-}, sa_psin, model="ksvm", search=2^{-}2, C=2^{6}.87, epsilon=2^{-}8)
# in this case: Aggregation should be -1 (default), 1 (class) or 3 (reg), see ref. paper.
I5=Importance(M3,sa_psin,method="DSA",Aggregation=3)
print("Input importances:")
print(round(I5$imp,digits=2)) # INS 2013 similar results
# 2D analysis (check reference for more details), RealL=L=7:
# need to aggregate results into a matrix of SA measure by using the agg_matrix_imp function.
```

```
# important notes:
# - agg_matrix_imp only works for the methods "DSA", "MSA" and "GSA".
# - reliable agg_matrix_imp results for "DSA" or "MSA" only for a
# a large LRandom value (e.g., LRandom=1000) or when LRandom=-1 (all training samples)
cm=agg_matrix_imp(I5)
print("show Table 8 DSA results (from the reference):")
print(round(cm$m1,digits=2))
print(round(cm$m2,digits=2))
# internal rminer function:
# show most relevant (darker) input pairs, in this case (x1,x2) > (x1,x3) > (x2,x3)
# to build a nice plot, a fixed threshold=c(0.05,0.05) is used. note that
# in the paper and for real data, we use threshold=0.1,
# which means threshold=rep(max(cm$m1,cm$m2)*threshold,2)
fcm=cmatrixplot(cm, threshold=c(0.05,0.05))
# 2D analysis using pair AT=c(x1,x2') (check reference for more details), RealL=7:
# nice 3D VEC surface plot:
\label{lem:vecplot} vecplot(I5,xval=c(1,2),graph="VEC3",xlab="x1",ylab="x2",zoom=1.1,
main="VEC surface of (x1,x2') influence on y")
# same influence but know shown using VEC contour:
par(mar=c(4.0,4.0,1.0,0.3)) # change the graph window space size
vecplot(I5,xval=c(1,2),graph="VECC",xlab="x1",ylab="x2",
 main="VEC surface of (x1,x2') influence on y")
# slower GSA:
I6=Importance(M3,sa_psin,method="GSA",interactions=1:4)
print("Input importances:")
print(round(I6$imp,digits=2)) # INS 2013 similar results
cm2=agg_matrix_imp(I6)
# compare cm2 with cm1, almost identical:
print(round(cm2$m1,digits=2))
print(round(cm2$m2,digits=2))
fcm2=cmatrixplot(cm2,threshold=0.1)
## End(Not run)
### 5th example, classification, 1D_SA, DSA, MSA and GSA:
## Not run:
data(sa_ssin_n2p)
# same model from Table 1 of the reference:
M4=fit(y^{-}, sa_ssin_n2p, model="ksvm", kpar=list(sigma=2^{-}8.25), C=2^{10})
I7=Importance(M4, sa_ssin_n2p, method="1D-SA")
print("1D-SA Input importances:")
print(round(I7$imp,digits=2)) # INS 2013 similar results (Table 6)
I8=Importance(M4, sa_ssin_n2p, method="GSA", interactions=1:4)
print("GSA Input importances:")
print(round(I8$imp,digits=2)) # INS 2013 similar results (Table 6)
19=Importance(M4, sa_ssin_n2p, method="DSA", LRandom=1000)
print("DSA Ns=1000 Input importances:")
print(round(I9$imp,digits=2)) # INS 2013 similar results (Table 6)
I10=Importance(M4, sa_ssin_n2p, method="DSA", LRandom=10)
```

```
print("DSA Ns=10 Input importances:")
print(round(I10$imp,digits=2)) # INS 2013 similar results (Table 6)
I11=Importance(M4, sa_ssin_n2p, method="MSA", LRandom=10)
print("MSA Ns=10 Input importances:")
print(round(I11$imp,digits=2)) # INS 2013 similar results (Table 6)
# 2D analysis:
cm3=agg_matrix_imp(I8)
fcm3=cmatrixplot(cm3,threshold=c(0.05,0.05))
cm4=agg_matrix_imp(I9)
fcm4=cmatrixplot(cm4,threshold=c(0.05,0.05))
## End(Not run)
### If you want to use Importance over your own model (different than rminer ones):
# 1st example, regression, uses the theoretical sin1reg function: x1=70% and x2=30%
data(sin1reg)
mypred=function(M,data)
{ return (M[1]*sin(pi*data[,1]/M[3])+M[2]*sin(pi*data[,2]/M[3])) }
M=c(0.7,0.3,2000)
# 4 is the column index of y
I=Importance(M,sin1reg,method="sens",measure="AAD",PRED=mypred,outindex=4)
print(I$imp) # x1=72.3% and x2=27.7%
L=list(runs=1,sen=t(I$imp),sresponses=I$sresponses)
mgraph(L,graph="IMP",leg=names(sin1reg),col="gray",Grid=10)
mgraph(L,graph="VEC",xval=1,Grid=10) # equal to:
par(mar=c(2.0,2.0,1.0,0.3)) # change the graph window space size
vecplot(I,graph="VEC",xval=1,Grid=10,main="VEC curve for x1 influence on y:")
### 2nd example, 3-class classification for iris and lda model:
## Not run:
data(iris)
library(MASS)
predlda=function(M,data) # the PRED function
{ return (predict(M,data)$posterior) }
LDA=lda(Species \sim .,iris, prior = c(1,1,1)/3)
# 4 is the column index of Species
I=Importance(LDA,iris,method="1D-SA",PRED=predlda,outindex=4)
vecplot(I,graph="VEC",xval=1,Grid=10,TC=1,
main="1-D VEC for Sepal.Lenght (x-axis) influence in setosa (prob.)")
## End(Not run)
### 3rd example, binary classification for setosa iris and lda model:
## Not run:
data(iris)
library(MASS)
iris2=iris;iris2$Species=factor(iris$Species=="setosa")
predlda2=function(M,data) # the PRED function
{ return (predict(M,data)$class) }
LDA2=lda(Species ~ .,iris2)
I=Importance(LDA2,iris2,method="1D-SA",PRED=predlda2,outindex=4)
```

imputation 33

```
vecplot(I,graph="VEC",xval=1,
main="1-D VEC for Sepal.Lenght (x-axis) influence in setosa (class)", Grid=10)
## End(Not run)
### Example with discrete inputs
## Not run:
data(iris)
ir1=iris
ir1[,1]=cut(ir1[,1],breaks=4)
ir1[,2]=cut(ir1[,2],breaks=4)
M=fit(Species~.,ir1,model="mlpe")
I=Importance(M, ir1, method="DSA")
# discrete example:
vecplot(I,graph="VEC",xval=1,TC=1,main="class: setosa (discrete x1)",data=ir1)
# continuous example:
vecplot(I,graph="VEC",xval=3,TC=1,main="class: setosa (cont. x1)",data=ir1)
## End(Not run)
```

imputation

Missing data imputation (e.g. substitution by value or hotdeck method).

# Description

Missing data imputation (e.g. substitution by value or hotdeck method).

# Usage

```
imputation(imethod = "value", D, Attribute = NULL, Missing = NA, Value = 1)
```

# **Arguments**

imethod

value – substitutes missing data by Value (with single element or several elements);
hotdeck – searches first the most similar example (i.e. using a k-nearest neighbor method – knn) in the dataset and replaces the missing data by the

value found in such example;

D dataset with missing data (data.frame)

imputation method type:

Attribute if NULL then all attributes (data columns) with missing data are replaced. Else,

Attribute is the attribute number (numeric) or name (character).

Missing missing data symbol

Value the substitution value (if imethod=value) or number of neighbors (k of knn).

34 imputation

# **Details**

Check the references.

#### Value

A data.frame without missing data.

# Note

```
See also http://hdl.handle.net/1822/36210 and http://www3.dsi.uminho.pt/pcortez/rminer.html
```

# Author(s)

```
Paulo Cortez http://www3.dsi.uminho.pt/pcortez/
```

#### References

• M. Brown and J. Kros.

Data mining and the impact of missing data. In Industrial Management & Data Systems, 103(8):611-621, 2003.

• This tutorial shows additional code examples:

P. Cortez.

A tutorial on using the rminer R package for data mining tasks. Teaching Report, Department of Information Systems, ALGORITMI Research Centre, Engi-

neering School, University of Minho, Guimaraes, Portugal, July 2015.

```
http://hdl.handle.net/1822/36210
```

## See Also

```
fit and delevels.
```

# **Examples**

```
d=matrix(ncol=5,nrow=5)
d[1,]=c(5,4,3,2,1)
d[2,]=c(4,3,4,3,4)
d[3,]=c(1,1,1,1,1)
d[4,]=c(4,NA,3,4,4)
d[5,]=c(5,NA,NA,2,1)
d=data.frame(d); d[,3]=factor(d[,3])
print(d)
print(imputation("value",d,3,Value="3"))
print(imputation("value",d,2,Value=median(na.omit(d[,2]))))
print(imputation("value",d,2,Value=c(1,2)))
print(imputation("hotdeck",d,"X2",Value=1))
print(imputation("hotdeck",d,Value=1))
```

Iforecast 35

```
## Not run:
# hotdeck 1-nearest neighbor substitution on a real dataset:
require(kknn)
d=read.table(
    file="http://archive.ics.uci.edu/ml/machine-learning-databases/autos/imports-85.data",
        sep=",",na.strings="?",stringsAsFactors=TRUE)
print(summary(d))
d2=imputation("hotdeck",d,Value=1)
print(summary(d2))
par(mfrow=c(2,1))
hist(d$V26)
hist(d$V26)
par(mfrow=c(1,1)) # reset mfrow
## End(Not run)
```

lforecast

Compute long term forecasts.

# Description

Performs multi-step forecasts by iteratively using 1-ahead predictions as inputs

# Usage

```
lforecast(M, data, start, horizon)
```

# **Arguments**

M fitted model, the object returned by fit.

data training data, typically built using CasesSeries.

start starting period (when out-of-samples start).

horizon number of multi-step predictions.

# **Details**

Check the reference for details.

# Value

Returns a numeric vector with the multi-step predictions.

# Author(s)

```
Paulo Cortez http://www3.dsi.uminho.pt/pcortez/
```

36 mgraph

# References

• This tutorial shows additional code examples:

P. Cortez.

A tutorial on using the rminer R package for data mining tasks.

Teaching Report, Department of Information Systems, ALGORITMI Research Centre, Engineering School, University of Minho, Guimaraes, Portugal, July 2015.

