Package 'SuperLearner'

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```
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Maintainer Eric Polley <polley.eric@mayo.edu>
Description Implements the super learner prediction method and contains a
      library of prediction algorithms to be used in the super learner.
License GPL-3
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      genefilter, ggplot2, glmnet, ipred, KernelKnn, kernlab, knitr,
      lattice, LogicReg, MASS, mlbench, nloptr, nnet, party,
      polspline, prettydoc, quadprog, randomForest, ranger,
      RhpcBLASctl, ROCR, rmarkdown, rpart, SIS, speedglm, spls, sva,
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VignetteBuilder knitr, rmarkdown
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```

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R topics documented:

create.Learner	. 3
create.SL.xgboost	
CV.SuperLearner	. 5
CVFolds	. 9
istWrappers	. 9
olot.CV.SuperLearner	. 10
predict.SL.bartMachine	. 11
predict.SL.biglasso	
predict.SL.extraTrees	
predict.SL.glm	
predict.SL.glmnet	
predict.SL.kernelKnn	. 14
predict.SL.ksvm	
predict.SL.lda	
predict.SL.lm	
predict.SL.qda	
predict.SL.ranger	
predict.SL.speedglm	. 17
predict.SL.speedlm	. 18
predict.SL.xgboost	. 18
predict.SuperLearner	. 19
recombineCVSL	. 20
recombineSL	. 23
SampleSplitSuperLearner	. 26
SL.bartMachine	. 30
SL.biglasso	
SL.cforest	
SL.extraTrees	
SL.glm	
SL.glmnet	
SL.kernelKnn	
SL.ksvm	
SL.lda	
SL.lm	
SL.qda	
SL.ranger	
SL.speedglm	
SL.speedlm	
SL.xgboost	
summary.CV.SuperLearner	
SuperLearner	
SuperLearner.control	
SuperLearner.CV.control	
SuperLearnerNews	
rimLogit	
write.method.template	. 58

create.Learner 3

$\label{eq:write.SL.template} write. SL. template \ .$ Index				•	• •		•	•	•	•	•	•	 •	•	•	•	٠	•	•	•	•	٠	٠	•	• •	62
create.Learner	Facto	ory J	for	lea	ırne	er w	vra	ірр	er	·s																

Description

Create custom learners and/or a sequence of learners with hyperparameter combinations defined over a grid.

Usage

```
create.Learner(base_learner, params = list(), tune = list(),
  env = parent.frame(), name_prefix = base_learner, detailed_names = F,
  verbose = F)
```

Arguments

base_learner Character string of the learner function that will be customized.

List with parameters to customize.

tune List of hyperparameter settings that will define custom learners.

env Environment in which to create the functions. Defaults to the current environment (e.g. often the global environment).

name_prefix The prefix string for the name of each function that is generated.

detailed_names Set to T to have the function names include the parameter configurations.

verbose Display extra details.

Value

Returns a list with expanded tuneGrid and the names of the created functions.

Examples

4 create.SL.xgboost

create.SL.xgboost

Factory for XGBoost SL wrappers

Description

Create multiple configurations of XGBoost learners based on the desired combinations of hyperparameters.

Usage

```
create.SL.xgboost(tune = list(ntrees = c(1000), max_depth = c(4), shrinkage =
  c(0.1), minobspernode = c(10)), detailed_names = F, env = .GlobalEnv,
  name_prefix = "SL.xgb")
```

Arguments

tune List of hyperparameter settings to test. If specified, each hyperparameter will need to be defined.

detailed_names Set to T to have the function names include the parameter configurations.

env Environment in which to create the SL.xgboost functions. Defaults to the global

environment.

name_prefix The prefix string for the name of each function that is generated.

Examples

```
# Create a new environment to store the learner functions.
# This keeps the global environment organized.
sl_{env} = new.env()
# Create 2 * 2 * 1 * 3 = 12 combinations of hyperparameters.
tune = list(ntrees = c(100, 500), max_depth = c(1, 2), minobspernode = 10,
            shrinkage = c(0.1, 0.01, 0.001)
# Generate a separate learner for each combination.
xgb_grid = create.SL.xgboost(tune = tune, env = sl_env)
# Review the function configurations.
xgb_grid
# Attach the environment so that the custom learner functions can be accessed.
attach(sl_env)
## Not run:
sl = SuperLearner(Y = Y, X = X, SL.library = xgb_grid$names)
## End(Not run)
detach(sl_env)
```

CV.SuperLearner

Function to get V-fold cross-validated risk estimate for super learner

Description

Function to get V-fold cross-validated risk estimate for super learner. This function simply splits the data into V folds and then calls SuperLearner. Most of the arguments are passed directly to SuperLearner.

Usage

```
CV.SuperLearner(Y, X, V = NULL, family = gaussian(), SL.library,
  method = "method.NNLS", id = NULL, verbose = FALSE,
  control = list(saveFitLibrary = FALSE), cvControl = list(),
  innerCvControl = list(),
  obsWeights = NULL, saveAll = TRUE, parallel = "seq", env = parent.frame())
```

Arguments

Y The outcome.

X The covariates.

V The number of folds for CV. SuperLearner. This argument will be depreciated and moved into the cvControl. If Both V and cvControl set the number of cross-validation folds, an error message will appear. The recommendation is to use cvControl. This is not the number of folds for SuperLearner. The number of folds for SuperLearner is controlled with innerCvControl.

family Currently allows gaussian or binomial to describe the error distribution. Link

function information will be ignored and should be contained in the method

argument below.

SL.library Either a character vector of prediction algorithms or a list containing character vectors. See details below for examples on the structure. A list of functions

included in the SuperLearner package can be found with listWrappers().

method A list (or a function to create a list) containing details on estimating the coeffi-

cients for the super learner and the model to combine the individual algorithms in the library. See ?method. template for details. Currently, the built in options are either "method.NNLS" (the default), "method.NNLS2", "method.NNloglik", "method.CC_LS", "method.CC_nloglik", or "method.AUC". NNLS and NNLS2 are non-negative least squares based on the Lawson-Hanson algorithm and the dual method of Goldfarb and Idnani, respectively. NNLS and NNLS2 will work for both gaussian and binomial outcomes. NNloglik is a non-negative binomial likelihood maximization using the BFGS quasi-Newton optimization method. NN* methods are normalized so weights sum to one. CC_LS uses Goldfarb and Idnani's quadratic programming algorithm to calculate the best convex combination of weights to minimize the squared error loss. CC_nloglik calculates the convex combination of weights that minimize the negative binomial log likelihood on the logistic scale using the sequential quadratic programming algorithm. AUC, which only works for binary outcomes, uses the Nelder-Mead

AUC).

Optional cluster identification variable. For the cross-validation splits, id forces observations in the same cluster to be in the same validation fold. id is passed to the prediction and screening algorithms in SL.library, but be sure to check the

method via the optim function to minimize rank loss (equivalent to maximizing

individual wrappers as many of them ignore the information.

verbose Logical; TRUE for printing progress during the computation (helpful for debug-

ging).

A list of parameters to control the estimation process. Parameters include saveFitLibrary

and trimLogit. See SuperLearner.control for details.

cvControl A list of parameters to control the outer cross-validation process. The outer

> cross-validation is the sample spliting for evaluating the SuperLearner. Parameters include V, stratifyCV, shuffle and validRows. See SuperLearner. CV.control

for details.

innerCvControl A list of lists of parameters to control the inner cross-validation process. It

should have V elements in the list, each a valid cvControl list. If only a single value, then replicated across all folds. The inner cross-validation are the values passed to each of the V SuperLearner calls. Parameters include V, stratifyCV,

shuffle and validRows. See SuperLearner.CV.control for details.

obsWeights Optional observation weights variable. As with id above, obsWeights is passed

to the prediction and screening algorithms, but many of the built in wrappers ignore (or can't use) the information. If you are using observation weights,

make sure the library you specify uses the information.

saveAll Logical; Should the entire SuperLearner object be saved for each fold?

id

control

parallel Options for parallel computation of the V-fold step. Use "seq" (the default) for

sequential computation. parallel = 'multicore' to use mclapply for the V-fold step (but note that SuperLearner() will still be sequential). The default for mclapply is to check the mc.cores option, and if not set to default to 2 cores. Be sure to set options()\$mc.cores to the desired number of cores if you don't want the default. Or parallel can be the name of a snow cluster and will use parLapply for the V-fold step. For both multicore and snow, the inner

SuperLearner calls will be sequential.

env Environment containing the learner functions. Defaults to the calling environ-

ment.

Details

The SuperLearner function builds a estimator, but does not contain an estimate on the performance of the estimator. Various methods exist for estimator performance evaluation. If you are familiar with the super learner algorithm, it should be no surprise we recommend using cross-validation to evaluate the honest performance of the super learner estimator. The function CV. SuperLearner computes the usual V-fold cross-validated risk estimate for the super learner (and all algorithms in SL.1ibrary for comparison).

Value

An object of class CV. SuperLearner (a list) with components:

call The matched call.

AllSL If saveAll = TRUE, a list with output from each call to SuperLearner, otherwise

NULL.

SL.predict The predicted values from the super learner when each particular row was part

of the validation fold.

discreteSL.predict

The traditional cross-validated selector. Picks the algorithm with the smallest cross-validated risk (in super learner terms, gives that algorithm coefficient 1

and all others 0).

whichDiscreteSL

A list of length V. The elements in the list are the algorithm that had the smallest cross-validated risk estimate for that fold.

library.predict

A matrix with the predicted values from each algorithm in SL.1ibrary. The columns are the algorithms in SL.1ibrary and the rows represent the predicted values when that particular row was in the validation fold (i.e. not used to fit

that estimator).

coef A matrix with the coefficients for the super learner on each fold. The columns

are the algorithms in SL.library the rows are the folds.

folds A list containing the row numbers for each validation fold.

V Number of folds for CV. SuperLearner.

libraryNames A character vector with the names of the algorithms in the library. The format is

'predictionAlgorithm_screeningAlgorithm' with '_All' used to denote the pre-

diction algorithm run on all variables in X.

SL.library Returns SL.library in the same format as the argument with the same name above.

Method A list with the method functions.

Y The outcome

Author(s)

Eric C Polley <polley.eric@mayo.edu>

See Also

SuperLearner

Examples

```
## Not run:
set.seed(23432)
## training set
n <- 500
p < -50
X <- matrix(rnorm(n*p), nrow = n, ncol = p)</pre>
colnames(X) <- paste("X", 1:p, sep="")</pre>
X <- data.frame(X)</pre>
Y \leftarrow X[, 1] + sqrt(abs(X[, 2] * X[, 3])) + X[, 2] - X[, 3] + rnorm(n)
## build Library and run Super Learner
SL.library <- c("SL.glm", "SL.randomForest", "SL.gam", "SL.polymars", "SL.mean")
test <- CV.SuperLearner(Y = Y, X = X, V = 10, SL.library = SL.library,
  verbose = TRUE, method = "method.NNLS")
test
summary(test)
## Look at the coefficients across folds
coef(test)
# Example with specifying cross-validation options for both
# CV.SuperLearner (cvControl) and the internal SuperLearners (innerCvControl)
test <- CV.SuperLearner(Y = Y, X = X, SL.library = SL.library,</pre>
  cvControl = list(V = 10, shuffle = FALSE),
  innerCvControl = list(list(V = 5)),
  verbose = TRUE, method = "method.NNLS")
## examples with snow
library(parallel)
cl <- makeCluster(2, type = "PSOCK") # can use different types here</pre>
clusterSetRNGStream(cl, iseed = 2343)
testSNOW <- CV.SuperLearner(Y = Y, X = X, SL.library = SL.library, method = "method.NNLS",
  parallel = cl)
summary(testSNOW)
stopCluster(cl)
## End(Not run)
```

CVFolds 9

CVFolds Generate list of row numbers for each fold in the cross-validation	Generate list of row numbers for each fold in the cross-validation
--	--

Description

Generate list of row numbers for each fold in the cross-validation. CVFolds is used in the SuperLearner to create the cross-validation splits.

