Package 'GAparsimony'

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Type Package

Title Searching Parsimony Models with Genetic Algorithms

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Description Methodology that combines feature selection, model tuning, and parsimonious model selection with Genetic Algorithms (GA) proposed in {Martinez-de-Pison} (2015) <<u>DOI:10.1016/j.asoc.2015.06.012</u>>. To this objective, a novel GA selection procedure is introduced based on separate cost and complexity evaluations.

Suggests parallel, doParallel, doRNG (>= 1.6), knitr (>= 1.8), lhs, MASS, caret, mlbench, e1071, nnet, kernlab

License GPL (>= 2)

Depends R (>= 3.0), methods, foreach, iterators

Imports stats, graphics, grDevices, utils

URL https://github.com/jpison/GAparsimony

Repository CRAN

NeedsCompilation no

Author F.J. Martinez-de-Pison [aut, cre]

Maintainer F.J. Martinez-de-Pison <fjmartin@unirioja.es>

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GAparsimony-package GAparsimony

Description

Combines feature selection, model tuning, and parsimonious model selection with GA optimization. GA selection procedure is based on separate cost and complexity evaluations. Therefore, the best individuals are initially sorted by an error fitness function, and afterwards, models with similar costs are rearranged according to modelcomplexity measurement so as to foster models of lesser complexity. The algorithm can be run sequentially or in parallel using an explicit master-slave parallelisation.

Details

GAparsimony package is a new GA wrapper automatic method that efficiently generated prediction models with reduced complexity and adequate generalization capacity. ga_parsimony function is primarily based on combining feature selection and model parameter tuning with a second novel GA selection process (ReRank algorithm) in order to achieve better overall parsimonious models. Unlike other GA methodologies that use a penalty parameter for combining loss and complexity measures into a unique fitness function, the main contribution of this package is that ga_parsimony selects the best models by considering cost and complexity separately. For this purpose, the ReRank algorithm rearranges individuals by their complexity when there is not a significant difference between their costs. Thus, less complex models with similar accuracy are promoted. Furthermore, because the penalty parameter is unnecessary, there is no consequent uncertainty associated with assigning a correct value beforehand. As a result, with GA-PARSIMONY, an automatic method for obtaining parsimonious models is finally made possible.

References

Sanz-Garcia A., Fernandez-Ceniceros J., Antonanzas-Torres F., Pernia-Espinoza A.V., Martinezde-Pison F.J. (2015). GA-PARSIMONY: A GA-SVR approach with feature selection and parameter optimization to obtain parsimonious solutions for predicting temperature settings in a continuous annealing furnace. Applied Soft Computing 35, 23-38. Fernandez-Ceniceros J., Sanz-Garcia A., Antonanzas-Torres F., Martinez-de-Pison F.J. (2015). A numerical-informational approach for characterising the ductile behaviour of the T-stub component. Part 2: Parsimonious soft-computingbased metamodel. Engineering Structures 82, 249-260. Antonanzas-Torres F., Urraca R., Antonanzas J., Fernandez-Ceniceros J., Martinez-de-Pison F.J. (2015). Generation of daily global solar irradiation with support vector machines for regression. Energy Conversion and Management 96, 277-286.

ga_parsimony

Author(s)

Francisco Javier Martinez de Pison Ascacibar <fjmartin@unirioja.es>

ga_parsimony GA-PARSIMONY

Description

A GA-based optimization method for searching accurate parsimonious models by combining feature selection, model tuning, and parsimonious model selection (PMS). PMS procedure is based on separate cost and complexity evaluations. The best individuals are initially sorted by an error fitness function, and afterwards, models with similar costs are rearranged according to their model complexity so as to foster models of lesser complexity. The algorithm can be run sequentially or in parallel using an explicit master-slave parallelisation.

Usage

```
ga_parsimony(fitness, ...,
min_param, max_param, nFeatures,
names_param=NULL, names_features=NULL,
object=NULL, iter_ini=NULL,
type_ini_pop="improvedLHS"
popSize = 50, pcrossover = 0.8, maxiter = 40,
feat_thres=0.90, rerank_error = 0.0, iter_start_rerank = 0,
pmutation = 0.10, feat_mut_thres=0.10, not_muted=3,
elitism = base::max(1, round(popSize * 0.20)),
population = parsimony_population,
selection = parsimony_nlrSelection,
crossover = parsimony_crossover,
mutation = parsimony_mutation,
keep_history = FALSE,
path_name_to_save_iter = NULL,
early_stop = maxiter, maxFitness = Inf, suggestions = NULL,
parallel = FALSE,
monitor = if (interactive()) parsimony_monitor else FALSE,
seed_ini = NULL, verbose=FALSE)
```