```
http://hdl.handle.net/1822/36210
```

• To check for more details:

P. Cortez.

Sensitivity Analysis for Time Lag Selection to Forecast Seasonal Time Series using Neural Networks and Support Vector Machines.

In Proceedings of the IEEE International Joint Conference on Neural Networks (IJCNN 2010), pp. 3694-3701, Barcelona, Spain, July, 2010. IEEE Computer Society, ISBN: 978-1-4244-6917-8 (DVD edition).

doi:10.1109/IJCNN.2010.5596890

#### See Also

```
fit, CasesSeries, predict.fit, mgraph.
```

#### **Examples**

```
ts=c(1,4,7,2,5,8,3,6,9,4,7,10,5,8,11,6,9)
d=CasesSeries(ts,c(1,2,3))
M=fit(y~.,d[1:7,],model="mlpe",search=2)
P1=predict(M,d[8:14,]) # single-step predictions
P2=lforecast(M,d,8,7) # multi-step predictions, horizon=7
print(mmetric(d$y[8:14],P1,"MAE"))
print(mmetric(d$y[8:14],P2,"MAE"))
L=vector("list",2); pred=vector("list",1);test=vector("list",1)
pred[[1]]=P1; test[[1]]=d$y[8:14]; L[[1]]=list(pred=pred,test=test,runs=1)
pred[[1]]=P2; test[[1]]=d$y[8:14]; L[[2]]=list(pred=pred,test=test,runs=1)
mgraph(L,graph="REG",Grid=10,leg=c("y","P1","P2"),col=c("black","cyan","blue"))
mgraph(L,graph="RSC",Grid=10,leg=c("P1","P2"),col=c("cyan","blue"))
```

mgraph

Mining graph function

# **Description**

Plots a graph given a mining list, list of several mining lists or given the pair y - target and x - predictions.

mgraph 37

## Usage

```
mgraph(y, x = NULL, graph, leg = NULL, xval = -1, PDF = "", PTS = -1,
    size = c(5, 5), sort = TRUE, ranges = NULL, data = NULL,
    digits = NULL, TC = -1, intbar = TRUE, lty = 1, col = "black",
    main = "", metric = "MAE", baseline = FALSE, Grid = 0,
    axis = NULL, cex = 1)
```

# **Arguments**

У

if there are predictions (!is.null(x)), y should be a numeric vector or factor with the target desired responses (or output values).

Else, y should be a list returned by the mining function or a vector list with several mining lists.

Х

the predictions (should be a numeric vector if task="reg", matrix if task="prob" or factor if task="class" (use if y is not a list).

graph

type of graph. Options are:

- ROC ROC curve (classification);
- LIFT LIFT accumulative curve (classification);
- IMP relative input importance barplot;
- REC REC curve (regression);
- VEC variable effect curve;
- RSC regression scatter plot;
- REP regression error plot;
- REG regression plot;
- DLC distance line comparison (for comparing errors in one line);

leg

legend of graph:

- if NULL not used;
- if -1 and graph="ROC" or "LIFT" the target class name is used;
- if -1 and graph="REG" leg=c("Target", "Predictions");
- if -1 and graph="RSC" leg=c("Predictions");
- if vector with "character" type (text) the text of the legend;
- if is list \$leg = vector with the text of the legend and \$pos is the position of the legend (e.g. "top" or c(4,5));

xval

auxiliary value, used by some graphs:

- VEC if -1 means perform several 1-D sensitivity analysis VEC curves, one for each attribute, if >0 means the attribute index (e.g. 1).
- ROC or LIFT or REC if -1 then xval=1. For these graphs, xval is the maximum x-axis value.
- IMP xval is the x-axis value for the legend of the attributes.
- REG xval is the set of plotted examples (e.g. 1:5), if -1 then all examples are used.
- DLC xval is the val of the mmetric function.

PDF

if "" then the graph is plotted on the screen, else the graph is saved into a pdf file with the name set in this argument.

38 mgraph

PTS	number of points in each line plot. If -1 then PTS=11 (for ROC, REC or LIFT) or PTS=6 (VEC).	
size	size of the graph, c(width,height), in inches.	
sort	if TRUE then sorts the data (works only for some graphs, e.g. VEC, IMP, REP).	
ranges	matrix with the attribute minimum and maximum ranges (only used by VEC).	
data	the training data, for plotting histograms and getting the minimum and maximum attribute ranges if not defined in ranges (only used by VEC).	
digits	the number of digits for the axis, can also be defined as $c(x$ -axis digits,y-axis digits) (only used by VEC).	
TC	target class (for multi-class classification class) from 1 to $Nc$ , where $Nc$ is the number of classes. If multi-class and TC==-1 then TC is set to the index of the last class.	
intbar	if $95\%$ confidence interval bars (according to t-student distribution) should be plotted as whiskers.	
lty	the same 1ty argument of the par function.	
col	color, as defined in the par function.	
main	the title of the graph, as defined in the plot function.	
metric	the error metric, as defined in mmetric (used by DLC).	
baseline	if the baseline should be plotted (used by ROC and LIFT).	
Grid	if >1 then there are GRID light gray squared grid lines in the plot.	
axis	Currently only used by IMP: numeric vector with the axis numbers $(1 - bottom, 3 - top)$ . If NULL then axis=c(1,3).	
cex	label font size	

# **Details**

Plots a graph given a mining list, list of several mining lists or given the pair y - target and x - predictions.

# Value

A graph (in screen or pdf file).

# Note

See also http://hdl.handle.net/1822/36210 and http://www3.dsi.uminho.pt/pcortez/rminer.html

# Author(s)

Paulo Cortez http://www3.dsi.uminho.pt/pcortez/

mgraph 39

#### References

To check for more details about rminer and for citation purposes:
 P. Cortez.

Data Mining with Neural Networks and Support Vector Machines Using the R/rminer Tool. In P. Perner (Ed.), Advances in Data Mining - Applications and Theoretical Aspects 10th Industrial Conference on Data Mining (ICDM 2010), Lecture Notes in Artificial Intelligence 6171, pp. 572-583, Berlin, Germany, July, 2010. Springer. ISBN: 978-3-642-14399-1.

@Springer: https://link.springer.com/chapter/10.1007/978-3-642-14400-4\_44
http://www3.dsi.uminho.pt/pcortez/2010-rminer.pdf

• This tutorial shows additional code examples:

P. Cortez.

A tutorial on using the rminer R package for data mining tasks.

Teaching Report, Department of Information Systems, ALGORITMI Research Centre, Engineering School, University of Minho, Guimaraes, Portugal, July 2015.

```
http://hdl.handle.net/1822/36210
```

#### See Also

fit, predict.fit, mining, mmetric, savemining and Importance.

## **Examples**

```
### regression
y=c(1,5,10,11,7,3,2,1); x=rnorm(length(y),0,1.0)+y
mgraph(y,x,graph="RSC",Grid=10,col=c("blue"))
mgraph(y,x,graph="REG",Grid=10,lty=1,col=c("black","blue"),
      leg=list(pos="topleft",leg=c("target","predictions")))
mgraph(y,x,graph="REP",Grid=10)
mgraph(y,x,graph="REP",Grid=10,sort=FALSE)
x2=rnorm(length(y),0,1.2)+y;x3=rnorm(length(y),0,1.4)+y;
L=vector("list",3); pred=vector("list",1); test=vector("list",1);
pred[[1]]=y; test[[1]]=x; L[[1]]=list(pred=pred,test=test,runs=1)
test[[1]]=x2; L[[2]]=list(pred=pred,test=test,runs=1)
test[[1]]=x3; L[[3]]=list(pred=pred,test=test,runs=1)
# distance line comparison graph:
mgraph(L,graph="DLC",metric="MAE",leg=c("x1","x2","x3"),main="MAE errors")
# new REC multi-curve single graph with NAREC (normalized Area of REC) values
# for maximum tolerance of val=0.5 (other val values can be used)
e1=mmetric(y,x,metric="NAREC",val=5)
e2=mmetric(y,x2,metric="NAREC",val=5)
e3=mmetric(y,x3,metric="NAREC",val=5)
11=paste("x1, NAREC=",round(e1,digits=2))
12=paste("x2, NAREC=",round(e2,digits=2))
13=paste("x3, NAREC=",round(e3,digits=2))
mgraph(L,graph="REC",leg=list(pos="bottom",leg=c(11,12,13)),main="REC curves")
### regression example with mining
```

```
## Not run:
data(sin1reg)
M1=mining(y^{-},sin1reg[,c(1,2,4)],model="mr",Runs=5)
M2=mining(y^{-}, sin1reg[,c(1,2,4)], model="mlpe", nr=3, maxit=50, size=4, Runs=5, feature="simp")
L=vector("list",2); L[[1]]=M2; L[[2]]=M1
mgraph(L,graph="REC",xval=0.1,leg=c("mlpe","mr"),main="REC curve")
mgraph(L,graph="DLC",metric="TOLERANCE",xval=0.01,
       leg=c("mlpe","mr"),main="DLC: TOLERANCE plot")
mgraph(M2,graph="IMP",xval=0.01,leg=c("x1","x2"),
       main="sin1reg Input importance",axis=1)
mgraph(M2,graph="VEC",xval=1,main="sin1reg 1-D VEC curve for x1")
mgraph(M2,graph="VEC",xval=1,
       main="sin1reg 1-D VEC curve and histogram for x1", data=sin1reg)
## End(Not run)
### classification example
## Not run:
data(iris)
M1=mining(Species~.,iris,model="rpart",Runs=5) # decision tree (DT)
M2=mining(Species~.,iris,model="ksvm",Runs=5) # support vector machine (SVM)
L=vector("list",2); L[[1]]=M2; L[[2]]=M1
mgraph(M1,graph="ROC",TC=3,leg=-1,baseline=TRUE,Grid=10,main="ROC")
mgraph(M1,graph="ROC",TC=3,leg=-1,baseline=TRUE,Grid=10,main="ROC",intbar=FALSE)
mgraph(L,graph="ROC",TC=3,leg=c("SVM","DT"),baseline=TRUE,Grid=10,
       main="ROC for virginica")
mgraph(L,graph="LIFT",TC=3,leg=list(pos=c(0.4,0.2),leg=c("SVM","DT")),
       baseline=TRUE,Grid=10,main="LIFT for virginica")
## End(Not run)
```

mining

Powerful function that trains and tests a particular fit model under several runs and a given validation method

## **Description**

Powerful function that trains and tests a particular fit model under several runs and a given validation method. Since there can be a huge number of models, the fitted models are not stored. Yet, several useful statistics (e.g. predictions) are returned.

# Usage

