Package 'semiArtificial'

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Description Contains methods to generate and evaluate semi-artificial data sets. Based on a given data set different methods learn data properties using machine learning algorithms and generate new data with the same properties. The package currently includes the following data generators: i) a RBF network based generator using rbfDDA() from package 'RSNNS', ii) a Random Forest based generator for both classification and regression problems iii) a density forest based generator for unsupervised data Data evaluation support tools include: a) single attribute based statistical evaluation: mean, median, standard deviation, skewness, kurtosis, medcouple, L/RMC, KS test, Hellinger distance b) evaluation based on clustering using Adjusted Rand Index (ARI) and FM c) evaluation based on classification performance with various learning models, e.g., random forests.
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<pre>URL http://lkm.fri.uni-lj.si/rmarko/software/</pre>
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semiArtificial-package

Generation and evaluation of semi-artificial data

Description

The package semiArtificial contains methods to generate and evaluate semi-artificial data sets. Different data generators take a data set as an input, learn its properties using machine learning algorithms and generates new data with the same properties.

Details

The package currently includes the following data generators:

- a RBF network based generator using rbfDDA model from RSNNS package.
- generator using density tree forest for unsupervised data,
- generator using random forest for classification and regression.

Data evaluation support tools include:

- statistical evaluation: mean, median, standard deviation, skewness, kurtosis, medcouple, L/RMC,
- evaluation based on clustering using Adjusted Rand Index (ARI) and Fowlkes-Mallows index (FM),
- evaluation based on prediction with a model, e.g., random forests.

Further software and development versions are available at http://lkm.fri.uni-lj.si/rmarko/software/.

Author(s)

Marko Robnik-Sikonja

References

Marko Robnik-Sikonja: Not enough data? Generate it!. *Technical Report, University of Ljubljana, Faculty of Computer and Information Science*, 2014

Other references are available from http://lkm.fri.uni-lj.si/rmarko/papers/

See Also

rbfDataGen, treeEnsemble, newdata, dataSimilarity, dsClustCompare, performanceCompare.

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cleanData	Rejection of new instances based on their distance to existing instances

Description

The function contains three data cleaning methods, the first two reject instances whose distance to their nearest neighbors in the existing data are too small or too large. The first checks distance between instances disregarding class, the second checks distances between instances taking only instances from the same class into account. The third method reassigns response variable using the prediction model stored in the generator teObject.

Usage

Arguments

teObject

An object of class TreeEnsemble containing a generator structure as returned by treeEnsemble. The teObject contains generator's training instances from which we compute a distance distribution of instances to their nearestInsK nearest instances. This distance distribution, computed on the training data of the generator, serves as a criterion to reject new instances from newdata, i.e. based on parameters below we reject the instances too close or to far away from their nearest neighbors in generator's training data. The computed distance distributions are stored and returned as cleaningObject component of returned list. If it is provided on subsequent calls, this reduces computational load.

newdat

A data. frame object with the (newly generated) data to be cleaned.

similarDropP

With numeric parameters similarDropP and dissimilarDropP (with the default value NA and the valid value range in [0, 1]) one removes instances in newdat too close to generator's training instances or too far away from these instances. The distance distribution is computed based on instances stored in teObject. For each instance in \$teObject\$ we store the distance to its nearestInsK nearest instances (disregarding the identical instances). These distances are sorted and represent a distribution of nearest distances for all training instances. The values similarDropP and dissimilarDropP represent a proportion of allowed smaller/larger distances computed on the generator's training data contained in the teObject.

dissimilarDropP

See similarDropP.

similarDropPclass

For classification problems only and similarly to the similarDropP and dissimilarDropP above, with the similarDropPclass and dissimilarDropPclass

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> (also in a [0, 1] range) we also removes instances in newdat too close to generator's training instances or too far away from these instances, but only taking near instances from the same class into account. The similarDropPclass contains either a single integer giving thresholds for all class values or a vector of thresholds, one for each class. If the vector is of insufficient length it is replicated using function rep. The generated distance distributions are stored in the cleaningObject component of the returned list.

dissimilarDropPclass

See similarDropPclass.

nearestInstK

An integer with default value of 1, controls how many generator's training instances we take into account when computing the distance distribution of nearest instances.

reassignResponse

is a logical value controlling whether the response variable of the newdat shall be set anew using a random forest prediction model or taken as it is. The default value reassign=FALSE means that values of response are not changed.

cleaningObject is a list object with a precomputed distance distributions and predictor from previous runs of the same function. If provided, this saves computation time.