Arguments

fitness the fitness function, any allowable R function which takes as input an individual chromosome which combines the model parameters to tune and the features to be selected. Fitness function returns a numerical vector with three values: "validation_cost": a robust validation cost measure, J (RMSE, AUC, Logloss). For example, n-repeated cross validation (CV) RMSE for regression or n-repeated CV Logloss or AUC for classification; "testing_cost": testing cost obtained with a testing dataset not included in the validation process. This value is only for checking the generalization capability of the model. NA value

| | can be supplied if there is not a testing data set; "model_complexity": model complexity. Can be the number of features, number of support vectors in SVM, sum of power of weights in ANNs, depth in Trees, generalised degrees of free- dom (GDF), or another complexity metrics o combination of them. Note: the chromosome is a concatenated real vector with the model param- eters (parameters-chromosome) and the binary selection of the input features (features-chromosome). For example, a chromosome defined as c(10, 0.01, 0,1,1,0,1,0,0) could corresponds to a SVR model parameters C=10 & gamma=0.01, and a selection of three input features (second, third and fifth) from a dataset of 7 features (0110100). |
|----------------|---|
| | additional arguments to be passed to the fitness function. This allows to write fitness functions that keep some variables fixed during the search. |
| min_param | a vector of length equal to the model parameters providing the minimum of the search space. |
| max_param | a vector of length equal to the model parameters providing the maximum of the search space. |
| nFeatures | a value specifying the number of maximum input features. |
| names_param | a vector with the name of the model parameters. |
| names_features | a vector with the name of the input features. |
| object | object of 'ga_parsimony' class to continue GA process. 'ga_parsimony@history' must be provided. Note: all GA settings are obtained from 'object' in order to continue the GA process. |
| iter_ini | Iteration/generation of 'object@history' to be used when 'object' is provided. If 'iter_ini==NULL' uses the last iteration of 'object'. |
| type_ini_pop | method to create the first population with 'parsimony_population' function. This function is called when iter_ini==0 and 'suggestions' are not provided. Meth- ods='randomLHS','geneticLHS','improvedLHS','maximinLHS','optimumLHS','random'. First 5 methods correspond with several latine hypercube sampling. |
| popSize | the population size. |
| pcrossover | the probability of crossover between pairs of chromosomes. Typically this is a large value and by default is set to 0.8. |
| maxiter | the maximum number of iterations to run before the GA process is halted. |
| feat_thres | proportion of selected features in the initial population. It is recommended a high percentage of selected features for the first generations. By default is set to 0.90. |
| rerank_error | when a value is provided, a second reranking process according to the model complexities is called by parsimony_rerank function. Its primary objective is to select individuals with high validation cost while maintaining the robustness of a parsimonious model. This function switches the position of two models if the first one is more complex than the latter and no significant difference is found between their fitness values in terms of cost. Therefore, if the absolute difference between the validation costs are lower than 'rerank_error' they are considered similar. Default value=0.01 |

ga_parsimony

iter_start_rerank iteration when ReRanking process is actived. Default=0. Sometimes is useful not to use ReRanking process in the first generations. the probability of mutation in a parent chromosome. Usually mutation occurs pmutation with a small probability. By default is set to 0.10. probability of the muted 'features-chromosome' to be one. Default value is set feat_mut_thres to 0.10. not_muted number of the best elitists that are not muted in each generation. Default value is set to 3. elitism the number of best individuals to survive at each generation. By default the top 20% individuals will survive at each iteration. population an R function for randomly generating an initial population. See parsimony_population for available functions. selection an R function performing selection, i.e. a function which generates a new population of individuals from the current population probabilistically according to individual fitness. See parsimony_nlrSelection for available functions. an R function performing crossover, i.e. a function which forms offsprings by crossover combining part of the genetic information from their parents. See parsimony_crossover for available functions. an R function performing mutation, i.e. a function which randomly alters the mutation values of some genes in a parent chromosome. See parsimony_mutation for available functions. keep_history If it is TRUE keeps in the list object@history each generation. This parameter must set TRUE in order to use 'plot' method or 'parsimony_importance' function. path_name_to_save_iter If it is not NULL save the 'ga parsimony' object to the 'path name to save iter' file at the end of each iteration. Note: use extension '.RData', example 'object.RData' the number of consecutive generations without any improvement in the best early_stop fitness value before the GA is stopped. maxFitness the upper bound on the fitness function after that the GA search is interrupted. Default value is set to +Inf a matrix of solutions strings to be included in the initial population. If provided suggestions the number of columns must match (object@nParams+object@nFeatures). Can be used a previous population, for example: 'ga_parsimony@history[[2]]\$population'. a logical argument specifying if parallel computing should be used (TRUE) or parallel not (FALSE, default) for evaluating the fitness function. This argument could also be used to specify the number of cores to employ; by default, this is taken from detectCores. Finally, the functionality of parallelization depends on system OS: on Windows only 'snow' type functionality is available, while on Unix/Linux/Mac OSX both 'snow' and 'multicore' (default) functionalities are available.