```
mining(x, data = NULL, Runs = 1, method = NULL, model = "default",
    task = "default", search = "heuristic", mpar = NULL,
    feature="none", scale = "default", transform = "none",
    debug = FALSE, ...)
```

#### **Arguments**

Χ

a symbolic description (formula) of the model to be fit. If x contains the data, then data=NULL (similar to x in ksvm, kernlab package).

data

an optional data frame (columns denote attributes, rows show examples) containing the training data, when using a formula.

Runs

number of runs used (e.g. 1, 5, 10, 20, 30)

method

a vector with c(vmethod,vpar,seed) or c(vmethod,vpar,window,increment), where vmethod is:

- all all *NROW* examples are used as both training and test sets (no *vpar* or *seed* is needed).
- holdout standard holdout method. If vpar<1 then NROW\*vpar random samples are used for training and the remaining rows are used for testing. Else, then NROW\*vpar random samples are used for testing and the remaining are used for training. For classification tasks (prob or class) a stratified sampling is assumed (equal to mode="stratified" in holdout).</li>
- holdoutrandom similar to holdout except that assumes always a random sampling (not stratified).
- holdoutorder similar to holdout except that instead of a random sampling, the first rows (until the split) are used for training and the remaining ones for testing (equal to mode="order" in holdout).
- holdoutinc incremental holdout retraining (e.g. used for stock market data). Here, *vpar* is the test size, *window* is the initial window size and *increment* is the number of samples added at each iteration. Note: argument Runs is automatically set when this option is used. See also holdout.
- holdoutrol rolling holdout retraining (e.g. used for stock market data). Here, *vpar* is the test size, *window* is the window size and *increment* is the number of samples added at each iteration. Note: argument Runs is automatically set when this option is used. See also holdout.
- kfold K-fold cross-validation method, where *vpar* is the number of folds. For classification tasks (prob or class) a stratified split is assumed (equal to mode="stratified" in crossvaldata).
- kfoldrandom similar to kfold except that assumes always a random sampling (not stratified).
- kfoldorder similar to kfold except that instead of a random sampling, the order of the rows is used to build the folds.

*vpar* – number used by *vmethod* (optional, if not defined 2/3 for holdout and 10 for kfold is assumed);

and seed (optional, if not defined then NA is assumed) is:

- NA random seed is adopted (default R method for generating random numbers);
- a vector of size Runs with fixed seed numbers for each Run;
- a number set.seed(number) is applied then a vector of seeds (of size Runs) is generated.

model

See fit for details.

task See fit for details. search See fit for details.

mpar Only kept for compatibility with previous rminer versions, as you should use

search instead of mpar. See fit for details.

feature See fit for more details about feature="none", "sabs" or "sbs" options.

For the mining function, additional options are feature=*fmethod*, where *fmethod* can be one of:

an oc one or.

- sens or sensg compute the 1-D sensitivity analysis input importances (\$sen), gradient measure.
- sensy compute the 1-D sensitivity analysis input importances (\$sen), variance measure.
- sensr compute the 1-D sensitivity analysis input importances (\$sen), range measure.
- simp, simpg or s equal to sensg but also computes the 1-D sensitivity responses (\$sresponses, useful for graph="VEC").
- simpv equal to sensv but also computes the 1-D sensitivity responses (useful for graph="VEC").
- simpr equal to sensr but also computes the 1-D sensitivity responses (useful for graph="VEC").

scale See fit for details. transform See fit for details.

debug If TRUE shows some information about each run.

... See fit for details.

#### **Details**

Powerful function that trains and tests a particular fit model under several runs and a given validation method (see [Cortez, 2010] for more details).

Several Runs are performed. In each run, the same validation method is adopted (e.g. holdout) and several relevant statistics are stored. Note: this function can require some computational effort, specially if a large dataset and/or a high number of Runs is adopted.

## Value

A list with the components:

- \$object fitted object values of the last run (used by multiple model fitting: "auto" mode). For "holdout", it is equal to a fit object, while for "kfold" it is a list.
- \$time vector with time elapsed for each run.
- \$test vector list, where each element contains the test (target) results for each run.
- \$pred vector list, where each element contains the predicted results for each test set and each run.
- \$error vector with a (validation) measure (often it is a error value) according to search\$metric for each run (valid options are explained in mmetric).

• \$mpar – vector list, where each element contains the fit model mpar parameters (for each run).

- \$model the model.
- \$task the task.
- \$method the external validation method.
- \$sen a matrix with the 1-D sensitivity analysis input importances. The number of rows is Runs times *vpar*, if kfold, else is Runs.
- \$sresponses a vector list with a size equal to the number of attributes (useful for graph="VEC"). Each element contains a list with the 1-D sensitivity analysis input responses (n name of the attribute; 1 number of levels; x attribute values; y 1-D sensitivity responses. Important note: sresponses (and "VEC" graphs) are only available if feature="sabs" or "simp" related (see feature).
- \$runs the Runs.
- \$attributes vector list with all attributes (features) selected in each run (and fold if kfold) if a feature selection algorithm is used.
- \$feature the feature.

#### Note

See also http://hdl.handle.net/1822/36210 and http://www3.dsi.uminho.pt/pcortez/rminer.html

## Author(s)

Paulo Cortez http://www3.dsi.uminho.pt/pcortez/

## References

To check for more details about rminer and for citation purposes:
 P. Cortez.

Data Mining with Neural Networks and Support Vector Machines Using the R/rminer Tool. In P. Perner (Ed.), Advances in Data Mining - Applications and Theoretical Aspects 10th Industrial Conference on Data Mining (ICDM 2010), Lecture Notes in Artificial Intelligence 6171, pp. 572-583, Berlin, Germany, July, 2010. Springer. ISBN: 978-3-642-14399-1. @Springer: https://link.springer.com/chapter/10.1007/978-3-642-14400-4\_44 http://www3.dsi.uminho.pt/pcortez/2010-rminer.pdf

• This tutorial shows additional code examples:

P. Cortez.

A tutorial on using the rminer R package for data mining tasks.

Teaching Report, Department of Information Systems, ALGORITMI Research Centre, Engineering School, University of Minho, Guimaraes, Portugal, July 2015.

http://hdl.handle.net/1822/36210

• For the grid search and other optimization methods: P. Cortez.

Modern Optimization with R.

```
Use R! series, Springer, 2nd edition, July 2021, ISBN 978-3-030-72818-2. 
https://link.springer.com/book/10.1007/978-3-030-72819-9
```

## See Also

fit, predict.fit, mparheuristic, mgraph, mmetric, savemining, holdout and Importance.

## **Examples**

```
### dontrun is used when the execution of the example requires some computational effort.
### simple regression example
set.seed(123); x1=rnorm(200,100,20); x2=rnorm(200,100,20)
y=0.7*sin(x1/(25*pi))+0.3*sin(x2/(25*pi))
# mining with an ensemble of neural networks, each fixed with size=2 hidden nodes
# assumes a default holdout (random split) with 2/3 for training and 1/3 for testing:
M=mining(y~x1+x2,Runs=2,model="mlpe",search=2)
print(M)
print(mmetric(M,metric="MAE"))
### more regression examples:
## Not run:
# simple nonlinear regression task; x3 is a random variable and does not influence y:
data(sin1reg)
# 5 runs of an external holdout with 2/3 for training and 1/3 for testing, fixed seed 12345
# feature selection: sabs method
# model selection: 5 searches for size, internal 2-fold cross validation fixed seed 123
                   with optimization for minimum MAE metric
M=mining(y~.,data=sin1reg,Runs=5,method=c("holdout",2/3,12345),model="mlpe",
      search=list(search=mparheuristic("mlpe",n=5),method=c("kfold",2,123),metric="MAE"),
         feature="sabs")
print(mmetric(M, metric="MAE"))
print(M$mpar)
print("median hidden nodes (size) and number of MLPs (nr):")
print(centralpar(M$mpar))
print("attributes used by the model in each run:")
print(M$attributes)
mgraph(M,graph="RSC",Grid=10,main="sin1 MLPE scatter plot")
mgraph(M,graph="REP",Grid=10,main="sin1 MLPE scatter plot",sort=FALSE)
mgraph(M,graph="REC",Grid=10,main="sin1 MLPE REC")
mgraph(M,graph="IMP",Grid=10,main="input importances",xval=0.1,leg=names(sin1reg))
# average influence of x1 on the model:
mgraph(M,graph="VEC",Grid=10,main="x1 VEC curve",xval=1,leg=names(sin1reg)[1])
## End(Not run)
### regression example with holdout rolling windows:
## Not run:
# simple nonlinear regression task; x3 is a random variable and does not influence y:
data(sin1reg)
# rolling with 20 test samples, training window size of 300 and increment of 50 in each run:
```

```
# note that Runs argument is automatically set to 14 in this example:
M=mining(y~.,data=sin1reg,method=c("holdoutrol",20,300,50),
         model="mlpe",debug=TRUE)
## End(Not run)
### regression example with all rminer models:
# simple nonlinear regression task; x3 is a random variable and does not influence y:
data(sin1reg)
models=c("naive","ctree","rpart","kknn","mlp","mlpe","ksvm","randomForest","mr","mars",
         "cubist", "pcr", "plsr", "cppls", "rvm")
for(model in models)
{
M=mining(y^{-}, data=sin1reg, method=c("holdout", 2/3, 12345), model=model)
 cat("model:",model,"MAE:",round(mmetric(M,metric="MAE")$MAE,digits=3),"\n")
}
## End(Not run)
### classification example (task="prob")
## Not run:
data(iris)
# 10 runs of a 3-fold cross validation with fixed seed 123 for generating the 3-fold runs
M=mining(Species~.,iris,Runs=10,method=c("kfold",3,123),model="rpart")
print(mmetric(M,metric="CONF"))
print(mmetric(M, metric="AUC"))
print(meanint(mmetric(M,metric="AUC")))
{\tt mgraph(M,graph="ROC",TC=2,baseline=TRUE,Grid=10,leg="Versicolor",}
       main="versicolor ROC")
mgraph(M,graph="LIFT",TC=2,baseline=TRUE,Grid=10,leg="Versicolor",
       main="Versicolor ROC")
M2=mining(Species~.,iris,Runs=10,method=c("kfold",3,123),model="ksvm")
L=vector("list",2)
L[[1]]=M;L[[2]]=M2
mgraph(L,graph="ROC",TC=2,baseline=TRUE,Grid=10,leg=c("DT","SVM"),main="ROC")
## End(Not run)
### other classification examples
## Not run:
### 1st example:
data(iris)
# 2 runs of an external 2-fold validation, random seed
# model selection: SVM model with rbfdot kernel, automatic search for sigma,
                   internal 3-fold validation, random seed, minimum "AUC" is assumed
# feature selection: none, "s" is used only to store input importance values
M=mining(Species~.,data=iris,Runs=2,method=c("kfold",2,NA),model="ksvm",
         search=list(search=mparheuristic("ksvm"), method=c("kfold",3)), feature="s")
print(mmetric(M,metric="AUC",TC=2))
mgraph(M,graph="ROC",TC=2,baseline=TRUE,Grid=10,leg="SVM",main="ROC",intbar=FALSE)
mgraph(M,graph="IMP",TC=2,Grid=10,main="input importances",xval=0.1,
```