Usage

```
CVFolds(N, id, Y, cvControl)
```

Arguments

N	Sample size

id Optional cluster id variable. If present, all observations in the same cluster will

always be in the same split.

Y outcome

cvControl Control parameters for the cross-validation step. See SuperLearner.CV.control

for details.

Value

validRows A list of length V where each element in the list is a vector with the row numbers

of the corresponding validation sample.

Author(s)

Eric C Polley <polley.eric@mayo.edu>

listWrappers	list all wrapper functions in SuperLearner

Description

List all wrapper functions in SuperLearner package

Usage

```
listWrappers(what = "both")
```

Arguments

what

What list to return. Can be both for both prediction algorithms and screening algorithms, SL for the prediction algorithms, screen for the screening algorithms, method for the estimation method details, or anything else will return a list of all (exported) functions in the SuperLearner package. Additional wrapper functions are available at https://github.com/ecpolley/SuperLearnerExtra.

Value

Invisible character vector with all exported functions in the SuperLearner package

Author(s)

```
Eric C Polley <polley.eric@mayo.edu>
```

See Also

SuperLearner

Examples

```
listWrappers(what = "SL")
listWrappers(what = "screen")
```

plot.CV.SuperLearner Graphical display of the V-fold CV risk estimates

Description

The function plots the V-fold cross-validated risk estimates for the super learner, the discrete super learner and each algorithm in the library. By default the estimates will be sorted and include an asymptotic 95% confidence interval.

Usage

```
## S3 method for class 'CV.SuperLearner'
plot(x, package = "ggplot2", constant = qnorm(0.975), sort = TRUE, ...)
```

Arguments

X	The output from CV. SuperLearner.
package	Either "ggplot2" or "lattice". The package selected must be available.
constant	A numeric value. The confidence interval is defined as p +/- constant * se, where p is the point estimate and se is the standard error. The default is the quantile of the standard normal corresponding to a 95% CI.
sort	Logical. Should the rows in the plot be sorted from the smallest to the largest point estimate. If FALSE, then the order is super learner, discrete super learner, then the estimators in SL.library.
	Additional arguments for summary.CV.SuperLearner

predict.SL.bartMachine 11

Details

see summary.CV.SuperLearner for details on how the estimates are computed

Value

Returns the plot (either a ggplot2 object (class ggplot) or a lattice object (class trellis))

Author(s)

```
Eric C Polley <polley.eric@mayo.edu>
```

See Also

```
summary.CV.SuperLearner and CV.SuperLearner
```

```
predict.SL.bartMachine
```

bartMachine prediction

Description

bartMachine prediction

Usage

```
## S3 method for class 'SL.bartMachine'
predict(object, newdata, family, X = NULL,
    Y = NULL, ...)
```

Arguments

object	SuperLearner object
newdata	Dataframe to predict the outcome
family	"gaussian" for regression, "binomial" for binary classification. (Not used)
X	Covariate dataframe (not used)
Υ	Outcome variable (not used)
	Additional arguments (not used)

12 predict.SL.extraTrees

predict.SL.biglasso
Prediction wrapper for SL.biglasso

Description

Prediction wrapper for SL.biglasso objects.

Usage

```
## S3 method for class 'SL.biglasso'
predict(object, newdata, ...)
```

Arguments

object SL.kernlab object

newdata Dataframe to generate predictions
... Unused additional arguments

See Also

```
SL.biglasso biglasso predict.biglasso
```

predict.SL.extraTrees extraTrees prediction on new data

Description

extraTrees prediction on new data

Usage

```
## S3 method for class 'SL.extraTrees'
predict(object, newdata, family, ...)
```

Arguments

object Model fit object from SuperLearner

newdata Dataframe

family Binomial or gaussian

. . . Any remaining arguments (not used).

predict.SL.glm 13

predict.SL.glm

Prediction for SL.glm

Description

Prediction for SL.glm

Usage

```
## S3 method for class 'SL.glm'
predict(object, newdata, ...)
```

Arguments

object SL.glm object

newdata Dataframe to generate predictions
... Unused additional arguments

See Also

```
{\tt SL.glm\ glm\ predict.glm\ SL.speedglm}
```

predict.SL.glmnet

Prediction for an SL.glmnet object

Description

Prediction for the glmnet wrapper.

Usage

```
## S3 method for class 'SL.glmnet'
predict(object, newdata, remove_extra_cols = T,
   add_missing_cols = T, ...)
```

Arguments

object Result object from SL.glmnet

newdata Dataframe or matrix that will generate predictions.

remove_extra_cols

Remove any extra columns in the new data that were not part of the original

model

add_missing_cols

Add any columns from original data that do not exist in the new data, and set

values to 0.

. . . Any additional arguments (not used).

14 predict.SL.ksvm

See Also

```
SL.glmnet
```

```
predict.SL.kernelKnn Prediction for SL.kernelKnn
```

Description

Prediction for SL.kernelKnn

Usage

```
## S3 method for class 'SL.kernelKnn'
predict(object, newdata, ...)
```

Arguments

object SL.kernelKnn object

newdata Dataframe to generate predictions
... Unused additional arguments

predict.SL.ksvm

Prediction for SL.ksvm

Description

Prediction for SL.ksvm

Usage

```
## S3 method for class 'SL.ksvm'
predict(object, newdata, family, coupler = "minpair", ...)
```

Arguments

object SL.kernlab object

newdata Dataframe to generate predictions

family Gaussian or binomial

coupler Coupling method used in the multiclass case, can be one of minpair or pkpd (see

kernlab package for details). For future usage.

... Unused additional arguments

See Also

SL.ksvm ksvm predict.ksvm

predict.SL.lda 15

predict.SL.lda

Prediction wrapper for SL.lda

Description

Prediction wrapper for SL.lda

Usage

```
## S3 method for class 'SL.lda'
predict(object, newdata, prior = object$object$prior,
  dimen = NULL, method = "plug-in", ...)
```

Arguments

object SL.lda object

newdata Dataframe to generate predictions

prior The prior probabilities of the classes, by default the proportions in the training

set or what was set in the call to lda.

dimen the dimension of the space to be used. If this is less than min(p, ng-1), only the

first dimen discriminant components are used (except for method="predictive"),

and only those dimensions are returned in x.

method This determines how the parameter estimation is handled. With "plug-in" (the

default) the usual unbiased parameter estimates are used and assumed to be correct. With "debiased" an unbiased estimator of the log posterior probabilities is used, and with "predictive" the parameter estimates are integrated out using a

vague prior.

... Unused additional arguments

See Also

```
SL.lda lda predict.lda
```

predict.SL.lm

Prediction for SL.lm

Description

Prediction for SL.lm

Usage

```
## S3 method for class 'SL.lm'
predict(object, newdata, ...)
```

16 predict.SL.qda

Arguments

object SL.lm object

newdata Dataframe to generate predictions
... Unused additional arguments

See Also

```
SL.lmlmpredict.lmSL.speedlm
```

predict.SL.qda

Prediction wrapper for SL.qda

Description

Prediction wrapper for SL.qda

Usage

```
## S3 method for class 'SL.qda'
predict(object, newdata, prior = object$object$prior,
  dimen = NULL, method = "plug-in", ...)
```

Arguments

object SL.lda object

newdata Dataframe to generate predictions

prior The prior probabilities of the classes, by default the proportions in the training

set or what was set in the call to lda.

dimen the dimension of the space to be used. If this is less than min(p, ng-1), only the

first dimen discriminant components are used (except for method="predictive"),

and only those dimensions are returned in x.

method This determines how the parameter estimation is handled. With "plug-in" (the

default) the usual unbiased parameter estimates are used and assumed to be correct. With "debiased" an unbiased estimator of the log posterior probabilities is used, and with "predictive" the parameter estimates are integrated out using a

vague prior.

... Unused additional arguments

See Also

SL.qda qda predict.qda

predict.SL.ranger 17

predict.SL.ranger

Prediction wrapper for ranger random forests

Description

Prediction wrapper for SL.ranger objects.

Usage

```
## S3 method for class 'SL.ranger'
predict(object, newdata, family, num.threads = 1,
  verbose = object$verbose, ...)
```

Arguments

object SL.kernlab object

newdata Dataframe to generate predictions

family Gaussian or binomial

verbose If TRUE output additional information during execution.

... Unused additional arguments

See Also

SL.ranger ranger predict.ranger

predict.SL.speedglm

Prediction for SL.speedglm

Description

Prediction for SL.speedglm

Usage

```
## S3 method for class 'SL.speedglm'
predict(object, newdata, ...)
```

Arguments

object SL.speedglm object

newdata Dataframe to generate predictions
... Unused additional arguments

See Also

```
SL.speedglm speedglm predict.speedglm
```

18 predict.SL.xgboost

Description

Prediction for SL.speedlm, a fast lm()

Usage

```
## S3 method for class 'SL.speedlm'
predict(object, newdata, ...)
```

Arguments

object SL.speedlm object

newdata Dataframe to generate predictions
... Unused additional arguments

See Also

```
SL.speedlm speedlm predict.speedlm SL.speedglm
```

predict.SL.xgboost

XGBoost prediction on new data

Description

XGBoost prediction on new data

Usage

```
## S3 method for class 'SL.xgboost'
predict(object, newdata, family, ...)
```

Arguments

object Model fit object from SuperLearner

newdata Dataframe that will be converted to an xgb.DMatrix

family Binomial or gaussian

. . . Any remaining arguments (not supported though).

predict.SuperLearner 19

predict.SuperLearner Predict method for SuperLearner object

Description

Obtains predictions on a new data set from a SuperLearner fit. May require the original data if one of the library algorithms uses the original data in its predict method.

Usage

```
## S3 method for class 'SuperLearner'
predict(object, newdata, X = NULL, Y = NULL,
    onlySL = FALSE, ...)
```

Arguments

object	Fitted object from SuperLearner
newdata	New X values for prediction
Χ	Original data set used to fit object, if needed by fit object.
Υ	Original outcome used to fit object, if needed by fit object.
onlySL	Logical. If TRUE, only compute predictions for algorithms with non-zero coefficients in the super learner object. Default is FALSE (computes predictions for all algorithms in library).
	Additional arguments passed to the predict.SL.* functions

Details

If newdata is omitted the predicted values from object are returned. Each algorithm in the Super Learner library needs to have a corresponding prediction function with the "predict." prefixed onto the algorithm name (e.g. predict.SL.glm for SL.glm).

Value

```
pred Predicted values from Super Learner fit
library.predict
Predicted values for each algorithm in library
```

Author(s)

```
Eric C Polley <polley.eric@mayo.edu>
```

See Also

SuperLearner

20 recombineCVSL

recombineCVSL

Recombine a CV.SuperLearner fit using a new metalearning method

Description

Function to re-compute the V-fold cross-validated risk estimate for super learner using a new metalearning method. This function takes as input an existing CV.SuperLearner fit and applies the recombineSL fit to each of the V Super Learner fits.