Details

The function uses the training instances stored in the generator teObject to compute distribution of distances from instances to their nearestInstK nearest instances. For classification problems the distributions can also be computed only for instances from the same class. Using these near distance distributions the function rejects all instances too close or too far away from existing instances.

The default value of similarDropP, dissimilarDropP, similarDropPclass, and dissimilarDropPclass is NA and means that the near/far values are not rejected. The same effect has value 0 for similarDropP and similarDropPclass, and value 1 for dissimilarDropP and dissimilarDropPclass.

Value

The method returns a list object with two components:

distant instances from newdata.

cleaningObject is a list containing computed distributions of nearest distances (also class-

based fro classification problems, and possibly a predictor used for reassigning

is a data. frame containing the instances left after rejection of too close or too

the response variable.

Author(s)

cleanData

Marko Robnik-Sikonja

See Also

treeEnsemble, newdata. TreeEnsemble.

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Examples

dataSimilarity

Evaluate statistical similarity of two data sets

Description

Use mean, standard deviation, skewness, kurtosis, Hellinger distance and KS test to compare similarity of two data sets.

Usage

```
dataSimilarity(data1, data2, dropDiscrete=NA)
```

Arguments

data1 A data. frame containing the reference data.

data2 A data.frame with the same number and names of columns as data1.

dropDiscrete A vector discrete attribute indices to skip in comparison. Typically we might

skip class, because its distribution was forced by the user.

Details

The function compares data stored in data1 with data2 on per attribute basis by computing several statistics: mean, standard deviation, skewness, kurtosis, Hellinger distance and KS test.

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Value

The method returns a list of statistics computed on both data sets:

A matrix with rows containing statistics (mean, standard deviation, skewness, stats1num

and kurtosis) computed on numeric attributes of data1.

equalInstances The number of instances in data2 equal to the instances in data1.

stats2num A matrix with rows containing statistics (mean, standard deviation, skewness,

and kurtosis) computed on numeric attributes of data2.

A vector with p-values of Kolmogorov-Smirnov two sample tests, performed on ksP

matching attributes from data1 and data2.

freq1 A list with value frequencies for discrete attributes in data1. A list with value frequencies for discrete attributes in data2. freq2

A list with differences in frequencies of discrete attributes' values between data1 dfreq

and data2.

dstatsNorm A matrix with rows containing difference between statistics (mean, standard

deviation, skewness, and kurtosis) computed on [0,1] normalized numeric at-

tributes for data1 and data2.

hellingerDist A vector with Hellinger distances between matching attributes from data1 and

data2.

Author(s)

Marko Robnik-Sikonja

See Also

newdata.RBFgenerator.

```
# use iris data set, split into training and testing data
set.seed(12345)
train <- sample(1:nrow(iris),size=nrow(iris)*0.5)</pre>
irisTrain <- iris[train,]</pre>
irisTest <- iris[-train,]</pre>
# create RBF generator
irisGenerator<- rbfDataGen(Species~.,irisTrain)</pre>
# use the generator to create new data
irisNew <- newdata(irisGenerator, size=100)</pre>
# compare statistics of original and new data
dataSimilarity(irisTest, irisNew)
```

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dsClustCompare	Evaluate clustering similarity of two data sets

Description

Similarity of two data sets is compared with a method using any of clustering comparison metrics: Adjusted Rand Index (ARI), Fowlkes-Mallows index(FM), Jaccard Index (J), or Variation of Information index (VI).

Usage

```
dsClustCompare(data1, data2)
```

Arguments

data1 A data. frame containing the reference data.

data2 A data. frame with the same number and names of columns as data1.

Details

The function compares data stored in data1 with data2 by first performing partitioning around medoids (PAM) clustering on data1. Instances from data2 are than assigned to the cluster with the closest medoid. In second step PAM clustering is performed on data2 and instances from data1 are assigned to the clusters with closest medoids. The procedure gives us two clusterings on the same instances which we can compare using any of ARI, FM, J, or VI. The higher the value of ARI/FM/J the more similar are the two data sets, and reverse is true for VI, where two perfectly matching partitions produce 0 score. For random clustering ARI returns a value around zero (negative values are possible) and for perfectly matching clustering ARI is 1. FM and J values are strictly in [0, 1].

Value

The method returns a value of a list containing ARI and/or FM, depending on the parameters.