| monitor | a logical or an R function which takes as input the current state of the ga_parsimony-class object and show the evolution of the search. By default, for interactive sessions, |
|----------|--|
| | the function parsimony_monitor depending on whether or not is an RStudio |
| | session, prints the average and best fitness values at each iteration. If set to plot |
| | these information are plotted on a graphical device. Other functions can be writ- |
| | ten by the user and supplied as argument. In non interactive sessions, by default |
| | monitor = FALSE so any output is suppressed. |
| seed_ini | an integer value containing the random number generator state. This argument can be used to replicate the results of a GA search. Note that if parallel computing is required, the doRNG package must be installed. |
| verbose | if it is TRUE shows additional information for debugging. |

Details

GAparsimony package is a new GA wrapper automatic procedure that efficiently generated prediction models with reduced complexity and adequate generalization capacity. ga_parsimony function is primarily based on combining feature selection and model parameter tuning with a second novel GA selection process (parsimony_rerank function), in order to achieve better overall parsimonious models. Unlike other GA methodologies that use a penalty parameter for combining loss and complexity measures into a unique fitness function, the main contribution of this package is that ga_parsimony selects the best models by considering cost and complexity separately. For this purpose, the ReRank algorithm rearranges individuals by their complexity when there is not a significant difference between their costs. Thus, less complex models with similar accuracy are promoted. Furthermore, because the penalty parameter is unnecessary, there is no consequent uncertainty associated with assigning a correct value beforehand. As a result, with GA-PARSIMONY, an automatic method for obtaining parsimonious models is finally made possible.

Value

Returns an object of class ga_parsimony-class. See ga_parsimony-class for a description of available slots information.

Author(s)

Francisco Javier Martinez de Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www. mineriadatos.com

References

Urraca R., Sodupe-Ortega E., Antonanzas E., Antonanzas-Torres F., Martinez-de-Pison, F.J. (2017). Evaluation of a novel GA-based methodology for model structure selection: The GA-PARSIMONY. Neurocomputing, Online July 2017. https://doi.org/10.1016/j.neucom.2016.08.154

Sanz-Garcia A., Fernandez-Ceniceros J., Antonanzas-Torres F., Pernia-Espinoza A.V., Martinez-de-Pison F.J. (2015). GA-PARSIMONY: A GA-SVR approach with feature selection and parameter optimization to obtain parsimonious solutions for predicting temperature settings in a continuous annealing furnace. Applied Soft Computing 35, 23-38.

Fernandez-Ceniceros J., Sanz-Garcia A., Antonanzas-Torres F., Martinez-de-Pison F.J. (2015). A numerical-informational approach for characterising the ductile behaviour of the T-stub component. Part 2: Parsimonious soft-computing-based metamodel. Engineering Structures 82, 249-260.

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Antonanzas-Torres F., Urraca R., Antonanzas J., Fernandez-Ceniceros J., Martinez-de-Pison F.J. (2015). Generation of daily global solar irradiation with support vector machines for regression. Energy Conversion and Management 96, 277-286.

See Also

ga_parsimony-class, summary.ga_parsimony, plot.ga_parsimony, parsimony_Population, parsimony_Selection, parsimony_Crossover, parsimony_Mutation, parsimony_importance, parsimony_rerank.

Examples

```
### Example 1: Classification ###
# This a toy example that shows how to search, for the *iris* database,
# a parsimony classification NNET model with 'GAparsimony'
# and 'caret' packages. Validation errors and iterations have been
# reduced to speedup the process
library(GAparsimony)
# Training and testing Datasets
library(caret)
data(iris)
# Z-score of input features
iris_esc <- data.frame(scale(iris[,1:4]),Species=iris[,5])</pre>
# Define an 70%/30% train_val/test split of the dataset
set.seed(1234)
inTraining <- createDataPartition(iris_esc$Species, p=.70, list=FALSE)</pre>
data_train <- iris_esc[ inTraining,]</pre>
data_test <- iris_esc[-inTraining,]</pre>
# Function to evaluate each SVM individual
# _____
fitness_SVM <- function(chromosome, ...)</pre>
{
# First two values in chromosome are 'C' & 'sigma' of 'svmRadial' method
tuneGrid <- data.frame(C=chromosome[1],sigma=chromosome[2])</pre>
# Next values of chromosome are the selected features (TRUE if > 0.50)
selec_feat <- chromosome[3:length(chromosome)]>0.50
# Return -Inf if there is not selected features
if (sum(selec_feat)<1) return(c(kappa_val=-Inf,kappa_test=-Inf,complexity=Inf))</pre>
# Extract features from the original DB plus response (last column)
data_train_model <- data_train[,c(selec_feat,TRUE)]</pre>
data_test_model <- data_test[,c(selec_feat,TRUE)]</pre>
```

```
# Validate each individual with only a 2-CV
# Yo obtain a robust validation measure
# use 'repeatedcv' with more folds and times
# (see 2nd and 3rd examples...)
train_control <- trainControl(method = "cv",number = 5)</pre>
# train the model
set.seed(1234)
model <- train(Species ~ ., data=data_train_model,</pre>
trControl=train_control,
method="svmRadial", metric="Kappa",
tuneGrid=tuneGrid, verbose=FALSE)
# Extract validation and test accuracy
accuracy_val <- model$results$Accuracy</pre>
accuracy_test <- postResample(pred=predict(model, data_test_model),</pre>
obs=data_test_model[,ncol(data_test_model)])[2]
# Obtain Complexity = Num_Features*1E6+Number of support vectors
complexity <- sum(selec_feat)*1E6+model$finalModel@nSV</pre>
# Return(validation accuracy, testing accuracy, model_complexity)
vect_errors <- c(accuracy_val=accuracy_val,</pre>
accuracy_test=accuracy_test,complexity=complexity)
return(vect_errors)
}
# -----
# Search the best parsimonious model with GA-PARSIMONY by using Feature Selection,
# Parameter Tuning and Parsimonious Model Selection
# -----
library(GAparsimony)
# Ranges of size and decay
min_param <- c(0.0001, 0.00001)</pre>
max_param <- c(0.9999, 0.99999)</pre>
names_param <- c("C","sigma")</pre>
# ga_parsimony can be executed with a different set of 'rerank_error' values
rerank_error <- 0.001
GAparsimony_model <- ga_parsimony(fitness=fitness_SVM,
                                min_param=min_param,
                                max_param=max_param,
                                names_param=names_param,
                                nFeatures=ncol(data_train)-1,
                               names_features=colnames(data_train)[-ncol(data_train)],
                                keep_history = TRUE,
                                rerank_error = rerank_error,
```