```
leg=names(iris),axis=1)
mgraph(M,graph="VEC",TC=2,Grid=10,main="Petal.Width VEC curve",
data=iris,xval=4)
### 2nd example, ordered kfold, k-nearest neigbor:
M=mining(Species~.,iris,Runs=1,method=c("kfoldo",3),model="knn")
# confusion matrix:
print(mmetric(M,metric="CONF"))
### 3rd example, use of all rminer models:
models=c("naive","ctree","rpart","kknn","mlp","mlpe","ksvm","randomForest","bagging",
         "boosting", "lda", "multinom", "naiveBayes", "qda")
for(model in models)
{
M=mining(Species~.,iris,Runs=1,method=c("kfold",3,123),model=model)
cat("model:",model,"ACC:",round(mmetric(M,metric="ACC")$ACC,digits=1),"\n")
}
## End(Not run)
### multiple models: automl or ensembles
## Not run:
data(iris)
d=iris
names(d)[ncol(d)]="y" # change output name
inputs=ncol(d)-1
metric="AUC"
# simple automl (1 search per individual model),
# internal holdout and external holdout:
sm=mparheuristic(model="automl", n=NA, task="prob", inputs=inputs)
mode="auto"
imethod=c("holdout",4/5,123) # internal validation method
emethod=c("holdout",2/3,567) # external validation method
search=list(search=sm,smethod=mode,method=imethod,metric=metric,convex=0)
M=mining(y^{-}.,data=d,model="auto",search=search,method=emethod,fdebug=TRUE)
# 1 single model was selected:
cat("best",emethod[1],"selected model:",M$object@model,"\n")
cat(metric,"=",round(as.numeric(mmetric(M,metric=metric)),2),"\n")
# simple automl (1 search per individual model),
# internal kfold and external kfold:
imethod=c("kfold",3,123) # internal validation method
emethod=c("kfold",5,567) # external validation method
search=list(search=sm,smethod=mode,method=imethod,metric=metric,convex=0)
M=mining(y^{-}, data=d, model="auto", search=search, method=emethod, fdebug=TRUE)
# kfold models were selected:
kfolds=as.numeric(emethod[2])
models=vector(length=kfolds)
for(i in 1:kfolds) models[i]=M$object$model[[i]]
cat("best",emethod[1],"selected models:",models,"\n")
```

```
cat(metric, "=",round(as.numeric(mmetric(M,metric=metric)),2),"\n")

# example with weighted ensemble:
M=mining(y~.,data=d,model="WE",search=search,method=emethod,fdebug=TRUE)
for(i in 1:kfolds) models[i]=M$object$model[[i]]
cat("best",emethod[1],"selected models:",models,"\n")
cat(metric,"=",round(as.numeric(mmetric(M,metric=metric)),2),"\n")

### End(Not run)

### for more fitting examples check the help of function fit: help(fit,package="rminer")
```

mmetric

Compute classification or regression error metrics.

# **Description**

Compute classification or regression error metrics.

## Usage

```
mmetric(y, x = NULL, metric, D = 0.5, TC = -1, val = NULL, aggregate = "no")
```

## **Arguments**

У

if there are predictions (!is.null(x)), y should be a numeric vector or factor with the target desired responses (or output values).

Else, y should be a list returned by the mining function.

Х

the predictions (should be a numeric vector if task="reg", matrix if task="prob" or factor if task="class" (used if y is not a list).

metric

a R function or a character.

Note: if a R function, then it should be set to provide lower values for better models if the intention is to be used within the search argument of fit and mining (i.e., "<" meaning).

Valid character options are (">" means "better" if higher value; "<" means "better" if lower value):

- ALL returns all classification or regression metrics (context dependent, multi-metric).
- if vector returns all metrics included in the vector, vector elements can be any of the options below (multi-metric).
- CONF confusion matrix (classification, matrix).
- ACC classification accuracy rate, equal to micro averaged F1 score (classification, ">", [0-%100]).
- macroACC macro average ACC score, for multiclass tasks (classification, ">", [0-%100]).

• weightedACC – weighted average ACC score, for multiclass tasks (classification, ">", [0-%100]).

- CE classification error or misclassification error rate (classification, "<", [0-%100]).
- MAEO mean absolute error for ordinal classification (classification, "<", [0-Inf[).</li>
- MSEO mean squared error for ordinal classification (classification, "<", [0-Inf[).
- KENDALL Kendalls's coefficient for ordinal classification or (mean if) ranking (classification, ">", [-1;1]). Note: if ranking, y is a matrix and mean metric is computed.
- SPEARMAN Mean Spearman's rho coefficient for ranking (classification, ">", [-1;1]). Note: if ranking, y is a matrix and mean metric is computed.
- BER balanced error rate (classification, "<", [0-%100]).
- KAPPA kappa index (classification, "<", [0-%100]).
- CRAMERV Cramer's V (classification, ">", [0,1.0]).
- ACCLASS classification accuracy rate per class (classification, ">", [0-%100]).
- BAL\_ACC balanced accuracy rate per class (classification, ">", [0-%100]).
- TPR true positive rate, sensitivity or recall (classification, ">", [0-%100]).
- macroTPR macro average TPR score, for multiclass tasks (classification, ">", [0-%100]).
- weightedTPR weighted average TPR score, for multiclass tasks (classification, ">", [0-%100]).
- TNR true negative rate or specificity (classification, ">", [0-%100]).
- macroTNR macro average TNR score, for multiclass tasks (classification, ">", [0-%100]).
- weightedTNR weighted average TNR score, for multiclass tasks (classification, ">", [0-%100]).
- microTNR micro average TNR score, for multiclass tasks (classification, ">", [0-%100]).
- PRECISION precision (classification, ">", [0-%100]).
- macroPRECISION macro average precision, for multiclass tasks (classification, ">", [0-%100]).
- weightedPRECISION weighted average precision, for multiclass tasks (classification, ">", [0-%100]).
- F1 F1 score (classification, ">", [0-%100]).
- macroF1 macro average F1 score, for multiclass tasks (classification, ">", [0-%100]).
- weightedF1 weighted average F1 score, for multiclass tasks (classification, ">", [0-%100]).
- MCC Matthews correlation coefficient (classification, ">", [-1,1]).
- BRIER overall Brier score (classification "prob", "<", [0,1.0]).
- BRIERCLASS Brier score per class (classification "prob", "<", [0,1.0]).

• ROC – Receiver Operating Characteristic curve (classification "prob", list with several components).

- AUC overall area under the curve (of ROC curve, classification "prob", ">", domain values: [0,1.0]).
- AUCCLASS area under the curve per class (of ROC curve, classification "prob", ">", domain values: [0,1.0]).
- NAUC normalized AUC (given a fixed val=FPR, classification "prob", ">", [0,1.0]).
- TPRATFPR the TPR (given a fixed val=FPR, classification "prob", ">", [0,1.0]).
- LIFT accumulative percent of responses captured (LIFT accumulative curve, classification "prob", list with several components).
- ALIFT area of the accumulative percent of responses captured (LIFT accumulative curve, classification "prob", ">", [0,1.0]).
- NALIFT normalized ALIFT (given a fixed val=percentage of examples, classification "prob", ">", [0,1.0]).
- ALIFTATPERC ALIFT value (given a fixed val=percentage of examples, classification "prob", ">", [0,1.0]).
- SAE sum absolute error/deviation (regression, "<", [0,Inf[).
- MAE mean absolute error (regression, "<", [0,Inf[).
- MdAE median absolute error (regression, "<", [0,Inf[).
- GMAE geometric mean absolute error (regression, "<", [0,Inf[).
- MaxAE maximum absolute error (regression, "<", [0,Inf[).
- NMAE normalized mean absolute error (regression, "<", [0%,Inf[). Note: by default, this metric assumes the range of y as the denominator of NMAE; a different range can be set by setting the optional val argument (see example).
- RAE relative absolute error (regression, "<", [0%,Inf[).
- SSE sum squared error (regression, "<", [0,Inf]).
- MSE mean squared error (regression, "<", [0,Inf]).
- MdSE median squared error (regression, "<", [0,Inf]).
- RMSE root mean squared error (regression, "<", [0,Inf[).
- GMSE geometric mean squared error (regression, "<", [0,Inf]).
- HRMSE Heteroscedasticity consistent root mean squared error (regression, "<", [0,Inf]).
- RSE relative squared error (regression, "<", [0%,Inf[).
- RRSE root relative squared error (regression, "<", [0%,Inf]).
- ME mean error (regression, "<", [0,Inf]).
- SMinkowski3 sum of Minkowski loss function (q=3, heavier penalty for large errors when compared with SSE, regression, "<", [0%,Inf]).
- MMinkowski3 mean of Minkowski loss function (q=3, heavier penalty for large errors when compared with SSE, regression, "<", [0%,Inf[).
- MdMinkowski3 median of Minkowski loss function (q=3, heavier penalty for large errors when compared with SSE, regression, "<", [0%,Inf[).

- COR Pearson correlation (regression, ">", [-1,1]).
- q2 =1-correlation^2 test error metric, as used by M.J. Embrechts (regression, "<", [0,1.0]).
- R2 coefficient of determination R^2 (regression, ">", squared pearson correlation coefficient: [0,1]).
- R22 2nd variant of coefficient of determination R^2 (regression, ">", most general definition that however can lead to negative values: ]-Inf,1]. In previous rminer versions, this variant was known as "R2").
- EV explained variance, 1 var(y-x)/var(y) (regression, ">", ]-Inf,1]).
- Q2  $R^2/SD$  test error metric, as used by M.J. Embrechts (regression, "<", [0,Inf]).
- REC Regression Error Characteristic curve (regression, list with several components).
- NAREC normalized REC area (given a fixed val=tolerance, regression, ">", [0,1.0]).
- TOLERANCE the tolerance (y-axis value) of a REC curve given a fixed val=tolerance value, regression, ">", [0,1.0]).
- TOLERANCEPERC the tolerance (y-axis value) of a REC curve given a percentage val= value (in terms of y range), regression, ">", [0,1.0]).
- MAPE Mean Absolute Percentage mmetric forecasting metric (regression, "<", [0%,Inf]).
- MdAPE Median Absolute Percentage mmetric forecasting metric (regression, "<"), [0%,Inf]).</li>
- RMSPE Root Mean Square Percentage mmetric forecasting metric (regression, "<", [0%,Inf[).
- RMdSPE Root Median Square Percentage mmetric forecasting metric (regression, "<", [0%,Inf[).
- SMAPE Symmetric Mean Absolute Percentage mmetric forecasting metric (regression, "<", [0%,200%]).
- SMdAPE Symmetric Median Absolute Percentage mmetric forecasting metric (regression, "<", [0%,200%]).
- MRAE Mean Relative Absolute mmetric forecasting metric (val should contain the last in-sample/training data value (for random walk) or full benchmark time series related with out-of-sample values, regression, "<", [0,Inf]).
- MdRAE Median Relative Absolute mmetric forecasting metric (val should contain the last in-sample/training data value (for random walk) or full benchmark time series, regression, "<", [0,Inf[).
- GMRAE Geometric Mean Relative Absoluate mmetric forecasting metric (val should contain the last in-sample/training data value (for random walk) or full benchmark time series, regression, "<", [0,Inf[).
- THEILSU2 Theils'U2 forecasting metric (val should contain the last insample/training data value (for random walk) or full benchmark time series, regression, "<", [0,Inf[).
- MASE MASE forecasting metric (val should contain the time series insamples or training data, regression, "<", [0,Inf[).

decision threshold (for task="prob", probabilistic classification) within [0,1]. D The class is TRUE if prob > D.

> target class index or vector of indexes (for multi-class classification class) from 1 to Nc. where Nc is the number of classes:<cr>

- if TC==-1 (the default value), then it is assumed:
  - if metric is "CONF" D is ignored and highest probability class is assumed (if TC>0, the metric is computed for positive TC class and D is used).
  - if metric is "ACC", "CE", "BER", "KAPPA", "CRAMERV", "BRIER", or "AUC" - the global metric (for all classes) is computed (if TC>0, the metric is computed for positive TC class).
  - if metric is "ACCLASS", "TPR", "TNR", "Precision", "F1", "MCC", "ROC", "BRIERCLASS", "AUCCLASS" - it returns one result per class (if TC>0, it returns negative (e.g. "TPR1") and positive (TC, e.g. "TPR2") result).
  - if metric is "NAUC", "TPRATFPR", "LIFT", "ALIFT", "NALIFT" or "ALIFTATPERC" – TC is set to the index of the last class.

val auxiliary value:

- when two or more metrics need different val values, then val should be a vector list, see example.
- if numeric or vector check the metric argument for specific details of each metric val meaning.

aggregate

character with type of aggregation performed when y is a mining list. Valid options are:

- no returns all metrics for all mining runs. If metric includes "CONF", "ROC", "LIFT" or "REC", it returns a vector list, else if metric includes a single metric, it returns a vector; else it returns a data.frame (runs x metrics).
- sum sums all run results.
- mean averages all run results.
- note: both "sum" and "mean" only work if only metric=="CONF" is used or if metric does not contain "ROC", "LIFT" or "REC".

# **Details**

Compute classification or regression error metrics:

- mmetric compute one or more classification/regression metrics given y and x OR a mining
- metrics deprecated function, same as mmetric(x,y,metric="ALL"), included here just for compatability purposes but will be removed from the package.

#### Value

Returns the computed error metric(s):

• one value if only one metric is requested (and y is not a mining list);

TC

- named vector if 2 or more elements are requested in metric (and y is not a mining list);
- list if there is a "CONF", "ROC", "LIFT" or "REC" request on metric (other metrics are stored in field \$res, and y is not a mining list).
- if y is a mining list then there can be several runs, thus:
  - a vector list of size y\$runs is returned if metric includes "CONF", "ROC", "LIFT" or "REC" and aggregate="no";
  - a data.frame is returned if aggregate="no" and metric does not include "CONF", "ROC",
    "LIFT" or "REC";
  - a table is returned if aggregate="sum" or "mean" and metric="CONF";
  - a vector or numeric value is returned if aggregate="sum" or "mean" and metric is not "CONF".

## Note

See also http://hdl.handle.net/1822/36210 and http://www3.dsi.uminho.pt/pcortez/rminer.html

## Author(s)

Paulo Cortez http://www3.dsi.uminho.pt/pcortez/

# References

• To check for more details about rminer and for citation purposes: P. Cortez.

Data Mining with Neural Networks and Support Vector Machines Using the R/rminer Tool. In P. Perner (Ed.), Advances in Data Mining - Applications and Theoretical Aspects 10th Industrial Conference on Data Mining (ICDM 2010), Lecture Notes in Artificial Intelligence 6171, pp. 572-583, Berlin, Germany, July, 2010. Springer. ISBN: 978-3-642-14399-1. @Springer: https://link.springer.com/chapter/10.1007/978-3-642-14400-4\_44 http://www3.dsi.uminho.pt/pcortez/2010-rminer.pdf

• This tutorial shows additional code examples:

P. Cortez.

A tutorial on using the rminer R package for data mining tasks. Teaching Report, Department of Information Systems, ALGORITMI Research Centre, Engineering School, University of Minho, Guimaraes, Portugal, July 2015.

http://hdl.handle.net/1822/36210

• About the Brier and Global AUC scores:

A. Silva, P. Cortez, M.F. Santos, L. Gomes and J. Neves. Rating Organ Failure via Adverse Events using Data Mining in the Intensive Care Unit. In Artificial Intelligence in Medicine, Elsevier, 43 (3): 179-193, 2008. doi:10.1016/j.artmed.2008.03.010

• About the classification and regression metrics:

I. Witten and E. Frank.

Data Mining: Practical machine learning tools and techniques.

Morgan Kaufmann, 2005.

• About the forecasting metrics:

R. Hyndman and A. Koehler

Another look at measures of forecast accuracy.

In International Journal of Forecasting, 22(4):679-688, 2006.

• About the ordinal classification metrics:

J.S. Cardoso and R. Sousa.

Measuring the Performance of Ordinal Classification.

In International Journal of Pattern Recognition and Artificial Intelligence, 25(8):1173-1195, 2011.

## See Also

fit, predict.fit, mining, mgraph, savemining and Importance.

## **Examples**