Author(s)

Marko Robnik-Sikonja

See Also

```
newdata.RBFgenerator.
```

```
# use iris data set
# create RBF generator
irisGenerator<- rbfDataGen(Species~.,iris)</pre>
```

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```
# use the generator to create new data
irisNew <- newdata(irisGenerator, size=200)
# compare ARI computed on clustering with original and new data
dsClustCompare(iris, irisNew)</pre>
```

newdata

Generate semi-artificial data using a generator

Description

Using a generator build with rbfDataGen or treeEnsemble the method generates size new instances.

Usage

Arguments

object	An object of class RBFgenerator or TreeEnsemble containing a generator structure as returned by rbfDataGen or treeEnsemble, respectively.
fillData	A dataframe with part of the values already specified. All missing values (i.e. NA values) are filled in by the generator.
size	A number of instances to generate. By default this is one instance, or in the case of existing fillData this is the number of rows in that dataframe.
var	For the generator of type RBF generator the parameter var determines the method of kernel width (variance) estimation. Supported options are "estimated" and "Silverman".
classProb	For classification problems, a vector of desired class value probability distribution. Default value classProb=NULL uses probability distribution of the generator's training instances.
defaultSpread	For the generator of type RBFgenerator the parameter is a numeric value replacing zero spread in case var="estimated" is used. The value defaultSpread=NULL keeps zero spread values.

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onlyPath For the generator of type TreeEnsemble and attribute density data in the leaves

(densityData="leaf"), the parameter is a boolean variable indicating if only attributes on the path from the root to the leaf are generated in the leaf. If onlyPath=FALSE all value are generated in the first randomly chosen leaf of a tree, else only attributes on the path are generated and then the next random tree

is selected.

predictClass For classification problems and the generator of type TreeEnsemble the param-

eter determines if the class value is set through prediction with the forest (the constructed generator serves as a predictor) or set according to the class value

distribution of the selected leaf.

.. Additional parameters passed to density estimation functions kde, logspline, and

quantile.

Details

The function uses the object structure as returned by rbfDataGen or treeEnsemble. In case of RBFgenerator the object contains descriptions of the Gaussian kernels, which model the original data. The kernels are used to generate a required number of new instances. The kernel width of provided kernels can be set in two ways. By setting var="estimated" the estimated spread of the training instances that have the maximal activation value for the particular kernel is used. Using var="Silverman" width is set by the generalization of Silverman's rule of thumb to multivariate case (unreliable for larger dimensions).

In case of TreeEnsemble generator no additional parameters are needed, except for the number of generated instances.

Value

The method returns a data. frame object with required number of instances.

Author(s)

Marko Robnik-Sikonja

See Also

rbfDataGen, treeEnsemble.

```
# inspect properties of the iris data set
plot(iris, col=iris$Species)
summary(iris)

# create RBF generator
irisRBF<- rbfDataGen(Species~.,iris)
# create treesemble generator
irisEnsemble<- treeEnsemble(Species~.,iris,noTrees=10)

# use the generator to create new data with both generators</pre>
```

```
irisNewRBF <- newdata(irisRBF, size=150)
irisNewEns <- newdata(irisEnsemble, size=150)

#inspect properties of the new data
plot(irisNewRBF, col = irisNewRBF$Species) #plot generated data
summary(irisNewRBF)
plot(irisNewEns, col = irisNewEns$Species) #plot generated data
summary(irisNewEns)</pre>
```

performanceCompare

Evaluate similarity of two data sets based on predictive performance

Description

Depending on the type of problem (classification or regression), a classification performance (accuracy, AUC, brierScore, etc) or regression performance (RMSE, MSE, MAE, RMAE, etc) on two data sets is used to compare the similarity of two data sets.

Usage

```
performanceCompare(data1, data2, formula, model="rf", stat=NULL, ...)
```

Arguments

data1	A data.frame containing the reference data.
data2	A data.frame with the same number and names of columns as data1.
formula	A formula specifying the response and predictive variables.
model	A predictive model used for performance comparison. The default value "rf" stands for random forest, but any classification or regression model supported by function CoreModel in CORElearn package can be used.
stat	A statistics used as performance indicator. The default value is NULL and means that for classification "accuracy" is used, and for regression "RMSE"" (relative mean squared error) is used. Other values supported and output by modelEval from CORElearn package can be used e.g., "AUC" or "brierScore".
	Additional parameters passed to CoreModel function.

Details

The function compares data stored in data1 with data2 by comparing models constructed on data1 and evaluated on both data1 and data2 with models built on data2 and evaluated on both data1 and data2. The difference between these performances are indicative on similarity of the data sets if used in machine learning and data mining. The performance indicator used is determined by parameter stat.

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Value

The method returns a list of performance indicators computed on both data sets:

diff.m1	The difference between performance of model built on data1 (and evaluated on both data1 and data2.)
diff.m2	The difference between performance of model built on data2 (and evaluated on both data1 and data2.)
perf.m1d1	The performance of model built on data1 on data1.
perf.m1d2	The performance of model built on data1 on data2.
perf.m2d1	The performance of model built on data2 on data1.
perf.m2d2	The performance of model built on data2 on data2.

Author(s)

Marko Robnik-Sikonja

See Also