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```
popSize = 20,
                                maxiter = 20,
                                early_stop=7,
                                feat_thres=0.90,# Perc selec features in first iter
                               feat_mut_thres=0.10,# Prob. feature to be 1 in mutation
                                not_muted=1,
                            parallel = FALSE, # speedup with 'n' cores or all with TRUE
                                seed_ini = 1234)
print(paste0("Best Parsimonious SVM with C=",
  GAparsimony_model@bestsolution['C'],
  " sigma=",
  GAparsimony_model@bestsolution['sigma'],
  "   ->  ",
  " AccuracyVal=",
  round(GAparsimony_model@bestsolution['fitnessVal'],6),
  " AccuracyTest=",
  round(GAparsimony_model@bestsolution['fitnessTst'],6),
  " Num Features=",
  round(GAparsimony_model@bestsolution['complexity']/1E6,0),
   " Complexity=",
  round(GAparsimony_model@bestsolution['complexity'],2)))
print(summary(GAparsimony_model))
print(parsimony_importance(GAparsimony_model))
 ### Example 2: Classification ###
 #This example shows how to search, for the *Sonar* database,
 #a parsimony classification SVM model with 'GAparsimony' and 'caret' packages.
 # Training and testing Datasets
 library(caret)
 library(GAparsimony)
 library(mlbench)
 data(Sonar)
 set.seed(1234)
 inTraining <- createDataPartition(Sonar$Class, p=.80, list=FALSE)</pre>
 data_train <- Sonar[ inTraining,]</pre>
 data_test <- Sonar[-inTraining,]</pre>
 # Function to evaluate each SVM individual
 # _____
 fitness_SVM <- function(chromosome, ...)</pre>
 {
```

First two values in chromosome are 'C' & 'sigma' of 'svmRadial' method

```
tuneGrid <- data.frame(C=chromosome[1],sigma=chromosome[2])</pre>
  # Next values of chromosome are the selected features (TRUE if > 0.50)
  selec_feat <- chromosome[3:length(chromosome)]>0.50
  # Return -Inf if there is not selected features
  if (sum(selec_feat)<1) return(c(kappa_val=-Inf,kappa_test=-Inf,complexity=Inf))</pre>
  # Extract features from the original DB plus response (last column)
 data_train_model <- data_train[,c(selec_feat,TRUE)]</pre>
  data_test_model <- data_test[,c(selec_feat,TRUE)]</pre>
  # How to validate each individual
  # 'repeats' could be increased to obtain a more robust validation metric. Also,
  # 'number' of folds could be adjusted to improve the measure.
  train_control <- trainControl(method = "repeatedcv",number = 10,repeats = 10)</pre>
  # train the model
  set.seed(1234)
 model <- train(Class ~ ., data=data_train_model, trControl=train_control,</pre>
                method="svmRadial", metric="Kappa",
 tuneGrid=tuneGrid, verbose=FALSE)
  # Extract kappa statistics (repeated k-fold CV and testing kappa)
 kappa_val <- model$results$Kappa</pre>
  kappa_test <- postResample(pred=predict(model, data_test_model),</pre>
                 obs=data_test_model[,ncol(data_test_model)])[2]
  # Obtain Complexity = Num_Features*1E6+Number of support vectors
  complexity <- sum(selec_feat)*1E6+model$finalModel@nSV</pre>
  # Return(validation error, testing error, model_complexity)
 vect_errors <- c(kappa_val=kappa_val,kappa_test=kappa_test,complexity=complexity)</pre>
  return(vect_errors)
# _____
# Search the best parsimonious model with GA-PARSIMONY by using Feature Selection,
# Parameter Tuning and Parsimonious Model Selection
# _____
library(GAparsimony)
# Ranges of size and decay
min_param <- c(00.0001, 0.00001)</pre>
max_param <- c(99.9999, 0.99999)</pre>
names_param <- c("C","sigma")</pre>
# ga_parsimony can be executed with a different set of 'rerank_error' values
rerank_error <- 0.001</pre>
# 40 individuals per population, 100 max generations with an early stopping
```