```
### pure binary classification
y=factor(c("a", "a", "a", "a", "b", "b", "b", "b"))
x=factor(c("a", "a", "b", "a", "b", "a", "b", "a"))
print(mmetric(y,x,"CONF")$conf)
print(mmetric(y,x,metric=c("ACC","TPR","ACCLASS")))
print(mmetric(y,x,"ALL"))
### probabilities binary classification
y=factor(c("a","a","a","a","b","b","b","b","b"))
px=matrix(nrow=8,ncol=2)
px[,1]=c(1.0,0.9,0.8,0.7,0.6,0.5,0.4,0.3)
px[,2]=1-px[,1]
print(px)
print(mmetric(y,px,"CONF")$conf)
print(mmetric(y,px,"CONF",D=0.5,TC=2)$conf)
print(mmetric(y,px,"CONF",D=0.3,TC=2)$conf)
print(mmetric(y,px,metric="ALL",D=0.3,TC=2))
print(mmetric(y,px,metric=c("ACC","AUC","AUCCLASS","BRIER","BRIERCLASS","CE"),D=0.3,TC=2))
# ACC and confusion matrix:
print(mmetric(y,px,metric=c("ACC","CONF"),D=0.3,TC=2))
# ACC and ROC curve:
print(mmetric(y,px,metric=c("ACC","ROC"),D=0.3,TC=2))
# ACC, ROC and LIFT curve:
print(mmetric(y,px,metric=c("ACC","ROC","LIFT"),D=0.3,TC=2))
### pure multi-class classification
```

```
'D', 'D', 'D', 'D', 'D', 'C', 'C', 'E', 'A', 'A', 'B', 'B')
y=factor(y)
x=factor(x)
print(mmetric(y,x,metric="CONF")$conf) # confusion matrix
print(mmetric(y,x,metric="CONF",TC=-1)$conf) # same thing
print(mmetric(y,x,metric="CONF",TC=1)$conf) # for target class TC=1: "A"
mshow=function(y,x,metric) print(round(mmetric(y,x,metric),digits=0))
mshow(y,x,"ALL")
mshow(y,x,c("ACCLASS","BAL_ACC","KAPPA"))
mshow(y,x,c("PRECISION")) # precision
mshow(y,x,c("TPR")) # recall
mshow(y,x,c("F1")) # F1 score
# micro (=ACC), macro and weighted average:
mshow(y,x,c("ACC","macroPRECISION","weightedPRECISION"))
mshow(y,x,c("ACC","macroTPR","weightedTPR"))
mshow(y,x,c("ACC","macroF1","weightedF1"))
mshow(y,x,c("ACC","macroACC","weightedACC"))
# several metrics in a single returned object:
print(mmetric(y,x,metric=c("CONF","macroF1","weightedF1","ACC")))
### probabilities multi-class
y=factor(c("a", "a", "b", "b", "c", "c"))
px=matrix(nrow=6,ncol=3)
px[,1]=c(1.0,0.7,0.5,0.3,0.1,0.7)
px[,2]=c(0.0,0.2,0.4,0.7,0.3,0.2)
px[,3]=1-px[,1]-px[,2]
print(px)
print(mmetric(y,px,metric="ALL",TC=-1,val=0.1))
print(mmetric(y,px,metric=c("AUC","AUCCLASS","NAUC"),TC=-1,val=0.1))
print(mmetric(y,px,metric=c("AUC","NAUC"),TC=3,val=0.1))
print(mmetric(y,px,metric=c("ACC","ACCLASS"),TC=-1))
print(mmetric(y,px,metric=c("CONF"),TC=3,D=0.5)$conf)
print(mmetric(y,px,metric=c("ACCLASS"),TC=3,D=0.5))
print(mmetric(y,px,metric=c("CONF"),TC=3,D=0.7)$conf)
print(mmetric(y,px,metric=c("ACCLASS"),TC=3,D=0.7))
### ordinal multi-class (example in Ricardo Sousa PhD thesis 2012)
y=ordered(c(rep("a",4),rep("b",6),rep("d",3)),levels=c("a","b","c","d"))
x=ordered(c(rep("c",(4+6)),rep("d",3)),levels=c("a","b","c","d"))
print(mmetric(y,x,metric="CONF")$conf)
print(mmetric(y,x,metric=c("CE","MAEO","MSEO","KENDALL")))
# note: only y needs to be ordered
x=factor(c(rep("b",4),rep("a",6),rep("d",3)),levels=c("a","b","c","d"))
print(mmetric(y,x,metric="CONF")$conf)
print(mmetric(y,x,metric=c("CE","MAEO","MSEO","KENDALL")))
```

```
print(mmetric(y,x,metric="ALL"))
### ranking (multi-class)
y=matrix(nrow=1,ncol=12);x=y
# http://www.youtube.com/watch?v=D56dvoVrBBE
y[1,]=1:12
x[1,]=c(2,1,4,3,6,5,8,7,10,9,12,11)
print(mmetric(y,x,metric="KENDALL"))
print(mmetric(y,x,metric="ALL"))
y=matrix(nrow=2,ncol=7);x=y
y[1,]=c(2,6,5,4,3,7,1)
y[2,]=7:1
x[1,]=1:7
x[2,]=1:7
print(mmetric(y,x,metric="ALL"))
### regression examples: y - desired values; x - predictions
y=c(95.01,96.1,97.2,98.0,99.3,99.7);x=95:100
print(mmetric(y,x,"ALL"))
print(mmetric(y,x,"MAE"))
mshow=function(y,x,metric) print(round(mmetric(y,x,metric),digits=2))
mshow(y,x,c("MAE","RMSE","RAE","RSE"))
# getting NMAE:
m=mmetric(y,x,"NMAE")
cat("NMAE:",round(m,digits=2)," (denominator=",diff(range(y)),")\n")
m=mmetric(y,x,"NMAE",val=5) # usage of different range
cat("NMAE:",round(m,digits=2)," (denominator=",5,")\n")
# get REC curve and other measures:
m=mmetric(y,x,c("REC","TOLERANCEPERC","MAE"),val=5)
print(m)
# correlation or similar measures:
mshow(y,x,c("COR","R2","R22","EV")) # ideal is close to 1
mshow(y,x,c("q2","Q2")) # ideal is close to 0
# other measures:
print(mmetric(y,x,c("TOLERANCE","NAREC"),val=0.5)) # if admitted/accepted absolute error is 0.5
print(mmetric(y,x,"TOLERANCEPERC",val=0.05)) # tolerance for a 5% of yrange
# tolerance for fixed 0.1 value and 5% of yrange:
print(mmetric(y,x,c("TOLERANCE","TOLERANCEPERC"),val=c(0.1,0.05)))
print(mmetric(y,x,"THEILSU2",val=94.1)) # val = 1-ahead random walk, c(y,94.1), same as below 
 print(mmetric(y,x,"THEILSU2",val=c(94.1,y[1:5]))) \ \# \ val = 1-ahead \ random \ walk \ (previous \ y \ values) 
print(mmetric(y,x,"MASE",val=c(88.1,89.9,93.2,94.1))) # val = in-samples
val=vector("list",length=4)
val[[2]]=0.5;val[[3]]=94.1;val[[4]]=c(88.1,89.9,93.2,94.1)
print(mmetric(y,x,c("MAE","NAREC","THEILSU2","MASE"),val=val))
# user defined error function example:
# myerror = number of samples with absolute error above 0.1% of y:
myerror=function(y,x){return (sum(abs(y-x)>(0.001*y)))}
print(mmetric(y,x,metric=myerror))
# example that returns a list since "REC" is included:
print(mmetric(y,x,c("MAE","REC","TOLERANCE","EV"),val=1))
```