```
newdata.RBFgenerator.
```

Examples

```
# use iris data set

# create RBF generator
irisGenerator<- rbfDataGen(Species~.,iris)

# use the generator to create new data
irisNew <- newdata(irisGenerator, size=200)

# compare statistics of original and new data
performanceCompare(iris, irisNew, Species~.)</pre>
```

rbfDataGen

A data generator based on RBF network

Description

Using given formula and data the method builds a RBF network and extracts its properties thereby preparing a data generator which can be used with newdata.RBFgenerator method to generate semi-artificial data.

Usage

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Arguments

formula A formula specifying the response and variables to be modeled.

data A data frame with training data.

eps The minimal probability considered in data generator to be larger than 0.

minSupport The minimal number of instances defining a Gaussian kernel to copy the kernel

to the data generator.

nominal The way how to treat nominal features. The option "asInteger" converts fac-

tors into integers and treats them as numeric features. The option "encodeBinary" converts each nominal attribute into a set of binary features, which encode the nominal value, e.g., for three valued attribute three binary attributes are con-

structed, each encoding a presence of one nominal value with 0 or 1.

Details

Parameter formula is used as a mechanism to select features (attributes) and the prediction variable (response, class). Only simple terms can be used and interaction terms are not supported. The simplest way is to specify just the response variable using e.g. class ~ .. See examples below.

A RBF network is build using rbfDDA from RSNNS package. The learned Gaussian kernels are extracted and used in data generation with newdata.RBFgenerator method.

Value

The created model is returned as a structure of class RBFgenerator, containing the following items:

noGaussians The number of extracted Gaussian kernels.

centers A matrix of Gaussian kernels' centers, with one row for each Gaussian kernel.

probs A vector of kernel probabilities. Probabilities are defined as relative frequencies

of training set instances with maximal activation in the given kernel.

unitClass A vector of class values, one for each kernel.

bias A vector of kernels' biases, one for each kernel. The bias is multiplied by the

kernel activation to produce output value of given RBF network unit.

spread A matrix of estimated variances for the kernels, one row for each kernel. The j-

th value in i-th row represents the variance of training instances for j-th attribute

with maximal activation in i-th Gaussian.

gNoActivated A vector containing numbers of training instances with maximal activation in

each kernel.

noAttr The number of attributes in training data.

datNames A vector of attributes' names.

originalNames A vector of original attribute names.

attrClasses A vector of attributes' classes (i.e., data types like numeric or factor).

attrLevels A list of levels for discrete attributes (with class factor).

attrOrdered A vector of type logical indicating whether the attribute is ordered (only possi-

ble for attributes of type factor.

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normParameters A list of parameters for normalization of attributes to [0,1].

noCol The number of columns in the internally generated data set.

isDiscrete A vector of type logical, each value indicating whether a respective attribute is

discrete.

noAttrGen The number of attributes to generate.

nominal The value of parameter nominal.

Author(s)

Marko Robnik-Sikonja

References

Marko Robnik-Sikonja: Not enough data? Generate it!. *Technical Report, University of Ljubljana, Faculty of Computer and Information Science*, 2014

Other references are available from http://lkm.fri.uni-lj.si/rmarko/papers/

See Also

newdata.RBFgenerator.

```
# use iris data set, split into training and testing, inspect the data
set.seed(12345)
train <- sample(1:nrow(iris),size=nrow(iris)*0.5)
irisTrain <- iris[train,]
irisTest <- iris[-train,]