```
# of 10 generations (CAUTION! 7.34 minutes with 8 cores)!!!!!
GAparsimony_model <- ga_parsimony(fitness=fitness_SVM,</pre>
```

}

set.seed(1234)

```
min_param=min_param,
                                 max_param=max_param,
                                 names_param=names_param,
                                 nFeatures=ncol(data_train)-1,
                              names_features=colnames(data_train)[-ncol(data_train)],
                                 keep_history = TRUE,
                                 rerank_error = rerank_error,
                                 popSize = 40,
                                 maxiter = 100,
                                 early_stop=10,
                                 feat_thres=0.90,# Perc selec features in first iter
                               feat_mut_thres=0.10,# Prob. feature to be 1 in mutation
                                 parallel = TRUE, seed_ini = 1234)
print(paste0("Best Parsimonious SVM with C=",
             GAparsimony_model@bestsolution['C'],
             " sigma=",
             GAparsimony_model@bestsolution['sigma'],
             " −> ",
             " KappaVal=",
             round(GAparsimony_model@bestsolution['fitnessVal'],6),
             " KappaTst=",
             round(GAparsimony_model@bestsolution['fitnessTst'],6),
             " Num Features=",
             round(GAparsimony_model@bestsolution['complexity']/1E6,0),
             " Complexity=",
             round(GAparsimony_model@bestsolution['complexity'],2)))
print(summary(GAparsimony_model))
# Plot GA evolution ('keep_history' must be TRUE)
elitists <- plot(GAparsimony_model)</pre>
# Percentage of appearance of each feature in elitists
print(parsimony_importance(GAparsimony_model))
### Example 3: Regression ###
# This example shows how to search, for the *Boston* database, a parsimony regressor ANN
# model with 'GAparsimony' and 'caret' packages.
# Load Boston database and scale it
library(MASS)
data(Boston)
Boston_scaled <- data.frame(scale(Boston))</pre>
# Define an 80%/20% train/test split of the dataset
```

```
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```

```
trainIndex <- createDataPartition(Boston[,"medv"], p=0.80, list=FALSE)</pre>
data_train <- Boston_scaled[trainIndex,]</pre>
data_test <- Boston_scaled[-trainIndex,]</pre>
# Restore 'Response' to original values
data_train[,ncol(data_train)] <- Boston$medv[trainIndex]</pre>
data_test[,ncol(data_test)] <- Boston$medv[-trainIndex]</pre>
print(dim(data_train))
print(dim(data_test))
# Function to evaluate each ANN individual
# ------
fitness_NNET <- function(chromosome, ...)</pre>
ł
  # First two values in chromosome are 'size' & 'decay' of 'nnet' method
  tuneGrid <- data.frame(size=round(chromosome[1]),decay=chromosome[2])</pre>
  # Next values of chromosome are the selected features (TRUE if > 0.50)
  selec_feat <- chromosome[3:length(chromosome)]>0.50
  if (sum(selec_feat)<1) return(c(rmse_val=-Inf,rmse_test=-Inf,complexity=Inf))</pre>
  # Extract features from the original DB plus response (last column)
  data_train_model <- data_train[,c(selec_feat,TRUE)]</pre>
  data_test_model <- data_test[,c(selec_feat,TRUE)]</pre>
  # How to validate each individual
  # 'repeats' could be increased to obtain a more robust validation metric. Also,
  # 'number' of folds could be adjusted to improve the measure.
  train_control <- trainControl(method = "repeatedcv",number = 10,repeats = 5)</pre>
  # train the model
  set.seed(1234)
  model <- train(medv ~ ., data=data_train_model, trControl=train_control,</pre>
                method="nnet", tuneGrid=tuneGrid, trace=FALSE, linout = 1)
  # Extract errors
  rmse_val <- model$results$RMSE</pre>
  rmse_test <- sqrt(mean((unlist(predict(model, newdata = data_test_model)) -</pre>
                          data_test_model$medv)^2))
  # Obtain Complexity = Num_Features*1E6+sum(neural_weights^2)
  complexity <- sum(selec_feat)*1E6+sum(model$finalModel$wts*model$finalModel$wts)</pre>
  # Return(-validation error, -testing error, model_complexity)
  # errors are negative because GA-PARSIMONY tries to maximize values
 vect_errors <- c(rmse_val=-rmse_test=-rmse_test, complexity=complexity)</pre>
  return(vect_errors)
}
# _____
# Search the best parsimonious model with GA-PARSIMONY by using Feature Selection,
# Parameter Tuning and Parsimonious Model Selection
# _____
library(GAparsimony)
```