```
### mining, several runs, prob multi-class
## Not run:
data(iris)
M=mining(Species~.,iris,model="rpart",Runs=2)
R=mmetric(M,metric="CONF",aggregate="no")
print(R[[1]]$conf)
print(R[[2]]$conf)
print(mmetric(M,metric="CONF",aggregate="mean"))
print(mmetric(M,metric="CONF",aggregate="sum"))
print(mmetric(M,metric=c("ACC","ACCLASS"),aggregate="no"))
print(mmetric(M,metric=c("ACC","ACCLASS"),aggregate="mean"))
print(mmetric(M,metric="ALL",aggregate="no"))
print(mmetric(M,metric="ALL",aggregate="mean"))
## End(Not run)
### mining, several runs, regression
## Not run:
data(sin1reg)
S=sample(1:nrow(sin1reg),40)
M=mining(y~.,data=sin1reg[S,],model="ksvm",search=2^3,Runs=10)
R=mmetric(M,metric="MAE")
print(mmetric(M,metric="MAE",aggregate="mean"))
miR=meanint(R) # mean and t-student confidence intervals
cat("MAE=",round(miR$mean,digits=2),"+-",round(miR$int,digits=2),"\n")
print(mmetric(M, metric=c("MAE", "RMSE")))
print(mmetric(M,metric=c("MAE","RMSE"),aggregate="mean"))
R=mmetric(M,metric="REC",aggregate="no")
print(R[[1]]$rec)
print(mmetric(M,metric=c("TOLERANCE","NAREC"),val=0.2))
print(mmetric(M,metric=c("TOLERANCE","NAREC"),val=0.2,aggregate="mean"))
## End(Not run)
```

mparheuristic

Function that returns a list of searching (hyper)parameters for a particular model (classification or regression) or for a multiple list of models (automl or ensembles).

# Description

Easy to use function that returns a list of searching (hyper)parameters for a particular model (classification or regression) or for a multiple list of models (automl or ensembles). The result is to be put in a search argument, used by fit or mining functions. Something like: search=list(search=mparheuristic(...),...).

#### Usage

#### **Arguments**

model

model type name. See fit for the individual model details (e.g., "ksvm"). For multiple models use:

- automl 5 individual machine learning algorithms: generalized linear model (GLM, via cv.glmnet), support vector machine (SVM, via ksvm), multi-layer perceptron (MLP, via mlpe), random forest (RF, via randomForest) and extreme gradient boosting (XG, via xgboost). The n="heuristic" setting (see below) is assumed for all algorithms, thus just one hyperparameter is tested for each model. This option is thus the fastest automl to run.
- autom12 same 5 individual machine learning algorithms as autom1. For each algorithm, a grid search is executed with 10 searches (same as: n="heuristic10"), except for ksvm, which uses 13 searches of an uniform design ("UD").
- autom13 same as autom12 except that a six extra stacking ensemble ("SE") model is performed using the 5 best tuned algorithm versions (GLM, SVM, MLP, RF and XG).
- a character vector with several models see the example section for a demonstration of this option.

number of searches or heuristic or numeric vector (either n or by should be used, n has prevalence over by). By default, the searches are linear for all models except for SVM several rbfdot kernel based models ("ksvm","rsvm","lssvm", which can assume 2^search-range; please check the result of this function to confirm if the search is linear or 2^search-range).

If this argument is 1 then the main hyperparameter of the model is set to the value of lower (if lower is not NA).

If this argument is a numeric vector, then the main hyperparameter of the model is set to this vector.

If this argument is a character type, then it is assumed to be an heuristic. Possible heuristic values are:

- heuristic only one model is fit, uses default rminer values, same as mparheuristic(model).
- heuristic5 5 hyperparameter searches from lower to upper, only works
  for the following models: ctree, rpart, kknn, ksvm, lssvm, mlp, mlpe,
  randomForest, multinom, rvm, xgboost. Notes: rpart different cp
  values (see rpart.control); ctree different mincriterion values (see
  ctree\_control); randomForest upper argument is limited by the number of inputs (mtry is searched); ksvm, lssvm or rvm the optional kernel
  argument can be used.
- heuristic10 same as heuristic5 but with 10 searches from lower to upper.

n

UD or UD1 - UD or UD1 uniform design search (only for ksvm and rbfdof kernel). This option assumes 2 hyperparameters for classification (sigma, C) and 3 hyperparameters (sigma, C, epsilon) for regression, thus task="reg" argument needs to be set when regression is used.

- xgb9 9 searches (3 for eta and 3 for max\_depth, works only when model=xgboost.
- mlp\_t heuristic 33 from Delgado 2014 paper, 10 searches, works only when model=mlp or model=mlpe.
- avNNet\_t heuristic 34 from Delgado 2014 paper, 9 searches, works only when model=mlpe.
- nnet\_t heuristic 36 from Delgado 2014 paper, 25 searches, works only when model=mlp or model=mlpe.
- svm\_C heuristic 48 from Delgado 2014 paper, 130 searches (may take time), works only when model=ksvm.
- svmRadial\_t heuristic 52 from Delgado 2014 paper, 25 searches, works only when model=ksvm.
- svmLinear\_t heuristic 54 from Delgado 2014 paper, 5 searches, works only when model=ksvm.
- svmPoly\_t heuristic 55 from Delgado 2014 paper, 27 searches, works only when model=ksvm.
- 1svmRadial\_t heuristic 56 from Delgado 2014 paper, 10 searches, works only when model=lssvm.
- rpart\_t heuristic 59 from Delgado 2014 paper, 10 searches, works only when model=rpart.
- rpart2\_t heuristic 60 from Delgado 2014 paper, 10 searches, works only when model=rpart.
- ctree\_t heuristic 63 from Delgado 2014 paper, 10 searches, works only when model=ctree.
- ctree2\_t heuristic 64 from Delgado 2014 paper, 10 searches, works only when model=ctree.
- rf\_t heuristic 131 from Delgado 2014 paper, 10 searches, works only when model=randomForest.
- knn\_R heuristic 154 from Delgado 2014 paper, 19 searches, works only when model=kknn.
- knn\_t heuristic 155 from Delgado 2014 paper, 10 searches, works only when model=kknn.
- multinom\_t heuristic 167 from Delgado 2014 paper, 10 searches, works only when model=multinom.

lower

lower bound for the (hyper)parameter (if NA a default value is assumed). If n=1 and !is.na(lower) then lower is the main hyperparameter value for some models (e.g., "kknn", "mlpe", "ksvm", "xgboost").

upper

upper bound for the (hyper)parameter (if NA a default value is assumed).

by

increment in the sequence (if NA a default value is assumed depending on n).

exponential

if an exponential scale should be used in the search sequence (the NA is a default value that assumes a linear scale unless model is a support vector machine).

kernel	optional kernel type, only used when model="ksvm", model="rsvm" or model="lssvm".
	Currently mapped kernels are "rbfdot" (Gaussian), "polydot" (polynomial)
	and "vanilladot" (linear); see ksvm for kernel details.
task	optional task argument, only used for uniform design (UD or UD1) (with "ksvm" and "rbfdot").
inputs	optional inputs argument: the number of inputs, only used by "randomForest".

#### **Details**

This function facilitates the definition of the search argument used by **fit** or **mining** functions. Using simple heuristics, reasonable (hyper)parameter search values are suggested for several rminer models. For models not mapped in this function, the function returns NULL, which means that no hyperparameter search is executed (often, this implies using rminer or R function default values).

The simple usage of heuristic assumes lower and upper bounds for a (hyper)parameter. If n=1, then rminer or R defaults are assumed. Else, a search is created using seq(lower, upper, by), where by was set by the used or computed from n. For some model="ksvm" setups,  $2^seq(...)$  is used for sigma and C,  $(1/10)^seq(...)$  is used for scale. Please check the resulting object to inspect the obtained final search values.

This function also allows to easily set multiple model searches, under the: "automl", "automl2", "automl3" or vector character options (see below examples).

#### Value

A list with one ore more (hyper)parameter values to be searched.

## Note

```
See also http://hdl.handle.net/1822/36210 and http://www3.dsi.uminho.pt/pcortez/rminer.html
```

#### Author(s)

```
Paulo Cortez http://www3.dsi.uminho.pt/pcortez/
```

## References

To check for more details about rminer and for citation purposes:
 P. Cortez.

Data Mining with Neural Networks and Support Vector Machines Using the R/rminer Tool. In P. Perner (Ed.), Advances in Data Mining - Applications and Theoretical Aspects 10th Industrial Conference on Data Mining (ICDM 2010), Lecture Notes in Artificial Intelligence 6171, pp. 572-583, Berlin, Germany, July, 2010. Springer. ISBN: 978-3-642-14399-1. @Springer: https://link.springer.com/chapter/10.1007/978-3-642-14400-4\_44 http://www3.dsi.uminho.pt/pcortez/2010-rminer.pdf

The automl is inspired in this work:
 L. Ferreira, A. Pilastri, C. Martins, P. Santos, P. Cortez.
 An Automated and Distributed Machine Learning Framework for Telecommunications Risk

Management. In J. van den Herik et al. (Eds.), Proceedings of 12th International Conference on Agents and Artificial Intelligence – ICAART 2020, Volume 2, pp. 99-107, Valletta, Malta, February, 2020, SCITEPRESS, ISBN 978-989-758-395-7.

@INSTICC: https://www.insticc.org/Primoris/Resources/PaperPdf.ashx?idPaper=89528

• This tutorial shows additional code examples:

P. Cortez.

A tutorial on using the rminer R package for data mining tasks.

Teaching Report, Department of Information Systems, ALGORITMI Research Centre, Engineering School, University of Minho, Guimaraes, Portugal, July 2015.

http://hdl.handle.net/1822/36210

Some lower/upper bounds and heuristics were retrieved from:
 M. Fernandez-Delgado, E. Cernadas, S. Barro and D. Amorim. Do we need hundreds of classifiers to solve real world classification problems?. In The Journal of Machine Learning Research, 15(1), 3133-3181, 2014.

## See Also

fit and mining.

## **Examples**