# inspect properties of the original data
plot(irisTrain, col=irisTrain$Species)
summary(irisTrain)

# create rbf generator
irisGenerator<- rbfDataGen(Species~.,irisTrain)

# use the generator to create new data
irisNew <- newdata(irisGenerator, size=200)

#inspect properties of the new data
plot(irisNew, col = irisNew$Species) #plot generated data
summary(irisNew)</pre>
```

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treeEnsemble

A data generator based on forest

Description

Using given formula and data the method treeEnsemble builds a tree ensemble and turns it into a data generator, which can be used with newdata method to generate semi-artificial data. The methods supports classification, regression, and unsupervised data, depending on the input and parameters. The method indAttrGen generates data from the same distribution as the input data, but assuming conditionally independent attributes.

Usage

Arguments

formula A formula specifying the response and variables to be modeled.

dataset A data frame with training data.

noTrees The number of trees in the ensemble.

minNodeWeight The minimal number of instances in a tree leaf.

noSelectedAttr Number of randomly selected attributes in each node which are considered as

possible splits. In general this should be a positive integer, but values 0, -1, and -2 are also possible. The default value is noSelectedAttr=0, which causes random selection of integer rounded \sqrt{a} attributes, where \$a\$ is the number of all attributes. Value -1 means that $1 + \log_2 a$ attributes are selected and value -2

means that all attributes are selected.

problemType The type of the problem modeled: classification, regression, or unsupervised

(density estimation). The default value "byResponse" indicates that the prob-

lem type is deducted based on formula and data.

densityData The type of generator data and place where new instances are generated: in the

leafs, top down from the root of the tree to the leaves, bottom up from the leaves to root. In case of value "no" the ensemble contains no generator data and can be used as an ordinary ensemble predictor (although probably slow, as it is written

entirely in R).

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cdfEstimation

The manner values are generated and the type of data stored in the generator: "ecdf" indicates values are generated from empirical cumulative distributions stored for each variable separately; "logspline" means that value distribution is modeled with logsplines, and "kde" indicates that Gaussian kernel density estimation is used.

densitySplitMethod

In case problemType="density" the parameters determines the criteria for selection of split in the density tree. Possible choices are balanced (a split value is chosen in such a way that the split is balanced), random (split value is chosen randomly) and maxVariance (split with maximal variance is chosen).

estimator

The attribute estimator used to select the node split in classification and regression trees. Function attrEval from CORElearn package is used, so the values have to be compatible with that function. The default value NULL chooses Gini index in case of classification problems and MSE (mean squared error in resulting splits) in case of regression.

... Further parameters to be passed onto probability density estimators.

Details

Parameter formula is used as a mechanism to select features (attributes) and the prediction variable (response) from the data. Only simple terms can be used and interaction terms are not supported. The simplest way is to specify just the response variable using e.g. class ~ .. For unsupervised problems all variables can be selected using formula ~ .. See examples below.

A forest of trees is build using R code. The base models of the ensemble are classification, regression or density trees with additional information stored at the appropriate nodes. New data can be generated using newdata method.

The method indAttrGen generates data from the same distribution as the input data (provided in dataset), but assumes conditional independence of attributes. This assumption makes the generated data a simple baseline generator. Internally, the method calls treeEnsemble with parameters noTrees=1, minNodeWeight=nrow(dataset), densityData="leaf".

Value

The created model is returned with additional data stored as a list and also in the trees. The model can be used with function newdata to generate new values.

Author(s)

Marko Robnik-Sikonja

References

Marko Robnik-Sikonja: Not enough data? Generate it!. *Technical Report, University of Ljubljana, Faculty of Computer and Information Science*, 2014

Other references are available from http://lkm.fri.uni-lj.si/rmarko/papers/

See Also

newdata.

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```
# use iris data set, split into training and testing, inspect the data
set.seed(12345)
train <- sample(1:nrow(iris),size=nrow(iris)*0.5)</pre>
irisTrain <- iris[train,]</pre>
irisTest <- iris[-train,]</pre>
# inspect properties of the original data
plot(iris[,-5], col=iris$Species)
summary(iris)
# create tree ensemble generator for classification problem
irisGenerator<- treeEnsemble(Species~., irisTrain, noTrees=10)</pre>
# use the generator to create new data
irisNew <- newdata(irisGenerator, size=200)</pre>
#inspect properties of the new data
plot(irisNew[,-5], col = irisNew$Species) # plot generated data
summary(irisNew)
## Not run:
# create tree ensemble generator for unsupervised problem
irisUnsupervised<- treeEnsemble(~.,irisTrain[,-5], noTrees=10)</pre>
irisNewUn <- newdata(irisUnsupervised, size=200)</pre>
plot(irisNewUn) # plot generated data
summary(irisNewUn)
# create tree ensemble generator for regression problem
CO2gen<- treeEnsemble(uptake~.,CO2, noTrees=10)
CO2New <- newdata(CO2gen, size=200)
plot(CO2) # plot original data
plot(CO2New) # plot generated data
summary(CO2)
summary(CO2New)
## End(Not run)
```

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