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```
# Ranges of size and decay
min_param <- c(1, 0.0001)</pre>
max_param <- c(25, 0.9999)
names_param <- c("size","decay")</pre>
# ga_parsimony can be executed with a different set of 'rerank_error' values
rerank_error <- 0.01</pre>
# 40 individuals per population, 100 max generations with an early stopping
# of 10 generations (CAUTION! 33.89 minutes with 8 cores)!!!!!
GAparsimony_model <- ga_parsimony(fitness=fitness_NNET,</pre>
                                   min_param=min_param,
                                   max_param=max_param,
                                   names_param=names_param,
                                   nFeatures=ncol(data_train)-1,
                                names_features=colnames(data_train)[-ncol(data_train)],
                                   keep_history = TRUE,
                                   rerank_error = rerank_error,
                                   popSize = 40,
                                   maxiter = 100, # Change to 100
                                   early_stop=10,
                                   feat_thres=0.90,# Perc selec features in first iter
                                feat_mut_thres=0.10,# Prob. feature to be 1 in mutation
                                   not_muted=2,
                                   parallel = TRUE, seed_ini = 1234)
print(paste0("Best Parsimonious ANN with ",
             round(GAparsimony_model@bestsolution['size']),
             " hidden neurons and decay=",
             GAparsimony_model@bestsolution['decay'],
             " −> ",
             " RMSEVal=",
             round(-GAparsimony_model@bestsolution['fitnessVal'],6),
             " RMSETst=",
             round(-GAparsimony_model@bestsolution['fitnessTst'],6)))
print(summary(GAparsimony_model))
# Plot GA evolution ('keep_history' must be TRUE)
elitists <- plot(GAparsimony_model)</pre>
# Percentage of appearance of each feature in elitists
print(parsimony_importance(GAparsimony_model))
```

Description

An S4 class for searching parsimonious models by feature selection and parameter tuning with genetic algorithms.

Objects from the Class

Objects can be created by calls to the ga_parsimony function.

Slots

- call an object of class "call" representing the matched call;
- min_param a vector of length equal to the model parameters providing the minimum of the search space;
- max_param a vector of length equal to the model parameters providing the maximum of the search space;
- nParams a value specifying the number of model parameter to be tuned;
- feat_thres proportion of selected features in the initial population. It is recommended a high percentage of selected features for the first generations;
- feat_mut_thres threshold to consider a random number between 0 and 1 is considered one if a value of the parameters-chromosome is muted. Default value is set to 0.5;
- not_muted number of the best elitists that are not muted. Default value is set to 3;
- rerank_error when a value distinct to zero is provided a second reranking process according to the model complexities is called by 'parsimonyReRank' function. Its primary objective is to select individuals with high validation cost while maintaining the robustness of a parsimonious model. This function switches the position of two models if the first one is more complex than the latter and no significant difference is found between their fitness values in terms of cost. Therefore, if the absolute difference between the validation costs are lower than 'rerank_error' they are considered similar. Default value=0.01;
- nFeatures a value specifying the number of maximum input features;
- names_param a vector with the name of the model parameters;
- names_features a vector with the name of the input features;
- popSize the population size;
- iter the actual (or final) iteration of GA search;
- iter_start_rerank iteration when ReRanking process is actived. Default=0. Sometimes is useful not to use ReRanking process in the first generations;
- early_stop the number of consecutive generations without any improvement in the best fitness value before the GA is stopped;
- maxiter the maximum number of iterations to run before the GA search is halted;

minutes_gen elapsed time of this generation (in minutes);

minutes_total total elapsed time (in minutes);

suggestions a matrix of user provided solutions and included in the initial population;

population the current (or final) population;

elitism the number of best fitness individuals to survive at each generation; pcrossover the crossover probability; pmutation the mutation probability; best_score the best validation score in the whole GA process; solution_best_score Solution with the best validation score in the whole GA process; fitnessval the values of validation cost for the current (or final) population; fitnesstst the values of testing cost for the current (or final) population; complexity the values of model complexities for the current (or final) population; summary a matrix of summary statistics for fitness values at each iteration (along the rows); bestSolList a list with the best solution of all iterations; bestfitnessTst the testing cost of the best solution at the last iteration; bestfitnessTst the testing cost of the best solution at the last iteration; bestcomplexity the model complexity of the best solution at the last iteration; bestsolution the best solution of all iteration;

Author(s)

Francisco Javier Martinez-de-Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www.mineriadatos.com

See Also

For examples of usage see ga_parsimony.

matrixNULL-class Virtual Class "matrixNULL" - Simple Class for matrix or NULL

Description

The class "matrixNULL" is a simple class union (setClassUnion) of "matrix" and "NULL".

Objects from the Class

Since it is a virtual Class, no objects may be created from it.

Examples

showClass("matrixNULL")

numericOrNA-class

Description

The class "numericOrNA" is a simple class union (setClassUnion) of "numeric" and "logical".

Objects from the Class

Since it is a virtual Class, no objects may be created from it.

Examples

```
showClass("numericOrNA")
```

parsimony_crossover Crossover operators in GA-PARSIMONY

Description

Functions implementing particular crossover genetic operator for GA-PARSIMONY. Method uses for model parameters Heuristic Blending and random swapping for binary selected features.

Usage