Usage

```
recombineCVSL(object, method = "method.NNloglik", verbose = FALSE,
 saveAll = TRUE, parallel = "seq")
```

Arguments

object

Fitted object from CV. SuperLearner.

method

A list (or a function to create a list) containing details on estimating the coefficients for the super learner and the model to combine the individual algorithms in the library. See ?method.template for details. Currently, the built in options are either "method.NNLS" (the default), "method.NNLS2", "method.NNloglik", "method.CC_LS", "method.CC_nloglik", or "method.AUC". NNLS and NNLS2 are non-negative least squares based on the Lawson-Hanson algorithm and the dual method of Goldfarb and Idnani, respectively. NNLS and NNLS2 will work for both gaussian and binomial outcomes. NNloglik is a non-negative binomial likelihood maximization using the BFGS quasi-Newton optimization method. NN* methods are normalized so weights sum to one. CC_LS uses Goldfarb and Idnani's quadratic programming algorithm to calculate the best convex combination of weights to minimize the squared error loss. CC nloglik calculates the convex combination of weights that minimize the negative binomial log likelihood on the logistic scale using the sequential quadratic programming algorithm. AUC, which only works for binary outcomes, uses the Nelder-Mead method via the optim function to minimize rank loss (equivalent to maximizing

verbose

logical; TRUE for printing progress during the computation (helpful for debugging).

saveAll

Logical; Should the entire SuperLearner object be saved for each fold?

parallel

Options for parallel computation of the V-fold step. Use "seq" (the default) for sequential computation. parallel = 'multicore' to use mclapply for the Vfold step (but note that SuperLearner() will still be sequential). Or parallel can be the name of a snow cluster and will use parLapply for the V-fold step. For both multicore and snow, the inner SuperLearner calls will be sequential.

recombineCVSL 21

Details

The function recombineCVSL computes the usual V-fold cross-validated risk estimate for the super learner (and all algorithms in SL.library for comparison), using a newly specified metalearning method. The weights for each algorithm in SL.library are re-estimated using the new metalearner, however the base learner fits are not regenerated, so this function saves a lot of computation time as opposed to using the CV.SuperLearner function with a new method argument. The output is identical to the output from the CV.SuperLearner function.

Value

An object of class CV. SuperLearner (a list) with components:

call The matched call.

AllSL If saveAll = TRUE, a list with output from each call to SuperLearner, otherwise

NULL.

SL.predict The predicted values from the super learner when each particular row was part

of the validation fold.

discreteSL.predict

The traditional cross-validated selector. Picks the algorithm with the smallest cross-validated risk (in super learner terms, gives that algorithm coefficient 1

and all others 0).

whichDiscreteSL

A list of length V. The elements in the list are the algorithm that had the smallest

cross-validated risk estimate for that fold.

library.predict

A matrix with the predicted values from each algorithm in SL.library. The columns are the algorithms in SL.library and the rows represent the predicted values when that particular row was in the validation fold (i.e. not used to fit

that estimator).

coef A matrix with the coefficients for the super learner on each fold. The columns

are the algorithms in SL. library the rows are the folds.

folds A list containing the row numbers for each validation fold.

V Number of folds for CV. SuperLearner.

libraryNames A character vector with the names of the algorithms in the library. The format is

'predictionAlgorithm_screeningAlgorithm' with '_All' used to denote the pre-

diction algorithm run on all variables in X.

SL.library Returns SL.library in the same format as the argument with the same name

above.

method A list with the method functions.

Y The outcome

Author(s)

Erin LeDell < ledell@berkeley.edu>

22 recombineCVSL

See Also

recombineSL

Examples

```
## Not run:
# Binary outcome example adapted from SuperLearner examples
set.seed(1)
N <- 200
X \leftarrow matrix(rnorm(N*10), N, 10)
X <- as.data.frame(X)</pre>
Y \leftarrow rbinom(N, 1, plogis(.2*X[, 1] + .1*X[, 2] - .2*X[, 3] +
  .1*X[, 3]*X[, 4] - .2*abs(X[, 4]))
SL.library <- c("SL.glmnet", "SL.glm", "SL.knn", "SL.gam", "SL.mean")
# least squares loss function
set.seed(1) # for reproducibility
cvfit_nnls <- CV.SuperLearner(Y = Y, X = X, V = 10, SL.library = SL.library,</pre>
 verbose = TRUE, method = "method.NNLS", family = binomial())
cvfit_nnls$coef
    SL.glmnet_All SL.glm_All SL.knn_All SL.gam_All SL.mean_All
# 1
        0.0000000 0.00000000 0.000000000 0.4143862 0.5856138
# 2
        0.0000000 0.00000000 0.304802397 0.3047478 0.3904498
# 3
        0.0000000 0.00000000 0.002897533 0.5544075 0.4426950
        0.0000000 0.20322642 0.000000000 0.1121891 0.6845845
# 5
        0.1743973 0.00000000 0.032471026 0.3580624 0.4350693
# 6
        0.0000000 0.00000000 0.099881535 0.3662309 0.5338876
        0.0000000 0.00000000 0.234876082 0.2942472 0.4708767
# 7
# 8
        0.0000000 0.06424676 0.113988158 0.5600208
                                                   0.2617443
# 9
        0.0000000 0.00000000 0.338030342 0.2762604
                                                    0.3857093
# 10
        0.3022442 0.00000000 0.294226204 0.1394534
                                                    0.2640762
# negative log binomial likelihood loss function
cvfit_nnloglik <- recombineCVSL(cvfit_nnls, method = "method.NNloglik")</pre>
cvfit_nnloglik$coef
    SL.glmnet_All SL.glm_All SL.knn_All SL.gam_All SL.mean_All
# 1
        0.0000000 0.0000000 0.00000000 0.5974799 0.40252010
# 2
        0.0000000 0.0000000 0.31177345 0.6882266 0.00000000
# 3
        0.0000000 0.0000000 0.01377469 0.8544238 0.13180152
# 4
        0.0000000 0.1644188 0.00000000 0.2387919 0.59678930
# 5
        0.2142254 0.0000000 0.00000000 0.3729426 0.41283197
# 6
        0.0000000 0.0000000 0.00000000 0.5847150
                                                  0.41528502
# 7
        0.0000000 0.0000000 0.47538172 0.5080311
                                                  0.01658722
# 8
        # 9
        0.0000000 0.0000000 0.45384961 0.2923480 0.25380243
# 10
        # If we use the same seed as the original `cvfit_nnls`, then
```

recombineSL 23

```
# the recombineCVSL and CV.SuperLearner results will be identical
# however, the recombineCVSL version will be much faster since
# it doesn't have to re-fit all the base learners, V times each.
set.seed(1)
cvfit_nnloglik2 \leftarrow CV.SuperLearner(Y = Y, X = X, V = 10, SL.library = SL.library,
 verbose = TRUE, method = "method.NNloglik", family = binomial())
cvfit_nnloglik2$coef
    SL.glmnet_All SL.glm_All SL.knn_All SL.gam_All SL.mean_All
# 1
        0.0000000 0.0000000 0.00000000 0.5974799 0.40252010
# 2
        0.0000000 0.0000000 0.31177345 0.6882266 0.00000000
# 3
        0.0000000 0.0000000 0.01377469 0.8544238
                                                 0.13180152
# 4
        0.0000000 0.1644188 0.00000000 0.2387919
                                                 0.59678930
# 5
        0.2142254 0.0000000 0.00000000 0.3729426
                                                 0.41283197
# 6
        0.0000000 0.0000000 0.00000000 0.5847150
                                                 0.41528502
# 7
        0.0000000 0.0000000 0.47538172 0.5080311
                                                 0.01658722
# 8
        0.0000000 0.0000000 0.00000000 1.0000000
                                                 0.00000000
# 9
        0.0000000 0.0000000 0.45384961 0.2923480
                                                 0.25380243
# 10
        ## End(Not run)
```

recombineSL

Recombine a SuperLearner fit using a new metalearning method

Description

The recombineSL function takes an existing SuperLearner fit and a new metalearning method and returns a new SuperLearner fit with updated base learner weights.

Usage

```
recombineSL(object, Y, method = "method.NNloglik", verbose = FALSE)
```

Arguments

object

Fitted object from SuperLearner.

Υ

The outcome in the training data set. Must be a numeric vector.

method

A list (or a function to create a list) containing details on estimating the coefficients for the super learner and the model to combine the individual algorithms in the library. See ?method.template for details. Currently, the built in options are either "method.NNLS" (the default), "method.NNLS2", "method.NNloglik", "method.CC_LS", "method.CC_nloglik", or "method.AUC". NNLS and NNLS2 are non-negative least squares based on the Lawson-Hanson algorithm and the dual method of Goldfarb and Idnani, respectively. NNLS and NNLS2 will work for both gaussian and binomial outcomes. NNloglik is a non-negative binomial likelihood maximization using the BFGS quasi-Newton optimization method. NN* methods are normalized so weights sum to one. CC_LS uses Goldfarb and

24 recombineSL

Idnani's quadratic programming algorithm to calculate the best convex combination of weights to minimize the squared error loss. CC_nloglik calculates the convex combination of weights that minimize the negative binomial log likelihood on the logistic scale using the sequential quadratic programming algorithm. AUC, which only works for binary outcomes, uses the Nelder-Mead method via the optim function to minimize rank loss (equivalent to maximizing AUC).

verbose

logical; TRUE for printing progress during the computation (helpful for debugging).

Details

recombineSL re-fits the super learner prediction algorithm using a new metalearning method. The weights for each algorithm in SL.library are re-estimated using the new metalearner, however the base learner fits are not regenerated, so this function saves a lot of computation time as opposed to using the SuperLearner function with a new method argument. The output is identical to the output from the SuperLearner function.

Value

call The matched call.

libraryNames A character vector with the names of the algorithms in the library. The format is

'predictionAlgorithm_screeningAlgorithm' with '_All' used to denote the pre-

diction algorithm run on all variables in X.

SL.library Returns SL.library in the same format as the argument with the same name

above.

SL.predict The predicted values from the super learner for the rows in newX.

coef Coefficients for the super learner.

library.predict

A matrix with the predicted values from each algorithm in SL.library for the

rows in newX.

Z The Z matrix (the cross-validated predicted values for each algorithm in SL.library).

cvRisk A numeric vector with the V-fold cross-validated risk estimate for each algo-

rithm in SL. library. Note that this does not contain the CV risk estimate for

the SuperLearner, only the individual algorithms in the library.

family Returns the family value from above

fitLibrary A list with the fitted objects for each algorithm in SL. library on the full train-

ing data set.

varNames A character vector with the names of the variables in X.

validRows A list containing the row numbers for the V-fold cross-validation step.

method A list with the method functions.

whichScreen A logical matrix indicating which variables passed each screening algorithm.

control The control list. cvControl The cvControl list.

recombineSL 25

```
errorsInCVLibrary
```

A logical vector indicating if any algorithms experienced an error within the CV step.

errorsInLibrary

A logical vector indicating if any algorithms experienced an error on the full

Author(s)

Erin LeDell < ledell@berkeley.edu>

References

van der Laan, M. J., Polley, E. C. and Hubbard, A. E. (2008) Super Learner, *Statistical Applications of Genetics and Molecular Biology*, **6**, article 25.

Examples

```
## Not run:
# Binary outcome example adapted from SuperLearner examples
set.seed(1)
N <- 200
X \leftarrow matrix(rnorm(N*10), N, 10)
X <- as.data.frame(X)</pre>
Y \leftarrow rbinom(N, 1, plogis(.2*X[, 1] + .1*X[, 2] - .2*X[, 3] +
  .1*X[, 3]*X[, 4] - .2*abs(X[, 4])))
SL.library <- c("SL.glmnet", "SL.glm", "SL.knn", "SL.gam", "SL.mean")
# least squares loss function
set.seed(1) # for reproducibility
fit_nnls <- SuperLearner(Y = Y, X = X, SL.library = SL.library,
  verbose = TRUE, method = "method.NNLS", family = binomial())
fit_nnls
                     Risk
                                Coef
#
# SL.glmnet_All 0.2439433 0.01293059
# SL.glm_All 0.2461245 0.08408060
# SL.knn_All 0.2604000 0.09600353
# SL.gam_All 0.2471651 0.40761918
# SL.mean_All 0.2486049 0.39936611
# negative log binomial likelihood loss function
fit_nnloglik <- recombineSL(fit_nnls, Y = Y, method = "method.NNloglik")</pre>
fit_nnloglik
                     Risk
                               Coef
# SL.glmnet_All 0.6815911 0.1577228
# SL.glm_All 0.6918926 0.0000000
# SL.knn_All
                     Inf 0.0000000
# SL.gam_All 0.6935383 0.6292881
```

```
# SL.mean_All
               0.6904050 0.2129891
# If we use the same seed as the original `fit_nnls`, then
# the recombineSL and SuperLearner results will be identical
# however, the recombineSL version will be much faster since
# it doesn't have to re-fit all the base learners.
fit_nnloglik2 <- SuperLearner(Y = Y, X = X, SL.library = SL.library,</pre>
  verbose = TRUE, method = "method.NNloglik", family = binomial())
fit_nnloglik2
                     Risk
                               Coef
# SL.glmnet_All 0.6815911 0.1577228
# SL.glm_All 0.6918926 0.0000000
# SL.knn_All
                      Inf 0.0000000
# SL.gam_All 0.6935383 0.6292881
# SL.mean_All 0.6904050 0.2129891
## End(Not run)
```

SampleSplitSuperLearner

Super Learner Prediction Function

Description

A Prediction Function for the Super Learner. The SuperLearner function takes a training set pair (X,Y) and returns the predicted values based on a validation set. SampleSplitSuperLearner uses sample split validation whereas SuperLearner uses V-fold cross-validation.