```
## "kknn"
s=mparheuristic("kknn",n="heuristic")
s=mparheuristic("kknn",n=1) # same thing
print(s)
s=mparheuristic("kknn",n="heuristic5")
print(s)
s=mparheuristic("kknn",n=5) # same thing
s=mparheuristic("kknn",lower=5,upper=15,by=2)
print(s)
# exponential scale:
s=mparheuristic("kknn",lower=1,upper=5,by=1,exponential=2)
print(s)
## "mlpe"
s=mparheuristic("mlpe")
print(s) # "NA" means set size with min(inputs/2,10) in fit
s=mparheuristic("mlpe",n="heuristic10")
print(s)
s=mparheuristic("mlpe",n=10) # same thing
s=mparheuristic("mlpe", n=10, lower=2, upper=20)
print(s)
# numeric (single number or vector) usage of n:
s=mparheuristic("mlpe",n=NA) #
```

```
print(s)
s=mparheuristic("mlpe",n=1,lower=NA) # same thing
print(s)
s=mparheuristic("mlpe",n=1,lower=2) # size=2
print(s)
s=mparheuristic("mlpe",n=1:9) # size=1:9
print(s)
## "randomForest", upper should be set to the number of inputs = max mtry
s=mparheuristic("randomForest",n=10,upper=6)
print(s)
## "ksvm"
s=mparheuristic("ksvm",n=10)
print(s)
s=mparheuristic("ksvm", n=10, kernel="vanilladot")
s=mparheuristic("ksvm",n=10,kernel="polydot")
print(s)
## lssvm
s=mparheuristic("lssvm",n=10)
print(s)
## rvm
s=mparheuristic("rvm",n=5)
s=mparheuristic("rvm",n=5,kernel="vanilladot")
print(s)
## "rpart" and "ctree" are special cases (see help(fit,package=rminer) examples):
s=mparheuristic("rpart",n=3) # 3 cp values
s=mparheuristic("ctree",n=3) # 3 mincriterion values
print(s)
### examples with fit
## Not run:
### classification
data(iris)
# ksvm and rbfdot:
model="ksvm";kernel="rbfdot"
s=mparheuristic(model,n="heuristic5",kernel=kernel)
print(s) # 5 sigma values
search=list(search=s,method=c("holdout",2/3,123))
# task "prob" is assumed, optimization of "AUC":
M=fit(Species~.,data=iris,model=model,search=search,fdebug=TRUE)
print(M@mpar)
# different lower and upper range:
s=mparheuristic(model,n=5,kernel=kernel,lower=-5,upper=1)
print(s) # from 2^-5 to 2^1
```

```
search=list(search=s,method=c("holdout",2/3,123))
# task "prob" is assumed, optimization of "AUC":
M=fit(Species~.,data=iris,model=model,search=search,fdebug=TRUE)
print(M@mpar)
# different exponential scale:
s=mparheuristic(model, n=5, kernel=kernel, lower=-4, upper=0, exponential=10)
print(s) # from 10^-5 to 10^1
search=list(search=s,method=c("holdout",2/3,123))
# task "prob" is assumed, optimization of "AUC":
M=fit(Species~.,data=iris,model=model,search=search,fdebug=TRUE)
print(M@mpar)
# "lssvm" Gaussian model, pure classification and ACC optimization, full iris:
model="lssvm";kernel="rbfdot"
s=mparheuristic("lssvm", n=3, kernel=kernel)
print(s)
search=list(search=s,method=c("holdout",2/3,123))
M=fit(Species~.,data=iris,model=model,search=search,fdebug=TRUE)
print(M@mpar)
# test several heuristic5 searches, full iris:
n="heuristic5";inputs=ncol(iris)-1
model=c("ctree","rpart","kknn","ksvm","lssvm","mlpe","randomForest")
for(i in 1:length(model))
 cat("--- i:",i,"model:",model[i],"\n")
 if(model[i]=="randomForest") s=mparheuristic(model[i],n=n,upper=inputs)
 else s=mparheuristic(model[i],n=n)
 print(s)
 search=list(search=s,method=c("holdout",2/3,123))
 M=fit(Species~.,data=iris,model=model[i],search=search,fdebug=TRUE)
 print(M@mpar)
 }
# test several Delgado 2014 searches (some cases launch warnings):
model=c("mlp","mlpe","mlp","ksvm","ksvm","ksvm",
        "ksvm","lssvm","rpart","rpart","ctree",
        "ctree","randomForest","kknn","kknn","multinom")
n=c("mlp_t","avNNet_t","nnet_t","svm_C","svmRadial_t","svmLinear_t",
    "svmPoly_t","lsvmRadial_t","rpart_t","rpart2_t","ctree_t",
    "ctree2_t", "rf_t", "knn_R", "knn_t", "multinom_t")
inputs=ncol(iris)-1
for(i in 1:length(model))
 {
 cat("--- i:",i,"model:",model[i],"heuristic:",n[i],"\n")
 if(model[i]=="randomForest") s=mparheuristic(model[i],n=n[i],upper=inputs)
 else s=mparheuristic(model[i],n=n[i])
 print(s)
 search=list(search=s,method=c("holdout",2/3,123))
 M=fit(Species~.,data=iris,model=model[i],search=search,fdebug=TRUE)
 print(M@mpar)
```

```
}
## End(Not run) #dontrun
### regression
## Not run:
data(sa_ssin)
s=mparheuristic("ksvm",n=3,kernel="polydot")
search=list(search=s,metric="MAE",method=c("holdout",2/3,123))
M=fit(y~.,data=sa_ssin,model="ksvm",search=search,fdebug=TRUE)
print(M@mpar)
# regression task, predict iris "Petal.Width":
data(iris)
ir2=iris[,1:4]
names(ir2)[ncol(ir2)]="y" # change output name
n=3; inputs=ncol(ir2)-1 # 3 hyperparameter searches
model=c("ctree","rpart","kknn","ksvm","mlpe","randomForest","rvm")
for(i in 1:length(model))
{
 cat("--- i:",i,"model:",model[i],"\n")
 if(model[i]=="randomForest") s=mparheuristic(model[i],n=n,upper=inputs)
 else s=mparheuristic(model[i],n=n)
 print(s)
 search=list(search=s,method=c("holdout",2/3,123))
 M=fit(y^{-}., data=ir2, model=model[i], search=search, fdebug=TRUE)
 print(M@mpar)
 }
## End(Not run) #dontrun
### multiple model examples:
## Not run:
data(iris)
inputs=ncol(iris)-1; task="prob"
# 5 machine learning (ML) algorithms, 1 heuristic hyperparameter per algorithm:
sm=mparheuristic(model="automl",task=task,inputs=inputs)
print(sm)
# 5 ML with 10/13 hyperparameter searches:
sm=mparheuristic(model="autom12",task=task,inputs=inputs)
# note: mtry only has 4 searches due to the inputs limit:
print(sm)
# regression example:
ir2=iris[,1:4]
inputs=ncol(ir2)-1; task="reg"
sm=mparheuristic(model="autom12",task=task,inputs=inputs)
# note: ksvm contains 3 UD hyperparameters (and not 2) since task="reg":
print(sm)
```

64 predict.fit

```
# 5 ML and stacking:
inputs=ncol(iris)-1; task="prob"
sm=mparheuristic(model="autom13", task=task,inputs=inputs)
# note: $1s only has 5 elements, one for each individual ML
print(sm)
# other manual design examples: ------
# 5 ML and three ensembles:
# the fit or mining functions will search for the best option
# between any of the 5 ML algorithms and any of the three
# ensemble approaches:
sm2=mparheuristic(model="automl3",task=task,inputs=inputs)
# note: ensembles need to be at the end of the $models field:
sm2$models=c(sm2$models,"AE","WE") # add AE and WE
sm2$smethod=c(sm2$smethod,rep("grid",2)) # add grid to AE and WE
# note: $1s only has 5 elements, one for each individual ML
print(sm2)
# 3 ML example:
models=c("cv.glmnet","mlpe","ksvm") # just 3 models
# note: in rminer the default cv.glmnet does not have "hyperparameters"
# since the cv automatically sets lambda
n=c(NA,10,"UD") # 10 searches for mlpe and 13 for ksvm
sm3=mparheuristic(model=models,n=n)
# note: $1s only has 5 elements, one for each individual ML
# usage in sm2 and sm3 for fit (see mining help for usages in mining):
method=c("holdout",2/3,123)
d=iris
names(d)[ncol(d)]="y" # change output name
s2=list(search=sm2, smethod="auto", method=method, metric="AUC", convex=0)
M2=fit(y~.,data=d,model="auto",search=s2,fdebug=TRUE)
s3=list(search=sm3, smethod="auto", method=method, metric="AUC", convex=0)
M3=fit(y~.,data=d,model="auto",search=s3,fdebug=TRUE)
## End(Not run)
```

predict.fit

predict method for fit objects (rminer)

#### **Description**

predict method for fit objects (rminer)

predict.fit 65

## **Arguments**

object a model object created by fit

newdata a data frame or matrix containing new data

#### **Details**

Returns predictions for a fit model. Note: the ... optional argument is currently only used by cubist model (see example).

#### Value

If task is prob returns a matrix, where each column is the class probability.

If task is class returns a factor.

If task is reg returns a numeric vector.

#### Methods

```
signature(object = "model") describe this method here
```

#### References

To check for more details about rminer and for citation purposes:
 P. Cortez.

Data Mining with Neural Networks and Support Vector Machines Using the R/rminer Tool. In P. Perner (Ed.), Advances in Data Mining - Applications and Theoretical Aspects 10th Industrial Conference on Data Mining (ICDM 2010), Lecture Notes in Artificial Intelligence 6171, pp. 572-583, Berlin, Germany, July, 2010. Springer. ISBN: 978-3-642-14399-1. @Springer: https://link.springer.com/chapter/10.1007/978-3-642-14400-4\_44 http://www3.dsi.uminho.pt/pcortez/2010-rminer.pdf

• This tutorial shows additional code examples:

P. Cortez.

A tutorial on using the rminer R package for data mining tasks.

Teaching Report, Department of Information Systems, ALGORITMI Research Centre, Engineering School, University of Minho, Guimaraes, Portugal, July 2015.