```
parsimony_crossover(object, parents, alpha=0.1, perc_to_swap=0.5, ...)
```

Arguments

| object | An object of class "ga_parsimony", usually resulting from a call to function ga_parsimony. |
|--------------|--|
| parents | A two-rows matrix of values indexing the parents from the current population. |
| alpha | A tuning parameter for the Heuristic Blending outer bounds [Michalewicz, 1991]. Typical and default value is 0.1. |
| perc_to_swap | Percentage of features for swapping in the crossovering process. |
| | Further arguments passed to or from other methods. |

Value

Return a list with two elements:

| children | Matrix of dimension 2 times the number of decision variables containing the generated offsprings; |
|------------|--|
| fitnessval | Vector of length 2 containing the fitness validation values for the offsprings. A value NA is returned if an offspring is different (which is usually the case) from the two parents. |
| fitnesstst | Vector of length 2 containing the fitness with the test database (if it was supplied), for the offsprings. A value NA is returned if an offspring is different (which is usually the case) from the two parents. |
| complexity | Vector of length 2 containing the model complexity for the offsprings. A value NA is returned if an offspring is different (which is usually the case) from the two parents. |

Author(s)

Francisco Javier Martinez de Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www. mineriadatos.com

See Also

ga_parsimony

parsimony_importance Percentage of appearance of each feature in elitist population

Description

Shows the percentage of appearance of each feature in the whole GA-PARSIMONY process but only for the elitist-population.

Usage

```
parsimony_importance(object, verbose=FALSE, ...)
```

Arguments

| object | An object of class "ga_parsimony" resulting from a call to function ga_parsimony with keep_history parameter set to TRUE. |
|---------|---|
| | with keep_history parameter set to TKOE. |
| verbose | If it is TRUE shows additional information. |
| | Further arguments passed to or from other methods. |

Details

parsimony_importance extracts elistist population from all generations. Obtains the percentage of appearance of each feature in the all GA process. Return the features higher-ordered.

Value

Return a vector with the higher-ordered percentage of appearance of each feature in the elitist-population and in the whole GA process.

Author(s)

Francisco Javier Martinez de Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www. mineriadatos.com

See Also

ga_parsimony

parsimony_monitor Functions for monitoring GA-PARSIMONY algorithm evolution

Description

Functions to print summary statistics of fitness values at each iteration of a GA search.

Usage

```
parsimony_monitor(object, digits = getOption("digits"), ...)
```

Arguments

| object | An object of class "ga_parsimony", usually resulting from a call to function ga_parsimony. |
|--------|--|
| digits | minimal number of significant digits. |
| | Further arguments passed to or from other methods. |

Value

These functions print a summary of current GA-PARSIMONY step on the console.

Author(s)

Francisco Javier Martinez de Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www. mineriadatos.com parsimony_Mutation Mutation operators in GA-PARSIMONY

Description

Functions implementing mutation genetic operator for GA-PARSIMONY. Method mutes a object@pmutation percentage of them. If the value corresponds to a model parameter, algorithm uses uniform random mutation. For binary select features, method sets to one if the random value between [0,1] is lower or equal to object@feat_mut_thres.

Usage

```
parsimony_mutation(object, ...)
```

Arguments

| object | An object of class "ga_parsimony", usually resulting from a call to function |
|--------|--|
| | ga_parsimony. |
| | Further arguments passed to or from other methods. |

Value

Return object with the population muted.

Author(s)

Francisco Javier Martinez de Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www. mineriadatos.com

See Also

ga_parsimony

parsimony_Population Population initialization in GA-PARSIMONY with a combined chromosome of model parameters and selected features

Description

Functions for creating an initial population to be used in the GA-PARSIMONY process.

Usage

```
parsimony_population(object, type_ini_pop="randomLHS", ...)
```

Arguments

| object | An object of class "ga_parsimony", usually resulting from a call to function ga_parsimony. |
|--------------|--|
| type_ini_pop | How to create the initial population. 'random' optiom initialize a random popu- lation between the predefined ranges. Values 'randomLHS', 'geneticLHS', 'im- provedLHS', 'maximinLHS' & 'optimumLHS' corresponds with several meth- ods of the Latin Hypercube Sampling (see 'lhs' package for more details). |
| | Further arguments passed to or from other methods. |

Details

parsimony_population generates a random population of object@popSize individuals. For each individual a random chromosome is generated with object@nParams real values in the range [object@min_param, object@max_param] plus object@nFeatures random binary values for feature selection. 'random' or Latin Hypercube Sampling can be used to create a efficient spread initial population.

Value

Return a matrix of dimension object@popSize rows and object@nParams+object@nFeatures columns.

Author(s)

Francisco Javier Martinez de Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www.mineriadatos.com

See Also

ga_parsimony

| parsimony_rerank | Function for reranking by complexity in parsimonious model selection |
|------------------|--|
| | process |

Description

Promotes models with similar fitness but lower complexity to top positions.

Usage

parsimony_rerank(object, verbose=FALSE, ...)

Arguments

| object | An object of class "ga_parsimony" resulting from a call to function ga_parsimony with keep_history parameter set to TRUE. |
|---------|---|
| verbose | If it is TRUE shows additional information. |
| | Further arguments passed to or from other methods. |

Details

This method corresponds with the second step of parsimonious model selection (PMS) procedure. PMS works in the following way: in each GA generation, best solutions are first sorted by their cost, J. Then, in a second step, individuals with less complexity are moved to the top positions when the absolute difference of their J is lower than a object@rerank_error threshold value. Therefore, the selection of less complex solutions among those with similar accuracy promotes the evolution of robust solutions with better generalization capabilities.

Value

Return a vector with the new position of the individuals.

Author(s)

Francisco Javier Martinez de Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www.mineriadatos.com

See Also

ga_parsimony

Examples

parsimony_Selection Selection operators in GA-PARSIMONY

Description

Functions implementing selection genetic operator in GA-PARSIMONY after parsimony_rerank process. Linear-rank or Nonlinear-rank selection (Michalewicz (1996)).

Usage