Usage

```
SampleSplitSuperLearner(Y, X, newX = NULL, family = gaussian(), SL.library,
method = "method.NNLS", id = NULL, verbose = FALSE,
control = list(), split = 0.8, obsWeights = NULL)
```

Arguments

Υ	The outcome in the training data set. Must be a numeric vector.
Χ	The predictor variables in the training data set, usually a data.frame.
newX	The predictor variables in the validation data set. The structure should match X . If missing, uses X for new X .
SL.library	Either a character vector of prediction algorithms or a list containing character vectors. See details below for examples on the structure. A list of functions included in the SuperLearner package can be found with listWrappers().
verbose	logical; TRUE for printing progress during the computation (helpful for debugging).

family

Currently allows gaussian or binomial to describe the error distribution. Link function information will be ignored and should be contained in the method argument below.

method

A list (or a function to create a list) containing details on estimating the coefficients for the super learner and the model to combine the individual algorithms in the library. See ?method.template for details. Currently, the built in options are either "method.NNLS" (the default), "method.NNLS2", "method.NNloglik", "method.CC_LS", or "method.CC_nloglik". NNLS and NNLS2 are non-negative least squares based on the Lawson-Hanson algorithm and the dual method of Goldfarb and Idnani, respectively. NNLS and NNLS2 will work for both gaussian and binomial outcomes. NNloglik is a non-negative binomial likelihood maximization using the BFGS quasi-Newton optimization method. NN* methods are normalized so weights sum to one. CC_LS uses Goldfarb and Idnani's quadratic programming algorithm to calculate the best convex combination of weights that minimize the negative binomial log likelihood on the logistic scale using the sequential quadratic programming algorithm.

id

Optional cluster identification variable. For the cross-validation splits, id forces observations in the same cluster to be in the same validation fold. id is passed to the prediction and screening algorithms in SL.library, but be sure to check the individual wrappers as many of them ignore the information.

obsWeights

Optional observation weights variable. As with id above, obsWeights is passed to the prediction and screening algorithms, but many of the built in wrappers ignore (or can't use) the information. If you are using observation weights, make sure the library you specify uses the information.

control

A list of parameters to control the estimation process. Parameters include saveFitLibrary and trimLogit. See SuperLearner.control for details.

split

Either a single value between 0 and 1 indicating the fraction of the samples for the training split. A value of 0.8 will randomly assign 80 percent of the samples to the training split and the other 20 percent to the validation split. Alternatively, split can be a numeric vector with the row numbers of X corresponding to the validation split. All other rows not in the vector will be considered in the training split.

Details

SuperLearner fits the super learner prediction algorithm. The weights for each algorithm in SL.library is estimated, along with the fit of each algorithm.

The prescreen algorithms. These algorithms first rank the variables in X based on either a univariate regression p-value of the randomForest variable importance. A subset of the variables in X is selected based on a pre-defined cut-off. With this subset of the X variables, the algorithms in SL.library are then fit.

The SuperLearner package contains a few prediction and screening algorithm wrappers. The full list of wrappers can be viewed with listWrappers(). The design of the SuperLearner package is such that the user can easily add their own wrappers. We also maintain a website with additional examples of wrapper functions at https://github.com/ecpolley/SuperLearnerExtra.

Value

call The matched call.

libraryNames A character vector with the names of the algorithms in the library. The format is

'predictionAlgorithm_screeningAlgorithm' with '_All' used to denote the pre-

diction algorithm run on all variables in X.

SL.library Returns SL.library in the same format as the argument with the same name

above.

SL. predict The predicted values from the super learner for the rows in newX.

coef Coefficients for the super learner.

library.predict

A matrix with the predicted values from each algorithm in SL.library for the

rows in newX.

Z The Z matrix (the cross-validated predicted values for each algorithm in SL.library).

cvRisk A numeric vector with the V-fold cross-validated risk estimate for each algo-

rithm in SL.1ibrary. Note that this does not contain the CV risk estimate for

the SuperLearner, only the individual algorithms in the library.

family Returns the family value from above

fitLibrary A list with the fitted objects for each algorithm in SL.library on the full train-

ing data set.

varNames A character vector with the names of the variables in X.

validRows A list containing the row numbers for the V-fold cross-validation step.

method A list with the method functions.

whichScreen A logical matrix indicating which variables passed each screening algorithm.

control The control list. split The split value.

errorsInCVLibrary

A logical vector indicating if any algorithms experienced an error within the CV

step.

errorsInLibrary

A logical vector indicating if any algorithms experienced an error on the full

data.

Author(s)

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References

van der Laan, M. J., Polley, E. C. and Hubbard, A. E. (2008) Super Learner, *Statistical Applications of Genetics and Molecular Biology*, **6**, article 25.

Examples

```
## Not run:
## simulate data
set.seed(23432)
## training set
n <- 500
p < -50
X <- matrix(rnorm(n*p), nrow = n, ncol = p)</pre>
colnames(X) <- paste("X", 1:p, sep="")</pre>
X <- data.frame(X)</pre>
Y \leftarrow X[, 1] + sqrt(abs(X[, 2] * X[, 3])) + X[, 2] - X[, 3] + rnorm(n)
## test set
m <- 1000
newX <- matrix(rnorm(m*p), nrow = m, ncol = p)</pre>
colnames(newX) <- paste("X", 1:p, sep="")</pre>
newX <- data.frame(newX)</pre>
newY <- newX[, 1] + sqrt(abs(newX[, 2] * newX[, 3])) + newX[, 2] -</pre>
  newX[, 3] + rnorm(m)
# generate Library and run Super Learner
SL.library <- c("SL.glm", "SL.randomForest", "SL.gam",</pre>
  "SL.polymars", "SL.mean")
test <- SampleSplitSuperLearner(Y = Y, X = X, newX = newX, SL.library = SL.library,</pre>
  verbose = TRUE, method = "method.NNLS")
test
# library with screening
SL.library <- list(c("SL.glmnet", "All"), c("SL.glm", "screen.randomForest",</pre>
  "All", "screen.SIS"), "SL.randomForest", c("SL.polymars", "All"), "SL.mean")
test <- SuperLearner(Y = Y, X = X, newX = newX, SL.library = SL.library,
  verbose = TRUE, method = "method.NNLS")
test
# binary outcome
set.seed(1)
N <- 200
X \leftarrow matrix(rnorm(N*10), N, 10)
X <- as.data.frame(X)</pre>
Y \leftarrow rbinom(N, 1, plogis(.2*X[, 1] + .1*X[, 2] - .2*X[, 3] +
  .1*X[, 3]*X[, 4] - .2*abs(X[, 4]))
SL.library <- c("SL.glmnet", "SL.glm", "SL.knn", "SL.gam", "SL.mean")
# least squares loss function
test.NNLS <- SampleSplitSuperLearner(Y = Y, X = X, SL.library = SL.library,
  verbose = TRUE, method = "method.NNLS", family = binomial())
test.NNLS
## End(Not run)
```

30 SL.bartMachine

Description

Support bayesian additive regression trees via the bartMachine package.

Usage

```
SL.bartMachine(Y, X, newX, family, obsWeights, id, num_trees = 50,
num_burn_in = 250, verbose = F, alpha = 0.95, beta = 2, k = 2,
q = 0.9, nu = 3, num_iterations_after_burn_in = 1000, ...)
```

Arguments

 ,	
Υ	Outcome variable
Χ	Covariate dataframe
newX	Optional dataframe to predict the outcome
family	"gaussian" for regression, "binomial" for binary classification
obsWeights	Optional observation-level weights (supported but not tested)
id	Optional id to group observations from the same unit (not used currently).
num_trees	The number of trees to be grown in the sum-of-trees model.
num_burn_in	Number of MCMC samples to be discarded as "burn-in".
verbose	Prints information about progress of the algorithm to the screen.
alpha	Base hyperparameter in tree prior for whether a node is nonterminal or not.
beta	Power hyperparameter in tree prior for whether a node is nonterminal or not.
k	For regression, k determines the prior probability that $E(Y X)$ is contained in the interval (y_min, y_max) , based on a normal distribution. For example, when k=2, the prior probability is 95%. For classification, k determines the prior probability that $E(Y X)$ is between (-3,3). Note that a larger value of k results in more shrinkage and a more conservative fit.
q	Quantile of the prior on the error variance at which the data-based estimate is placed. Note that the larger the value of \mathbf{q} , the more aggressive the fit as you are placing more prior weight on values lower than the data-based estimate. Not used for classification.
nu	Degrees of freedom for the inverse chi^2 prior. Not used for classification.
num_iterations_	_after_burn_in

Number of MCMC samples to draw from the posterior distribution of f(x).

Additional arguments (not used)

SL.biglasso 31

SL.biglasso	SL wrapper for biglasso

Description

SL wrapper for biglasso

Usage

```
SL.biglasso(Y, X, newX, family, obsWeights, penalty = "lasso",
   alg.logistic = "Newton", screen = "SSR", alpha = 1, nlambda = 100,
   eval.metric = "default", ncores = 1, nfolds = 5, ...)
```

Arguments

nfolds

rguments	
Υ	Outcome variable
Χ	Training dataframe
newX	Test dataframe
family	Gaussian or binomial
obsWeights	Observation-level weights
penalty	The penalty to be applied to the model. Either "lasso" (default), "ridge", or "enet" (elastic net).
alg.logistic	The algorithm used in logistic regression. If "Newton" then the exact hessian is used (default); if "MM" then a majorization-minimization algorithm is used to set an upper-bound on the hessian matrix. This can be faster, particularly in data-larger-than-RAM case.
screen	"SSR" (default) is the sequential strong rule; "SEDPP" is the (sequential) EDPP rule. "SSR-BEDPP", "SSR-Dome", and "SSR-Slores" are our newly proposed screening rules which combine the strong rule with a safe rule (BEDPP, Dome test, or Slores rule). Among the three, the first two are for lasso-penalized linear regression, and the last one is for lasso-penalized logistic regression. "None" is to not apply a screening rule.
alpha	The elastic-net mixing parameter that controls the relative contribution from the lasso (11) and the ridge (12) penalty.
nlambda	The number of lambda values to check. Default is 100.
eval.metric	The evaluation metric for the cross-validated error and for choosing optimal lambda. "default" for linear regression is MSE (mean squared error), for logistic regression is misclassification error. "MAPE", for linear regression only, is the Mean Absolute Percentage Error.
ncores	The number of cores to use for parallel execution across a cluster created by the parallel package.

The number of cross-validation folds. Default is 5. Any additional arguments, not currently used.

32 SL.cforest

References

Zeng Y, Breheny P (2017). biglasso: Extending Lasso Model Fitting to Big Data. https://CRAN.R-project.org/package=biglasso.

See Also

```
predict.SL.biglasso biglasso cv.biglasso predict.biglasso SL.glmnet
```

Examples

SL.cforest

cforest party

Description

These defaults emulate cforest_unbiased() but allow customization.