```
http://hdl.handle.net/1822/36210
```

## See Also

```
fit, mining, mgraph, mmetric, savemining, CasesSeries, lforecast and Importance.
```

# Examples

```
### simple classification example with logistic regression
data(iris)
M=fit(Species~.,iris,model="lr")
P=predict(M,iris)
```

66 savemining

```
print(mmetric(iris$Species,P,"CONF")) # confusion matrix
### simple regression example
data(sa_ssin)
H=holdout(sa_ssin$y,ratio=0.5,seed=12345)
Y=sa_ssin[H$ts,]$y # desired test set
# fit multiple regression on training data (half of samples)
M=fit(y^{-}.,sa\_ssin[H$tr,],model="mr") # multiple regression
P1=predict(M,sa_ssin[H$ts,]) # predictions on test set
print(mmetric(Y,P1,"MAE")) # mean absolute error
### fit cubist model
M=fit(y~.,sa_ssin[H$tr,],model="cubist") #
P2=predict(M,sa_ssin[H$ts,],neighbors=3) #
print(mmetric(Y,P2,"MAE")) # mean absolute error
P3=predict(M,sa_ssin[H$ts,],neighbors=7) #
print(mmetric(Y,P3,"MAE")) # mean absolute error
### check fit for more examples
```

savemining

Load/save into a file the result of a fit (model) or mining functions.

## **Description**

Load/save into a file the result of a fit (model) or mining functions.

## Usage

```
savemining(mmm_mining, file, ascii = TRUE)
```

## **Arguments**

mmm\_mining the list object that is returned by the mining function.

file filename that should include an extension

ascii if TRUE then ascii format is used to store the file (larger file size), else a binary

format is used.

## **Details**

```
Very simple functions that do what their names say. Additional usages are: loadmining(file) savemodel(MM_model,file,ascii=FALSE) loadmodel(file)
```

## Value

loadmining returns a mining mining list, while loadmodel returns a model object (from fit).

sa\_fri1 67

## Author(s)

```
Paulo Cortez http://www3.dsi.uminho.pt/pcortez/
```

#### References

See fit.

## See Also

fit, predict.fit, mining, mgraph, mmetric, savemining, Importance.

## **Examples**

```
### dontrun is used here to avoid the creation of a new file
### in the CRAN servers. The example should work fine:
## Not run:
data(iris)
M=fit(Species~.,iris,model="rpart")
tempdirpath=tempdir()
filename=paste(tempdirpath,"/iris.model",sep="")
savemodel(M,filename) # saves to file
M=NULL # cleans M
M=loadmodel(filename) # load from file
print(M)
## End(Not run)
```

sa\_fri1

Synthetic regression and classification datasets for measuring input importance of supervised learning models

# Description

5 Synthetic regression (sa\_fri1, sa\_ssin, sa\_psin, sa\_int2, sa\_tree) and 4 classification (sa\_ssin\_2, sa\_ssin\_n2p, sa\_int2\_3c, sa\_int2\_8p) datasets for measuring input importance of supervised learning models

# Usage

```
data(sa_fri1)
```

## **Format**

A data frame with 1000 observations on the following variables.

```
xn input (numeric or factor, depends on the dataset)
```

y output target (numeric or factor, depends on the dataset)

68 sin1reg

# **Details**

Check reference or source for full details

## **Source**

See references

## References

• To cite the Importance function, sensitivity analysis methods or synthetic datasets, please use: P. Cortez and M.J. Embrechts.

Using Sensitivity Analysis and Visualization Techniques to Open Black Box Data Mining Models.

```
In Information Sciences, Elsevier, 225:1-17, March 2013. doi:10.1016/j.ins.2012.10.039
```

# **Examples**

```
data(sa_ssin)
print(summary(sa_ssin))
## Not run: plot(sa_ssin$x1,sa_ssin$y)
```

sin1reg

sin1 regression dataset

# **Description**

Simple synthetic dataset with 1000 points, where y=0.7\*sin(pi\*x1/2000)+0.3\*sin(pi\*x2/2000)

# Usage

```
data(sin1reg)
```

# **Format**

The format is: chr "sin1reg"

# **Details**

Simple synthetic dataset with 1000 points, where y=0.7\*sin(pi\*x1/2000)+0.3\*sin(pi\*x2/2000)

#### Source

See references

69 vecplot

## References

• To cite the Importance function, sensitivity analysis methods or synthetic datasets, please use: P. Cortez and M.J. Embrechts.

Using Sensitivity Analysis and Visualization Techniques to Open Black Box Data Mining Models.

```
In Information Sciences, Elsevier, 225:1-17, March 2013.
doi:10.1016/j.ins.2012.10.039
```

## **Examples**

```
data(sin1reg)
print(summary(sin1reg))
```

vecplot

VEC plot function (to use in conjunction with Importance function).

# **Description**

VEC plot function (to use in conjunction with Importance function).

#### **Usage**

```
vecplot(I, graph = "VEC", leg = NULL, xval = 1, sort = FALSE, data = NULL,
digits = c(1, 1), TC = 1, intbar = NULL, lty = 1, pch = 19, col = NULL,
datacol = NULL, main = "", main2 = "", Grid = 0,
xlab = "", ylab = "", zlab = "",
levels = NULL, levels2 = NULL, showlevels = FALSE,
screen = list(z = 40, x = -60), zoom = 1, cex = 1)
```

#### **Arguments**

Ι the output list of the Importance function. graph

- type of VEC graph:
  - VECB 1-D VEC curve with box plots (only valid for SA methods: "DSA", "MSA");
  - VEC3 2-D VEC surface;

• VEC – 1-D VEC curve;

• VECC – 2-D VEC contour;

leg see mgraph

xval the attribute input index (e.g. 1), only used if graph="VEC" or (graph="VEC3"

or "VECC" and length(interactions)=1, see Importance). if a vector, then

several VEC curves are plotted (in this case, x-axis is scaled).

if factor inputs are sorted: sort

70 vecplot

• increasing – sorts the first attribute (if factor) according to the response values, increasing order;

- decreasing similar to increasing but uses reverse order;
- TRUE similar to increasing;
- increasing2 sorts the second attribute (for graph="VEC3" or "VECC", if factor, according to the response values), increasing order;
- decreasing2 similar to increasing2 but uses reverse order;
- FALSE no sort is used;

pch point type for the graph="VEC" curve, can be a vector if there are several VEC

curve plots

col color (e.g. "black", "grayrange", "white")
datacol color of the data histogram for graph="VEC"

main see mgraph

main2 key title for graph="VECC"

Grid see mgraph
xlab x-axis label
ylab y-axis label
zlab z-axis label

levels if x1 is factor you can choose the order of the levels to this argument levels2 if x2 is factor you can choose the order of the levels to this argument

showlevels if you want to show the factor levels in x1 or x2 axis in graph="VEC3":

- FALSE or TRUE do not (do) show the levels in x1, x2 and z axis for factor variables;
- vector with 3 logical values if you want to show the levels in each of the x1, x2 or z axis for factor variables (e.g. c(FALSE, FALSE, TRUE) only shows for z-axis).

screen select the perspective angle of the VEC3 graph:

- x assumes list(z=0, x=-90, y=0);
- X assumes list(x=-75);
- y assumes list(z=0, x=-90, y=-90);
- Y assumes list(z=10, x=-90, y=-90);
- z assumes list(z=0, x=0, y=0);
- xy assumes list(z=10, x=-90, y=-45);
- else you need to specify a list with z, x an y angles, see wireframe

zoom of the wireframe (graph="VEC3")

cex label font size

vecplot 71

# **Details**

For examples and references check: Importance

## Value

A VEC curve/surface/contour plot.

# Author(s)

```
Paulo Cortez http://www3.dsi.uminho.pt/pcortez/
```

# References

• To cite the Importance function or sensitivity analysis method, please use:

P. Cortez and M.J. Embrechts.

Using Sensitivity Analysis and Visualization Techniques to Open Black Box Data Mining Models.

In Information Sciences, Elsevier, 225:1-17, March 2013.

doi:10.1016/j.ins.2012.10.039

# See Also

Importance

# **Index**

y onlot	lforecast, 35
* aplot	mgraph, 36
mgraph, 36	mining, 40
vecplot, 69 * classif	mparheuristic, 56
	predict.fit,64
fit, 7	savemining, 66
Importance, 26	vecplot, 69
mgraph, 36	* regression
mining, 40	* regression fit, 7
mmetric, 47	lforecast, 35
mparheuristic, 56	
predict.fit,64	mgraph, 36 mining, 40
savemining, 66	<u> </u>
vecplot, 69	mmetric, 47 mparheuristic, 56
* datasets	predict.fit, 64
CasesSeries, 2	savemining, 66
sa_fri1,67	vecplot, 69
sin1reg,68	* ts
* file	CasesSeries, 2
savemining, 66	lforecast, 35
* manip	Trorecast, 33
delevels, 5	bagging, 8
holdout, 23	boosting, 8
imputation, 33	boosting, o
* methods	CasesSeries, 2, 15, 35, 36, 65
predict.fit,64	centralpar (mining), 40
* models	cppls, 9
crossvaldata, 3	crossval, 5
* neural	crossvaldata, 3, 13, 41
fit, <b>7</b>	ctree, 8
Importance, 26	ctree_control, 57
lforecast, 35	cubist, 9
mgraph, 36	cv.glmnet, 8
mining, 40	2 6
mparheuristic, 56	data.frame, 5
predict.fit,64	delevels, 5, 34
savemining, 66	, ,
vecplot, 69	factor, <i>5</i> , <i>10</i>
* nonlinear	fit, 3-6, 7, 25, 27-29, 34-36, 39, 41, 42, 44,
fit,7	47, 53, 56, 57, 59, 60, 65–67

INDEX 73

holdout, 4, 5, 15, 23, 41, 44	sa_int2_3c (sa_fri1), 67 sa_int2_8p (sa_fri1), 67
Importance, 9, 15, 25, 26, 39, 44, 53, 65, 67, 69, 71	sa_psin (sa_fri1), 67 sa_ssin (sa_fri1), 67
imputation, $6,33$	sa_ssin_2 (sa_fri1), 67 sa_ssin_n2p (sa_fri1), 67
kknn, 8 ksvm, 8, 10, 13, 41, 59	sa_tree (sa_fri1), 67 savemining, 15, 25, 29, 39, 44, 53, 65, 66, 67
lda, 9 lforecast, 3, 15, 35, 65	savemodel (savemining), 66 sin1reg, 68
list, 9–11 lm, 9	vecplot, 28, 29, 69 vector, 10, 12
loadmining (savemining), 66 loadmodel (savemining), 66	wireframe, 70
lssvm, 8	xgboost, 8
mars, 9 metrics (mmetric), 47	•
mgraph, 15, 25, 29, 36, 36, 44, 53, 65, 67, 69,	
mining, 4, 5, 9, 11, 12, 15, 25, 29, 36–39, 40, 47, 51, 53, 56, 59, 60, 65–67	
mmetric, 11, 12, 15, 25, 29, 37–39, 42, 44, 47, 65, 67	
model-class (fit), 7 mparheuristic, 10, 11, 14, 15, 44, 56 multinom, 9	
$\begin{array}{c} \text{naiveBayes, } 9 \\ \text{nnet, } 8,  9,  13 \end{array}$	
par, 38	
pcr, 9 plot, 38	
plsr, 9 predict, model-method (predict.fit), 64 predict-methods (predict.fit), 64 predict.fit, 3, 5, 15, 25, 36, 39, 44, 53, 64,	
67 qda, 9	
${\tt randomForest}, 8$	
rpart, 8, 13 rpart.control, 57 rvm, 9	
sa_fri1, 67 sa_int2 (sa_fri1), 67	