```
parsimony_lrSelection(object, r = 2/(object@popSize*(object@popSize-1)),
q = 2/object@popSize, ...)
parsimony_nlrSelection(object, q = 0.25, ...)
```

Arguments

| object | An object of class "ga_parsimony", usually resulting from a call to function ga_parsimony. |
|--------|--|
| r | A tuning parameter for the specific selection operator. |
| q | A tuning parameter for the specific selection operator. |
| | Further arguments passed to or from other methods. |

Value

Return a list with four elements:

| population | a matrix of dimension object@popSize times the number of decision variables containing the selected individuals or strings; |
|------------|---|
| fitnessval | a vector of length object@popSize containing the fitness validation values for the selected individuals; |
| fitnesstst | a vector of length object@popSize containing the fitness with the test database (if it was supplied), for the selected individuals; |
| complexity | a vector of length object@popSize containing the model complexity for the selected individuals. |

Author(s)

Francisco Javier Martinez de Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www. mineriadatos.com

See Also

ga_parsimony

plot.ga_parsimony-method

Plot of GA evolution of elitists

Description

The plot method for ga_parsimony-class objects gives a evolution plot of the validation and testing errors, and the number of model features selected of elitists.

Usage

```
## S4 method for signature 'ga_parsimony'
plot(x, general_cex = 0.7, min_ylim=NULL, max_ylim=NULL,
min_iter=NULL, max_iter=NULL,
main_label="Boxplot cost evolution",
iter_auto_ylim=3, steps=5, pos_cost_num=-3.1,
pos_feat_num=-1.7, digits_plot=4, width_plot=12,
height_plot=6, window=TRUE, ...)
```

Arguments

| х | An object of class "ga_parsimony". |
|---------------------|--|
| general_cex | Main text scale. |
| min_ylim | Min limit on the y-axis. |
| max_ylim | Max limit on the y-axis. |
| min_iter | Min GA iteration to visualize. |
| <pre>max_iter</pre> | Max GA iteration to visualize. |
| main_label | Main plot title. |
| iter_auto_ylim | If it is not NULL, GA iteration to choose the min limit of y-axis. |
| steps | Number of divisions in y-axis. |
| pos_cost_num | Relative position of numbers in cost axis. |
| pos_feat_num | Relative position of numbers in feature axis. |
| digits_plot | Number of digits to visualize. |
| width_plot | Figure width in inches. |
| height_plot | Figure height in inches. |
| window | If TRUE shows a new window. |
| | Further arguments, currently not used. |

Details

Plot method shows the evolution of validation and testing errors, and the number of model features selected of elitists. White and grey box-plots represent validation and testing errors of elitists evolution, respectively. Continuous and dashed-dotted lines show the validation and testing error of the best individual for each generation, respectively. Finally, the shaded area delimits the maximum and minimum number of features, and the dashed line, the number fo features of the best individual.

Value

The method invisibly return a list with the elistists validation error, testing error and model complexity in the whole GA process.

Author(s)

Francisco Javier Martinez de Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www. mineriadatos.com

See Also

ga_parsimony, ga_parsimony-class.

summary.ga_parsimony-method
 Summary for GA-PARSIMONY

Description

Summary method for class ga_parsimony-class.

Usage

```
## S4 method for signature 'ga_parsimony'
summary(object, ...)
## S3 method for class 'summary.ga_parsimony'
print(x, digits = getOption("digits"), ...)
```

Arguments

| an object of class ga_parsimony-class. |
|--|
| an object of class summary.ga_parsimony. |
| number of significant digits. |
| further arguments passed to or from other methods. |
| |

Value

The summary function returns an object of class ga_parsimony-class which can be printed by the corresponding print method. The function also returns invisibly a list with the information from the genetic algorithm search.

Author(s)

Francisco Javier Martinez de Pison. <fjmartin@unirioja.es>. EDMANS Group. http://www. mineriadatos.com

See Also

ga_parsimony

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