Usage

```
SL.cforest(Y, X, newX, family, obsWeights, id, ntree = 1000,
  mtry = max(floor(ncol(X)/3), 1), mincriterion = 0, teststat = "quad",
  testtype = "Univ", replace = F, fraction = 0.632, ...)
```

SL.extraTrees 33

Arguments

Υ	Outcome variable
Χ	Covariate dataframe

newX Optional dataframe to predict the outcome

. . .

family "gaussian" for regression, "binomial" for binary classification obsWeights Optional observation-level weights (supported but not tested)

id Optional id to group observations from the same unit (not used currently).

ntree Number of trees

mtry Number of randomly selected features per node

mincriterion See ?cforest_control
teststat See ?cforest_control
testtype See ?cforest_control
replace See ?cforest_control
fraction See ?cforest_control

... Remaining arguments (unused)

Description

Supports the Extremely Randomized Trees package for SuperLearning, which is a variant of random forest

Usage

```
SL.extraTrees(Y, X, newX, family, obsWeights, id, ntree = 500, mtry = if
  (family$family == "gaussian") max(floor(ncol(X)/3), 1) else
  floor(sqrt(ncol(X))), nodesize = if (family$family == "gaussian") 5 else 1,
  numRandomCuts = 1, evenCuts = FALSE, numThreads = 1, quantile = FALSE,
  subsetSizes = NULL, subsetGroups = NULL, tasks = NULL,
  probOfTaskCuts = mtry/ncol(X), numRandomTaskCuts = 1, verbose = FALSE,
  ...)
```

Arguments

Υ	Outcome variable
Χ	Covariate dataframe

newX Optional dataframe to predict the outcome

family "gaussian" for regression, "binomial" for binary classification.
obsWeights Optional observation-level weights (supported but not tested)

34 SL.extraTrees

id Optional id to group observations from the same unit (not used currently).

ntree Number of trees (default 500).

mtry Number of features tested at each node. Default is ncol(x) / 3 for regression and

sqrt(ncol(x)) for classification.

nodesize The size of leaves of the tree. Default is 5 for regression and 1 for classification.

numRandomCuts the number of random cuts for each (randomly chosen) feature (default 1, which

corresponds to the official ExtraTrees method). The higher the number of cuts

the higher the chance of a good cut.

evenCuts if FALSE then cutting thresholds are uniformly sampled (default). If TRUE

then the range is split into even intervals (the number of intervals is numRan-

domCuts) and a cut is uniformly sampled from each interval.

numThreads the number of CPU threads to use (default is 1).

quantile if TRUE then quantile regression is performed (default is FALSE), only for re-

gression data. Then use predict(et, newdata, quantile=k) to make predictions for

k quantile.

subsetSizes subset size (one integer) or subset sizes (vector of integers, requires subset-

Groups), if supplied every tree is built from a random subset of size subsetSizes.

NULL means no subsetting, i.e. all samples are used.

subsetGroups list specifying subset group for each sample: from samples in group g, each tree

will randomly select subsetSizes[g] samples.

tasks vector of tasks, integers from 1 and up. NULL if no multi-task learning. (untested)

probOfTaskCuts probability of performing task cut at a node (default mtry / ncol(x)). Used only

if tasks is specified. (untested)

numRandomTaskCuts

number of times task cut is performed at a node (default 1). Used only if tasks

is specified. (untested)

verbose Verbosity of model fitting.

... Any remaining arguments (not supported though).

Details

If Java runs out of memory: java.lang.OutOfMemoryError: Java heap space, then (assuming you have free memory) you can increase the heap size by: options(java.parameters = "-Xmx2g") before calling library(extraTrees),

References

Geurts, P., Ernst, D., & Wehenkel, L. (2006). Extremely randomized trees. Machine learning, 63(1), 3-42.

Simm, J., de Abril, I. M., & Sugiyama, M. (2014). Tree-based ensemble multi-task learning method for classification and regression. IEICE TRANSACTIONS on Information and Systems, 97(6), 1677-1681.

See Also

extraTrees predict.SL.extraTrees predict.extraTrees

SL.glm 35

Examples

```
data(Boston, package = "MASS")
Y = Boston$medv
# Remove outcome from covariate dataframe.
X = Boston[, -14]
set.seed(1)
# Sample rows to speed up example.
row_subset = sample(nrow(X), 30)
sl = SuperLearner(Y[row_subset], X[row_subset, ], family = gaussian(),
cvControl = list(V = 2), SL.library = c("SL.mean", "SL.extraTrees"))
print(sl)
```

SL.glm

Wrapper for glm

Description

Wrapper for generalized linear models via glm().

Note that for outcomes bounded by [0, 1] the binomial family can be used in addition to gaussian.

Usage

```
SL.glm(Y, X, newX, family, obsWeights, model = TRUE, ...)
```

Arguments

Υ	Outcome variable
Χ	Training dataframe
newX	Test dataframe
family	Gaussian or binomial
obsWeights	Observation-level weights
model	Whether to save model.matrix of data in fit object. Set to FALSE to save memory.
	Any remaining arguments, not used.

References

Fox, J. (2015). Applied regression analysis and generalized linear models. Sage Publications.

36 SL.glmnet

See Also

```
predict.SL.glm glm predict.glm SL.speedglm
```

Examples

SL.glmnet

Elastic net regression, including lasso and ridge

Description

Penalized regression using elastic net. Alpha = 0 corresponds to ridge regression and alpha = 1 corresponds to Lasso.

See vignette("glmnet_beta",package = "glmnet") for a nice tutorial on glmnet.

Usage

```
SL.glmnet(Y, X, newX, family, obsWeights, id, alpha = 1, nfolds = 10,
    nlambda = 100, useMin = TRUE, loss = "deviance", ...)
```

Arguments

alpha

Υ	Outcome variable
Χ	Covariate dataframe
newX	Dataframe to predict the outcome
family	"gaussian" for regression, "binomial" for binary classification. Untested options: "multinomial" for multiple classification or "mgaussian" for multiple response, "poisson" for non-negative outcome with proportional mean and variance, "cox".
obsWeights	Optional observation-level weights
id	Optional id to group observations from the same unit (not used currently).

Elastic net mixing parameter, range [0, 1]. 0 = ridge regression and 1 = lasso.

SL.glmnet 37

nfolds	Number of folds for internal cross-validation to optimize lambda.
nlambda	Number of lambda values to check, recommended to be 100 or more.
useMin	If TRUE use lambda that minimizes risk, otherwise use 1 standard-error rule which chooses a higher penalty with performance within one standard error of the minimum (see Breiman et al. 1984 on CART for background).
loss	Loss function, can be "deviance", "mse", or "mae". If family = binomial can also be "auc" or "class" (misclassification error).
	Any additional arguments are passed through to cv.glmnet.

References

Friedman, J., Hastie, T., & Tibshirani, R. (2010). Regularization paths for generalized linear models via coordinate descent. Journal of statistical software, 33(1), 1.

Hoerl, A. E., & Kennard, R. W. (1970). Ridge regression: Biased estimation for nonorthogonal problems. Technometrics, 12(1), 55-67.

Tibshirani, R. (1996). Regression shrinkage and selection via the lasso. Journal of the Royal Statistical Society. Series B (Methodological), 267-288.

Zou, H., & Hastie, T. (2005). Regularization and variable selection via the elastic net. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 67(2), 301-320.

See Also

```
predict.SL.glmnet cv.glmnet glmnet
```

38 SL.kernelKnn

SL.kernelKnn SL wrapper for KernelKNN	SL.kernelKnn	SL wrapper for KernelKNN	
---------------------------------------	--------------	--------------------------	--

Description

Wrapper for a configurable implementation of k-nearest neighbors. Supports both binomial and gaussian outcome distributions.

Usage

```
SL.kernelKnn(Y, X, newX, family, k = 10, method = "euclidean", weights_function = NULL, extrema = F, h = 1, ...)
```

Arguments

Υ	Outcome variable	
Χ	Training dataframe	
newX	Test dataframe	
family	Gaussian or binomial	
k	Number of nearest neighbors to use	
method	Distance method, can be 'euclidean' (default), 'manhattan', 'chebyshev', 'canberra', 'braycurtis', 'pearson_correlation', 'simple_matching_coefficient', 'minkowski' (by default the order 'p' of the minkowski parameter equals k), 'hamming', 'mahalanobis', 'jaccard_coefficient', 'Rao_coefficient'	
weights_function		
	Weighting method for combining the nearest neighbors. Can be 'uniform' (default), 'triangular', 'epanechnikov', 'biweight', 'triweight', 'tricube', 'gaussian', 'cosine', 'logistic', 'gaussianSimple', 'silverman', 'inverse', 'exponential'.	
extrema	if TRUE then the minimum and maximum values from the k-nearest-neighbors will be removed (can be thought as outlier removal).	
h	the bandwidth, applicable if the weights_function is not NULL. Defaults to 1.0.	
	Any additional parameters, not currently passed through.	

Value

List with predictions and the original training data & hyperparameters.

```
# Load a test dataset.
data(PimaIndiansDiabetes2, package = "mlbench")
data = PimaIndiansDiabetes2
```

SL.ksvm

SL.ksvm

Wrapper for Kernlab's SVM algorithm

Description

Wrapper for Kernlab's support vector machine algorithm.

Usage

```
SL.ksvm(Y, X, newX, family, type = NULL, kernel = "rbfdot",
   kpar = "automatic", scaled = T, C = 1, nu = 0.2, epsilon = 0.1,
   cross = 0, prob.model = family$family == "binomial",
   class.weights = NULL, cache = 40, tol = 0.001, shrinking = T, ...)
```

Υ	Outcome variable	
Χ	Training dataframe	
newX	Test dataframe	
family	Gaussian or binomial	
type	ksvm can be used for classification, for regression, or for novelty detection. Depending on whether y is a factor or not, the default setting for type is C-svc or eps-svr, respectively, but can be overwritten by setting an explicit value. See ?ksvm for more details.	
kernel	the kernel function used in training and predicting. This parameter can be set to any function, of class kernel, which computes the inner product in feature space between two vector arguments. See ?ksvm for more details.	
kpar	the list of hyper-parameters (kernel parameters). This is a list which contains the parameters to be used with the kernel function. See ?ksvm for more details.	
scaled	A logical vector indicating the variables to be scaled. If scaled is of length 1, the value is recycled as many times as needed and all non-binary variables are scaled. Per default, data are scaled internally (both x and y variables) to zero mean and unit variance. The center and scale values are returned and used for later predictions.	

40 SL.ksvm

С	cost of constraints violation (default: 1) this is the 'C'-constant of the regularization term in the Lagrange formulation.
nu	parameter needed for nu-svc, one-svc, and nu-svr. The nu parameter sets the upper bound on the training error and the lower bound on the fraction of data points to become Support Vectors (default: 0.2).
epsilon	epsilon in the insensitive-loss function used for eps-svr, nu-svr and eps-bsvm (default: 0.1)
cross	if a integer value k>0 is specified, a k-fold cross validation on the training data is performed to assess the quality of the model: the accuracy rate for classification and the Mean Squared Error for regression
prob.model	if set to TRUE builds a model for calculating class probabilities or in case of regression, calculates the scaling parameter of the Laplacian distribution fitted on the residuals. Fitting is done on output data created by performing a 3-fold cross-validation on the training data. (default: FALSE)
class.weights	a named vector of weights for the different classes, used for asymmetric class sizes. Not all factor levels have to be supplied (default weight: 1). All components have to be named.
cache	cache memory in MB (default 40)
tol	tolerance of termination criterion (default: 0.001)
shrinking	option whether to use the shrinking-heuristics (default: TRUE)
	Any additional parameters, not currently passed through.

Value

List with predictions and the original training data & hyperparameters.

References

Hsu, C. W., Chang, C. C., & Lin, C. J. (2016). A practical guide to support vector classification. http://www.csie.ntu.edu.tw/~cjlin/papers/guide/guide.pdf

Scholkopf, B., & Smola, A. J. (2001). Learning with kernels: support vector machines, regularization, optimization, and beyond. MIT press.

Vapnik, V. N. (1998). Statistical learning theory (Vol. 1). New York: Wiley.

Zeileis, A., Hornik, K., Smola, A., & Karatzoglou, A. (2004). kernlab-an S4 package for kernel methods in R. Journal of statistical software, 11(9), 1-20.

See Also

```
predict.SL.ksvm ksvm predict.ksvm
```

```
data(Boston, package = "MASS")
Y = Boston$medv
# Remove outcome from covariate dataframe.
```

SL.lda 41

SL.lda

SL wrapper for MASS:lda

Description

Linear discriminant analysis, used for classification.

Usage

```
SL.lda(Y, X, newX, family, obsWeights = rep(1, nrow(X)), id = NULL,
  verbose = F, prior = as.vector(prop.table(table(Y))), method = "mle",
  tol = 1e-04, CV = F, nu = 5, ...)
```

Υ	Outcome variable
Χ	Training dataframe
newX	Test dataframe
family	Binomial only, cannot be used for regression.
obsWeights	Observation-level weights
id	Not supported.
verbose	If TRUE, display additional output during execution.
prior	the prior probabilities of class membership. If unspecified, the class proportions for the training set are used. If present, the probabilities should be specified in the order of the factor levels.
method	"moment" for standard estimators of the mean and variance, "mle" for MLEs, "mve" to use cov.mve, or "t" for robust estimates based on a t distribution.
tol	tolerance
CV	If true, returns results (classes and posterior probabilities) for leave-one-out cross-validation. Note that if the prior is estimated, the proportions in the whole dataset are used.
nu	degrees of freedom for method = "t".
• • •	Any additional arguments, not currently used.

42 SL.lm

References

James, G., Witten, D., Hastie, T., & Tibshirani, R. (2013). An Introduction to Statistical Learning (Vol. 6). New York: Springer. Section 4.4.

See Also

```
predict.SL.lda lda predict.lda SL.qda
```

Examples

SL.1m

 $Wrapper\, for\, lm$

Description

Wrapper for OLS via lm(), which may be faster than glm().

Usage

```
SL.lm(Y, X, newX, family, obsWeights, model = TRUE, ...)
```

Υ	Outcome variable
Χ	Training dataframe
newX	Test dataframe
family	Gaussian or binomial
obsWeights	Observation-level weights
model	Whether to save model.matrix of data in fit object. Set to FALSE to save memory.
	Any remaining arguments, not used.

SL.qda 43

References

Fox, J. (2015). Applied regression analysis and generalized linear models. Sage Publications.

See Also

```
predict.SL.lm lm predict.lm SL.speedlm
```

Examples

SL.qda

SL wrapper for MASS:qda

Description

Quadratic discriminant analysis, used for classification.

Usage

```
SL.qda(Y, X, newX, family, obsWeights = rep(1, nrow(X)), verbose = F,
  id = NULL, prior = as.vector(prop.table(table(Y))), method = "mle",
  tol = 1e-04, CV = F, nu = 5, ...)
```

Υ	Outcome variable
X	Training dataframe
newX	Test dataframe
family	Binomial only, cannot be used for regression.
obsWeights	Observation-level weights
verbose	If TRUE, display additional output during execution.
id	Not supported.

SL.ranger

prior	the prior probabilities of class membership. If unspecified, the class proportions for the training set are used. If present, the probabilities should be specified in the order of the factor levels.
method	"moment" for standard estimators of the mean and variance, "mle" for MLEs, "mve" to use cov.mve, or "t" for robust estimates based on a t distribution.
tol	tolerance
CV	If true, returns results (classes and posterior probabilities) for leave-one-out cross-validation. Note that if the prior is estimated, the proportions in the whole dataset are used.
nu	degrees of freedom for method = "t".
	Any additional arguments, not currently used.

References

James, G., Witten, D., Hastie, T., & Tibshirani, R. (2013). An Introduction to Statistical Learning (Vol. 6). New York: Springer. Section 4.4.

See Also

```
predict.SL.qda qda predict.qda SL.lda
```

Examples

SL.ranger

SL wrapper for ranger

Description

Ranger is a fast implementation of Random Forest (Breiman 2001) or recursive partitioning, particularly suited for high dimensional data.

Extending code by Eric Polley from the SuperLearnerExtra package.

SL.ranger 45

Usage

```
SL.ranger(Y, X, newX, family, obsWeights, num.trees = 500,
   mtry = floor(sqrt(ncol(X))), write.forest = TRUE,
   probability = family$family == "binomial",
   min.node.size = ifelse(family$family == "gaussian", 5, 1), replace = TRUE,
   sample.fraction = ifelse(replace, 1, 0.632), num.threads = 1,
   verbose = T, ...)
```

Arguments

Y Outcome variable

X Training dataframe

newX Test dataframe

family Gaussian or binomial

obsWeights Observation-level weights

num. trees Number of trees.

mtry Number of variables to possibly split at in each node. Default is the (rounded

down) square root of the number variables.

write.forest Save ranger.forest object, required for prediction. Set to FALSE to reduce mem-

ory usage if no prediction intended.

probability Grow a probability forest as in Malley et al. (2012).

min.node.size Minimal node size. Default 1 for classification, 5 for regression, 3 for survival,

and 10 for probability.

replace Sample with replacement.

sample.fraction

Fraction of observations to sample. Default is 1 for sampling with replacement

and 0.632 for sampling without replacement.

num. threads Number of threads to use.

verbose If TRUE, display additional output during execution.

... Any additional arguments, not currently used.

References

Breiman, L. (2001). Random forests. Machine learning 45:5-32.

Wright, M. N. & Ziegler, A. (2016). ranger: A Fast Implementation of Random Forests for High Dimensional Data in C++ and R. Journal of Statistical Software, in press. http://arxiv.org/abs/1508.04409.

See Also

```
SL.ranger ranger predict.ranger
```

SL.speedglm

Examples

SL.speedglm

Wrapper for speedglm

Description

Speedglm is a fast version of glm()

Usage

```
SL.speedglm(Y, X, newX, family, obsWeights, maxit = 25, k = 2, ...)
```

Arguments

Υ	Outcome variable
Χ	Training dataframe
newX	Test dataframe
family	Gaussian or binomial
obsWeights	Observation-level weights
maxit	Maximum number of iterations before stopping.
k	numeric, the penalty per parameter to be used; the default $k=2$ is the classical AIC.
	Any remaining arguments, not used.

References

Enea, M. A. R. C. O. (2013). Fitting linear models and generalized linear models with large data sets in R. Statistical Methods for the Analysis of Large Datasets: book of short papers, 411-414.

SL.speedlm 47

See Also

predict.SL.speedglm speedglm predict.speedglm

SL.speedlm Wrapper for speedlm

Description

Speedlm is a fast version of lm()

Usage

```
SL.speedlm(Y, X, newX, family, obsWeights, ...)
```

Arguments

Y Outcome variable

X Training dataframe

newX Test dataframe

family Gaussian or binomial

obsWeights Observation-level weights

... Any remaining arguments, not used.

References

Enea, M. A. R. C. O. (2013). Fitting linear models and generalized linear models with large data sets in R. Statistical Methods for the Analysis of Large Datasets: book of short papers, 411-414.

See Also

```
predict.SL.speedlm speedlm predict.speedlm SL.speedglm
```

SL.xgboost XGBoost SuperLearner wrapper

Description

Supports the Extreme Gradient Boosting package for SuperLearnering, which is a variant of gradient boosted machines (GBM).

Usage

```
SL.xgboost(Y, X, newX, family, obsWeights, id, ntrees = 1000, max_depth = 4,
    shrinkage = 0.1, minobspernode = 10, params = list(), nthread = 1,
    verbose = 0, save_period = NULL, ...)
```

Arguments

Υ Outcome variable Χ Covariate dataframe Optional dataframe to predict the outcome newX "gaussian" for regression, "binomial" for binary classification, "multinomial" for family multiple classification (not yet supported). obsWeights Optional observation-level weights (supported but not tested) Optional id to group observations from the same unit (not used currently). id ntrees How many trees to fit. Low numbers may underfit but high numbers may overfit, depending also on the shrinkage. max_depth How deep each tree can be. 1 means no interactions, aka tree stubs. How much to shrink the predictions, in order to reduce overfitting. shrinkage minobspernode Minimum observations allowed per tree node, after which no more splitting will occur. params Many other parameters can be customized. See https://xgboost.readthedocs. io/en/latest/parameter.html nthread How many threads (cores) should xgboost use. Generally we want to keep this to 1 so that XGBoost does not compete with SuperLearner parallelization.

verbose Verbosity of XGB fitting.

save_period How often (in tree iterations) to save current model to disk during processing. If

NULL does not save model, and if 0 saves model at the end.

... Any remaining arguments (not supported though).

Details

The performance of XGBoost, like GBM, is sensitive to the configuration settings. Therefore it is best to create multiple configurations using create.SL.xgboost and allow the SuperLearner to choose the best weights based on cross-validated performance.

If you run into errors please first try installing the latest version of XGBoost from drat as described here: https://xgboost.readthedocs.io/en/latest/build.html

summary.CV.SuperLearner

Summary Function for Cross-Validated Super Learner

Description

summary method for the CV. SuperLearner function

Usage

```
## $3 method for class 'CV.SuperLearner'
summary(object, obsWeights = NULL, ...)
## $3 method for class 'summary.CV.SuperLearner'
print(x, digits, ...)
```

Arguments

object An object of class "CV.SuperLearner", the result of a call to CV. SuperLearner.

An object of class "summary.CV.SuperLearner", the result of a call to summary.CV.SuperLearner.

obsWeights Optional vector for observation weights.

digits The number of significant digits to use when printing.

... additional arguments ...

Details

Summary method for CV. SuperLearner. Calculates the V-fold cross-validated estimate of either the mean squared error or the -2*log(L) depending on the loss function used.

Value

summary.CV.SuperLearner returns a list with components

call The function call from CV. SuperLearner

method Describes the loss function used. Currently either least squares of negative log

Likelihood.

V Number of folds

Risk.SL Risk estimate for the super learner

Risk dSL Risk estimate for the discrete super learner (the cross-validation selector)

Risk.library A matrix with the risk estimates for each algorithm in the library

Table A table with the mean risk estimate and standard deviation across the folds for

the super learner and all algorithms in the library

Author(s)

```
Eric C Polley <eric.polley@nih.gov>
```

See Also

CV.SuperLearner

SuperLearner

Super Learner Prediction Function

Description

A Prediction Function for the Super Learner. The SuperLearner function takes a training set pair (X,Y) and returns the predicted values based on a validation set.

Usage

```
SuperLearner(Y, X, newX = NULL, family = gaussian(), SL.library,
method = "method.NNLS", id = NULL, verbose = FALSE,
control = list(), cvControl = list(), obsWeights = NULL, env = parent.frame())
```

Arguments

Y The outcome in the training data set. Must be a numeric vector.

X The predictor variables in the training data set, usually a data.frame.

newX The predictor variables in the validation data set. The structure should match X.

If missing, uses X for newX.

SL.1ibrary Either a character vector of prediction algorithms or a list containing character

vectors. See details below for examples on the structure. A list of functions included in the SuperLearner package can be found with listWrappers().

metaded in the superseason package can be round with 115 cm apper 5().

verbose logical; TRUE for printing progress during the computation (helpful for debug-

ging).

family Currently allows gaussian or binomial to describe the error distribution. Link

function information will be ignored and should be contained in the method

argument below.

method A list (or a function to create a list) containing details on estimating the coefficients for the super learner and the model to combine the individual algorithms

in the library. See ?method.template for details. Currently, the built in options are either "method.NNLS" (the default), "method.NNLS2", "method.NNloglik", "method.CC_LS", "method.CC_nloglik", or "method.AUC". NNLS and NNLS2 are non-negative least squares based on the Lawson-Hanson algorithm and the dual method of Goldfarb and Idnani, respectively. NNLS and NNLS2 will work for both gaussian and binomial outcomes. NNloglik is a non-negative binomial likelihood maximization using the BFGS quasi-Newton optimization method. NN* methods are normalized so weights sum to one. CC_LS uses Goldfarb and Idnani's quadratic programming algorithm to calculate the best convex combination of weights to minimize the squared error loss. CC_nloglik calculates the convex combination of weights that minimize the negative binomial log likelihood on the logistic scale using the sequential quadratic programming algorithm. AUC, which only works for binary outcomes, uses the Nelder-Mead method via the optim function to minimize rank loss (equivalent to maximizing

AUC).

id Optional cluster identification variable. For the cross-validation splits, id forces observations in the same cluster to be in the same validation fold. id is passed to the prediction and screening algorithms in SL.library, but be sure to check the individual wrappers as many of them ignore the information. obsWeights Optional observation weights variable. As with id above, obsWeights is passed to the prediction and screening algorithms, but many of the built in wrappers ignore (or can't use) the information. If you are using observation weights, make sure the library you specify uses the information. control A list of parameters to control the estimation process. Parameters include saveFitLibrary and trimLogit. See SuperLearner.control for details. A list of parameters to control the cross-validation process. Parameters include cvControl V, stratifyCV, shuffle and validRows. See SuperLearner.CV.control for details. env Environment containing the learner functions. Defaults to the calling environ-

Details

SuperLearner fits the super learner prediction algorithm. The weights for each algorithm in SL.1ibrary is estimated, along with the fit of each algorithm.

The prescreen algorithms. These algorithms first rank the variables in X based on either a univariate regression p-value of the randomForest variable importance. A subset of the variables in X is selected based on a pre-defined cut-off. With this subset of the X variables, the algorithms in SL.library are then fit.

The SuperLearner package contains a few prediction and screening algorithm wrappers. The full list of wrappers can be viewed with listWrappers(). The design of the SuperLearner package is such that the user can easily add their own wrappers. We also maintain a website with additional examples of wrapper functions at https://github.com/ecpolley/SuperLearnerExtra.

Value

call	The matched call.	
libraryNames	A character vector with the names of the algorithms in the library. The format is 'predictionAlgorithm_screeningAlgorithm' with '_All' used to denote the prediction algorithm run on all variables in X.	
SL.library	Returns SL.1ibrary in the same format as the argument with the same name above.	
SL.predict	The predicted values from the super learner for the rows in newX.	
coef	Coefficients for the super learner.	
library.predict		
	A matrix with the predicted values from each algorithm in SL.library for the rows in newX.	
Z	The Z matrix (the cross-validated predicted values for each algorithm in SL.library).	
cvRisk	A numeric vector with the V-fold cross-validated risk estimate for each algorithm in SL.library. Note that this does not contain the CV risk estimate for the SuperLearner, only the individual algorithms in the library.	

family Returns the family value from above

fitLibrary A list with the fitted objects for each algorithm in SL.library on the full train-

ing data set.

cvFitLibrary A list with fitted objects for each algorithm in SL.library on each of V different

training data sets.

varNames A character vector with the names of the variables in X.

validRows A list containing the row numbers for the V-fold cross-validation step.

method A list with the method functions.

whichScreen A logical matrix indicating which variables passed each screening algorithm.

control The control list.

cvControl The cvControl list.

errorsInCVLibrary

A logical vector indicating if any algorithms experienced an error within the CV

step.

errorsInLibrary

A logical vector indicating if any algorithms experienced an error on the full

data.

env Environment passed into function which will be searched to find the learner

functions. Defaults to the calling environment.

times A list that contains the execution time of the SuperLearner, plus separate times

for model fitting and prediction.

Author(s)

Eric C Polley <polley.eric@mayo.edu>

References

van der Laan, M. J., Polley, E. C. and Hubbard, A. E. (2008) Super Learner, *Statistical Applications of Genetics and Molecular Biology*, **6**, article 25.

```
## Not run:
## simulate data
set.seed(23432)
## training set
n <- 500
p <- 50
X <- matrix(rnorm(n*p), nrow = n, ncol = p)
colnames(X) <- paste("X", 1:p, sep="")
X <- data.frame(X)
Y <- X[, 1] + sqrt(abs(X[, 2] * X[, 3])) + X[, 2] - X[, 3] + rnorm(n)
## test set
m <- 1000
newX <- matrix(rnorm(m*p), nrow = m, ncol = p)</pre>
```

```
colnames(newX) <- paste("X", 1:p, sep="")</pre>
newX <- data.frame(newX)</pre>
newY \leftarrow newX[, 1] + sqrt(abs(newX[, 2] * newX[, 3])) + newX[, 2] -
  newX[, 3] + rnorm(m)
# generate Library and run Super Learner
SL.library <- c("SL.glm", "SL.randomForest", "SL.gam",
  "SL.polymars", "SL.mean")
test <- SuperLearner(Y = Y, X = X, newX = newX, SL.library = SL.library,</pre>
  verbose = TRUE, method = "method.NNLS")
test
# library with screening
SL.library <- list(c("SL.glmnet", "All"), c("SL.glm", "screen.randomForest",</pre>
  "All", "screen.SIS"), "SL.randomForest", c("SL.polymars", "All"), "SL.mean")
test <- SuperLearner(Y = Y, X = X, newX = newX, SL.library = SL.library,</pre>
  verbose = TRUE, method = "method.NNLS")
test
# binary outcome
set.seed(1)
N <- 200
X <- matrix(rnorm(N*10), N, 10)</pre>
X <- as.data.frame(X)</pre>
Y <- rbinom(N, 1, plogis(.2*X[, 1] + .1*X[, 2] - .2*X[, 3] +
  .1*X[, 3]*X[, 4] - .2*abs(X[, 4])))
SL.library <- c("SL.glmnet", "SL.glm", "SL.knn", "SL.gam", "SL.mean")
# least squares loss function
test.NNLS <- SuperLearner(Y = Y, X = X, SL.library = SL.library,</pre>
  verbose = TRUE, method = "method.NNLS", family = binomial())
test.NNLS
# negative log binomial likelihood loss function
test.NNloglik <- SuperLearner(Y = Y, X = X, SL.library = SL.library,</pre>
  verbose = TRUE, method = "method.NNloglik", family = binomial())
test.NNloglik
# 1 - AUC loss function
test.AUC <- SuperLearner(Y = Y, X = X, SL.library = SL.library,
  verbose = TRUE, method = "method.AUC", family = binomial())
test.AUC
# 2
# adapted from library(SIS)
set.seed(1)
# training
b \leftarrow c(2, 2, 2, -3*sqrt(2))
n <- 150
p <- 200
truerho <- 0.5
corrmat <- diag(rep(1-truerho, p)) + matrix(truerho, p, p)</pre>
```

```
corrmat[, 4] = sqrt(truerho)
corrmat[4, ] = sqrt(truerho)
corrmat[4, 4] = 1
cholmat <- chol(corrmat)</pre>
x \leftarrow matrix(rnorm(n*p, mean=0, sd=1), n, p)
x <- x
feta <- x[, 1:4]
fprob <- exp(feta) / (1 + exp(feta))</pre>
y <- rbinom(n, 1, fprob)
# test
m <- 10000
newx <- matrix(rnorm(m*p, mean=0, sd=1), m, p)</pre>
newx <- newx
newfeta <- newx[, 1:4]</pre>
newfprob <- exp(newfeta) / (1 + exp(newfeta))</pre>
newy <- rbinom(m, 1, newfprob)</pre>
DATA2 <- data.frame(Y = y, X = x)
newDATA2 <- data.frame(Y = newy, X=newx)</pre>
create.SL.knn <- function(k = c(20, 30)) {
    for(mm in seq(length(k))){
         eval(parse(text = paste('SL.knn.', k[mm], '<- function(..., k = ', k[mm], k[mm], '<- function(..., k = ', k[mm], k[m], k[m],
              ') SL.knn(..., k = k)', sep = '')), envir = .GlobalEnv)
    invisible(TRUE)
create.SL.knn(c(20, 30, 40, 50, 60, 70))
# library with screening
SL.library <- list(c("SL.glmnet", "All"), c("SL.glm", "screen.randomForest"),</pre>
    "SL.randomForest", "SL.knn", "SL.knn.20", "SL.knn.30", "SL.knn.40",
     "SL.knn.50", "SL.knn.60", "SL.knn.70",
    c("SL.polymars", "screen.randomForest"))
test <- SuperLearner(Y = DATA2$Y, X = DATA2[, -1], newX = newDATA2[, -1],
    SL.library = SL.library, verbose = TRUE, family = binomial())
test
## examples with multicore
set.seed(23432, "L'Ecuyer-CMRG") # use L'Ecuyer for multicore seeds. see ?set.seed for details
## training set
n <- 500
p <- 50
X <- matrix(rnorm(n*p), nrow = n, ncol = p)</pre>
colnames(X) <- paste("X", 1:p, sep="")</pre>
X <- data.frame(X)</pre>
Y \leftarrow X[, 1] + sqrt(abs(X[, 2] * X[, 3])) + X[, 2] - X[, 3] + rnorm(n)
## test set
m <- 1000
newX <- matrix(rnorm(m*p), nrow = m, ncol = p)</pre>
colnames(newX) <- paste("X", 1:p, sep="")</pre>
```

```
newX <- data.frame(newX)</pre>
newY \leftarrow newX[, 1] + sqrt(abs(newX[, 2] * newX[, 3])) + newX[, 2] - newX[, 3] + rnorm(m)
# generate Library and run Super Learner
SL.library <- c("SL.glm", "SL.randomForest", "SL.gam",</pre>
  "SL.polymars", "SL.mean")
testMC <- mcSuperLearner(Y = Y, X = X, newX = newX, SL.library = SL.library,</pre>
 method = "method.NNLS")
testMC
## examples with snow
library(parallel)
cl <- makeCluster(2, type = "PSOCK") # can use different types here</pre>
clusterSetRNGStream(cl, iseed = 2343)
# make SL functions available on the clusters, use assignment to avoid printing
foo <- clusterEvalQ(cl, library(SuperLearner))</pre>
testSNOW <- snowSuperLearner(cluster = cl, Y = Y, X = X, newX = newX,</pre>
 SL.library = SL.library, method = "method.NNLS")
testSNOW
stopCluster(cl)
## snow example with user-generated wrappers
# If you write your own wrappers and are using snowSuperLearner()
# These new wrappers need to be added to the SuperLearner namespace and exported to the clusters
# Using a simple example here, but can define any new SuperLearner wrapper
my.SL.wrapper <- function(...) SL.glm(...)</pre>
# assign function into SuperLearner namespace
environment(my.SL.wrapper) <-asNamespace("SuperLearner")</pre>
cl <- makeCluster(2, type = "PSOCK") # can use different types here</pre>
clusterSetRNGStream(cl, iseed = 2343)
# make SL functions available on the clusters, use assignment to avoid printing
foo <- clusterEvalQ(cl, library(SuperLearner))</pre>
clusterExport(cl, c("my.SL.wrapper")) # copy the function to all clusters
testSNOW <- snowSuperLearner(cluster = cl, Y = Y, X = X, newX = newX,</pre>
 SL.library = c("SL.glm", "SL.mean", "my.SL.wrapper"), method = "method.NNLS")
testSNOW
stopCluster(cl)
## timing
replicate(5, system.time(SuperLearner(Y = Y, X = X, newX = newX,
 SL.library = SL.library, method = "method.NNLS")))
replicate(5, system.time(mcSuperLearner(Y = Y, X = X, newX = newX,
 SL.library = SL.library, method = "method.NNLS")))
cl <- makeCluster(2, type = 'PSOCK')</pre>
# make SL functions available on the clusters, use assignment to avoid printing
foo <- clusterEvalQ(cl, library(SuperLearner))</pre>
replicate(5, system.time(snowSuperLearner(cl, Y = Y, X = X, newX = newX,
 SL.library = SL.library, method = "method.NNLS")))
stopCluster(cl)
```

End(Not run)

SuperLearner.control Control parameters for the SuperLearner

Description

Control parameters for the SuperLearner

Usage

```
SuperLearner.control(saveFitLibrary = TRUE, saveCVFitLibrary = FALSE, trimLogit = 0.001)
```

Arguments

saveFitLibrary Logical. Should the fit for each algorithm be saved in the output from SuperLearner. saveCVFitLibrary

Logical. Should cross-validated fits for each algorithm be saved in the output

from SuperLearner.

trimLogit number between 0.0 and 0.5. What level to truncate the logit transformation to

maintain a bounded loss function when using the NNloglik method.

Value

A list containing the control parameters.

SuperLearner.CV.control

Control parameters for the cross validation steps in SuperLearner

Description

Control parameters for the cross validation steps in SuperLearner

Usage

```
SuperLearner.CV.control(V = 10L, stratifyCV = FALSE, shuffle = TRUE,
  validRows = NULL)
```

SuperLearnerNews 57

Arguments

V Integer. Number of splits for the	e V-fold cross-validation step. The default is 10.
-------------------------------------	--

In most cases, between 10 and 20 splits works well.

stratifyCV Logical. Should the data splits be stratified by a binary response? Attempts to

maintain the same ratio in each training and validation sample.

shuffle Logical. Should the rows of X be shuffled before creating the splits.

validRows A List. Use this to pass pre-specified rows for the sample splits. The length of

the list should be V and each entry in the list should contain a vector with the

row numbers of the corresponding validation sample.

Value

A list containing the control parameters

SuperLearnerNews Show the NEW

Show the NEWS file for the SuperLearner package

Description

Show the NEWS file of the SuperLearner package. The function is simply a wrapper for the RShowDoc function

Usage

```
SuperLearnerNews(...)
SuperLearnerDocs(what = 'SuperLearnerR.pdf', ...)
```

Arguments

... additional arguments passed to RShowDoc

what specify what document to open. Currently supports the NEWS file and the PDF

files 'SuperLearner.pdf' and 'SuperLearnerR.pdf'.

Value

A invisible character string given the path to the SuperLearner NEWS file

58 write.method.template

trimLogit

truncated-probabilities logit transformation

Description

computes the logit transformation on the truncated probabilities

Usage

```
trimLogit(x, trim = 1e-05)
```

Arguments

x vector of probabilities.trim value to truncate probabilities at. Currently symmetric truncation (trim and 1-trim).

Value

logit transformed values

Examples

write.method.template Method to estimate the coefficients for the super learner

Description

These functions contain the information on the loss function and the model to combine algorithms

Usage

```
write.method.template(file = "", ...)

## a few built in options:
method.NNLS()
method.NNLS2()
method.NNloglik()
method.CC_LS()
method.CC_nloglik()
method.CC_nloglik()
method.AUC(nlopt_method=NULL, optim_method="L-BFGS-B", bounds=c(0, Inf), normalize=TRUE)
```

write.method.template 59

Arguments

file A connection, or a character string naming a file to print to. Passed to cat.

optim_method Passed to the optim call method. See optim for details.

nlopt_method Either optim_method or nlopt_method must be provided, the other must be

NULL

bounds Bounds for parameter estimates

normalize Logical. Should the parameters be normalized to sum up to 1

... Additional arguments passed to cat.

Details

A SuperLearner method must be a list (or a function to create a list) with exactly 3 elements. The 3 elements must be named require, computeCoef and computePred.

Value

A list containing 3 elements:

require A character vector listing any required packages. Use NULL if no additional

packages are required

computeCoef A function. The arguments are: Z, Y, libraryNames, obsWeights, control,

verbose. The value is a list with two items: cvRisk and coef. This function computes the coefficients of the super learner. As the super learner minimizes the cross-validated risk, the loss function information is contained in this func-

tion as well as the model to combine the algorithms in SL.library.

computePred A function. The arguments are: predY, coef, control. The value is a numeric

vector with the super learner predicted values.

Author(s)

Eric C Polley <Polley.Eric@mayo.edu>

See Also

SuperLearner

```
write.method.template(file = '')
```

60 write.screen.template

write.screen.template screening algorithms for SuperLearner

Description

Screening algorithms for SuperLearner to be used with SL.library.

Usage

```
write.screen.template(file = "", ...)
```

Arguments

file A connection, or a character string naming a file to print to. Passed to cat.

... Additional arguments passed to cat

Details

Explain structure of a screening algorithm here:

Value

whichVariable

A logical vector with the length equal to the number of columns in X. TRUE indicates the variable (column of X) should be included.

Author(s)

```
Eric C Polley <polley.eric@mayo.edu>
```

See Also

SuperLearner

```
write.screen.template(file = '')
```

write.SL.template 61

write.SL.template

Wrapper functions for prediction algorithms in SuperLearner

Description

Template function for SuperLearner prediction wrappers and built in options.

Usage

```
write.SL.template(file = "", ...)
```

Arguments

file A connection, or a character string naming a file to print to. Passed to cat.

... Additional arguments passed to cat

Details

Describe SL.* structure here

Value

A list with two elements:

pred The predicted values for the rows in newX.

fit A list. Contains all objects necessary to get predictions for new observations

from specific algorithm.

Author(s)

Eric C Polley <polley.eric@mayo.edu>

See Also

SuperLearner

```
write.SL.template(file = '')
```

Index

*Topic methods	ksvm, <i>14</i> , <i>40</i>
summary.CV.SuperLearner,48	
*Topic models	1da, <i>15</i> , <i>42</i>
CV.SuperLearner, 5	listWrappers,9
predict.SuperLearner, 19	lm, <i>16</i> , <i>43</i>
recombineCVSL, 20	
recombineSL, 23	mcSuperLearner (SuperLearner), 50
SampleSplitSuperLearner, 26	method.AUC(write.method.template), 58
SuperLearner, 50	<pre>method.CC_LS (write.method.template), 58</pre>
trimLogit, 58	<pre>method.CC_nloglik</pre>
*Topic plot	(write.method.template), 58
plot.CV.SuperLearner, 10	method.NNloglik
*Topic utilities	(write.method.template), 58
CVFolds, 9	method.NNLS(write.method.template), 58
listWrappers, 9	method.NNLS2(write.method.template), 58
SuperLearner.control, 56	method.template
SuperLearner.CV.control, 56	(write.method.template), 58
SuperLearnerNews, 57	
write.method.template, 58	optim, <i>59</i>
write.screen.template,60	
write.SL.template, 61	plot.CV.SuperLearner, 10
	predict.biglasso, 12,32
All(write.screen.template),60	predict.extraTrees, <i>34</i>
biglasso, <i>12</i> , <i>32</i>	predict.glm, <i>13</i> , <i>36</i>
	predict.ksvm, <i>14</i> , <i>40</i>
cat, <i>59–61</i>	predict.lda, <i>15</i> , <i>42</i>
coef.CV.SuperLearner (CV.SuperLearner),	predict.lm, <i>16</i> , <i>43</i>
5	predict.qda, <i>16</i> , <i>44</i>
coef.SuperLearner (SuperLearner), 50	predict.ranger, 17, 45
create.Learner, 3	<pre>predict.SL.bartMachine, 11</pre>
create.SL.xgboost, 4	<pre>predict.SL.bayesglm</pre>
cv.biglasso, 32	(write.SL.template), 61
cv.glmnet, 37	predict.SL.biglasso, 12, 32
CV. SuperLearner, 5, 11, 49	<pre>predict.SL.caret (write.SL.template), 61</pre>
CVFolds, 9	<pre>predict.SL.cforest (write.SL.template),</pre>
C11 01u3, 7	61
extraTrees, 34	<pre>predict.SL.earth(write.SL.template), 61</pre>
	<pre>predict.SL.extraTrees, 12, 34</pre>
glm, 13, 36	<pre>predict.SL.gam (write.SL.template), 61</pre>
glmnet, <i>37</i>	<pre>predict.SL.gbm (write.SL.template), 61</pre>

INDEX 63

predict.SL.glm, 13, 36	SampleSplitSuperLearner, 26
predict.SL.glmnet, 13, 37	screen.corP(write.screen.template),60
predict.SL.ipredbagg	<pre>screen.corRank(write.screen.template),</pre>
(write.SL.template),61	60
predict.SL.kernelKnn,14	<pre>screen.glmnet(write.screen.template),</pre>
<pre>predict.SL.knn (write.SL.template), 61</pre>	60
predict.SL.ksvm, 14, 40	screen.randomForest
predict.SL.lda, 15, 42	(write.screen.template), 60
predict.SL.leekasso	screen.SIS(write.screen.template), 60
(write.SL.template), 61	screen.template
predict.SL.lm, 15, 43	(write.screen.template), 60
<pre>predict.SL.loess(write.SL.template), 61</pre>	<pre>screen.ttest(write.screen.template), 60</pre>
<pre>predict.SL.logreg (write.SL.template),</pre>	SL.bartMachine, 30
61	SL.bayesglm(write.SL.template), 61
<pre>predict.SL.mean (write.SL.template), 61</pre>	SL.biglasso, <i>12</i> , 31
<pre>predict.SL.nnet(write.SL.template), 61</pre>	SL.caret(write.SL.template), 61
<pre>predict.SL.nnls(write.SL.template), 61</pre>	SL.cforest, 32
predict.SL.polymars	SL.earth(write.SL.template), 61
(write.SL.template), 61	SL.extraTrees, 33
predict.SL.qda, 16, 44	SL.gam(write.SL.template), 61
predict.SL.randomForest	SL.gbm(write.SL.template), 61
(write.SL.template), 61	SL.glm, 13, 35
predict.SL.ranger, 17	SL.glm.interaction(write.SL.template),
<pre>predict.SL.ridge (write.SL.template), 61</pre>	61
<pre>predict.SL.rpart(write.SL.template), 61</pre>	SL.glmnet, <i>14</i> , <i>32</i> , 36
predict.SL.speedglm, 17, 47	SL.ipredbagg(write.SL.template), 61
predict.SL.speedlm, 18, 47	SL.kernelKnn, 38
<pre>predict.SL.step(write.SL.template), 61</pre>	SL.knn(write.SL.template), 61
<pre>predict.SL.stepAIC(write.SL.template),</pre>	SL.ksvm, <i>14</i> , 39
61	SL.lda, 15, 41, 44
<pre>predict.SL.svm (write.SL.template), 61</pre>	SL.leekasso(write.SL.template), 61
<pre>predict.SL.template</pre>	SL.1m, 16, 42
(write.SL.template), 61	SL.loess(write.SL.template),61
predict.SL.xgboost, 18	SL.logreg(write.SL.template), 61
predict.speedglm, 17, 47	SL.mean(write.SL.template), 61
predict.speedlm, 18,47	SL.nnet(write.SL.template), 61
predict.SuperLearner, 19	SL.nnls(write.SL.template), 61
print.CV.SuperLearner	SL.polymars (write.SL.template), 61
(CV.SuperLearner), 5	SL.qda, 16, 42, 43
print.summary.CV.SuperLearner	SL.randomForest (write.SL.template), 61
(summary.CV.SuperLearner), 48	SL.ranger, 17, 44, 45
print.SuperLearner (SuperLearner), 50	SL.ridge(write.SL.template),61
	SL.rpart(write.SL.template),61
qda, <i>16</i> , <i>44</i>	SL.rpartPrune (write.SL.template), 61
	SL.speedglm, 13, 17, 18, 36, 46, 47
ranger, 17, 45	SL.speedlm, 16, 18, 43, 47
recombineCVSL, 20	SL.step(write.SL.template), 61
recombineSL, 22, 23	SL.stepAIC(write.SL.template), 61

INDEX

```
SL.svm(write.SL.template), 61
SL.template (write.SL.template), 61
SL.xgboost, 47
snowSuperLearner (SuperLearner), 50
speedglm, 17, 47
speedlm, 18, 47
summary.CV.SuperLearner, 11,48
SuperLearner, 8–10, 19, 50, 59–61
SuperLearner.control, 6, 27, 51, 56
SuperLearner.CV.control, 6, 9, 51, 56
SuperLearnerDocs (SuperLearnerNews), 57
SuperLearnerNews, 57
trimLogit, 58
write.method.template, 58
write.screen.template, 60
write.SL.template, 61
```