# Package 'SuperLearner'

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<b>Description</b> 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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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 = 20, family = gaussian(), SL.library,
  method = "method.NNLS", id = NULL, verbose = FALSE,
  control = list(saveFitLibrary = FALSE), cvControl = list(),
  obsWeights = NULL, saveAll = TRUE, parallel = "seq")
```

# **Arguments**

Υ	The outcome.
Χ	The covariates.
V	The number of folds for CV.SuperLearner. This is not the number of folds for SuperLearner. The number of folds for SuperLearner is controlled with cvControl.
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 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",

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"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.

verbose

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

control

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 cross-validation process. 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?

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.

#### 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).

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#### 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, other-

wise 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

```
set.seed(23432)
## training set
n <- 500
p <- 50</pre>
```

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```
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)

# build Library and run Super Learner
SL.library <- c("SL.glm", "SL.randomForest", "SL.gam", "SL.polymars", "SL.mean")
## Not run:
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)

## End(Not run)</pre>
```

**CVFolds** 

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.
Υ	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 <eric.polley@nih.gov>
```

#### 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.

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#### 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

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

#### **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 <eric.polley@nih.gov>
```

#### See Also

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

```
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
X Original data set used to fit object
Y Original outcome used to fit object

onlySL Logical. If TRUE, only compute predictions for algorithms with non-zero coef-

ficients 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 <eric.polley@nih.gov>
```

#### See Also

SuperLearner

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 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.NNLS2", "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).

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

ging).

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 V-fold 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.

# 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, other-

wise 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>

#### See Also

recombineSL

```
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$coef
    SL.glmnet_All SL.glm_All SL.knn_All SL.gam_All SL.mean_All
# 1
        0.0000000 0.00000000 0.000000000 0.4143862 0.5856138
# 2
        0.0000000 0.00000000 0.304802397 0.3047478
                                                  0.3904498
# 3
        0.0000000 0.00000000 0.002897533 0.5544075
                                                 0.4426950
# 4
        0.0000000 0.20322642 0.000000000 0.1121891
                                                   0.6845845
# 5
        0.1743973 0.00000000 0.032471026 0.3580624
                                                   0.4350693
# 6
        0.0000000 0.00000000 0.099881535 0.3662309
                                                   0.5338876
# 7
        0.0000000 0.00000000 0.234876082 0.2942472
                                                   0.4708767
# 8
        0.0000000 0.06424676 0.113988158 0.5600208
                                                   0.2617443
# 9
        0.0000000 0.00000000 0.338030342 0.2762604
                                                   0.3857093
# 10
        0.3022442 0.00000000 0.294226204 0.1394534
                                                   0.2640762
# negative log binomial likelihood loss function
cvfit_nnloglik <- recombineCVSL(cvfit_nnls, method = "method.NNloglik")</pre>
cvfit_nnloglik$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 \quad 0.1644188 \ 0.00000000 \quad 0.2387919 \quad 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 \quad 0.0000000 \quad 0.47538172 \quad 0.5080311 \quad 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
# 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.
cvfit_nnloglik2 <- CV.SuperLearner(Y = Y, X = X, V = 10, SL.library = SL.library,</pre>
 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
        # 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.

Y 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 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).

AUC

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

ging).

#### **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.

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)

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. http://www.bepress.com/sagmb/vol6/iss1/art25

```
## 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 <- 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")</pre>
# least squares loss function
set.seed(1) # for reproducibility
fit_nnls <- SuperLearner(Y = Y, X = X, SL.library = SL.library,</pre>
  verbose = TRUE, method = "method.NNLS", family = binomial())
fit_nnls
                     Risk
# SL.glmnet_All 0.2439433 0.01293059
# SL.glm_All 0.2461245 0.08408060
             0.2604000 0.09600353
# SL.knn_All
# 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.
set.seed(1)
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 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().

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 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", 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.1ibrary 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)

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

#### 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. http://www.bepress.com/sagmb/vol6/iss1/art25

```
## 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 \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 <- SampleSplitSuperLearner(Y = Y, X = X, newX = newX, SL.library = SL.library,
  verbose = TRUE, method = "method.NNLS")
test
# library with screening
SL.library <- list(c("SL.glmnet", "All"), c("SL.glm", "screen.randomForest",
  "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 <- matrix(rnorm(N*10), N, 10)</pre>
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)
```

summary.CV.SuperLearner

Summary Function for Cross-Validated Super Learner

# Description

summary method for the CV. SuperLearner function

#### Usage

```
## S3 method for class 'CV.SuperLearner'
summary(object, obsWeights = NULL, ...)
## S3 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.

x 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)
```

#### **Arguments**

id

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

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

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.

cvControl A list of parameters to control the cross-validation process. Parameters include

 $\label{thm:control} \textit{V}, \textit{stratifyCV}, \textit{shuffle} \textit{ and } \textit{validRows}. \textit{ See SuperLearner.CV}. \textit{control} \textit{ for } \\$ 

details.

#### **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.

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

#### 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. http://www.bepress.com/sagmb/vol6/iss1/art25

```
## 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 \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,
  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 \leftarrow matrix(rnorm(N*10), N, 10)
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,</pre>
  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 <- matrix(rnorm(n*p, mean=0, sd=1), n, p)</pre>
x <- x
feta <- x[, 1:4]
fprob <- exp(feta) / (1 + exp(feta))</pre>
y \leftarrow 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],</pre>
      ') 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)
## 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)
testSNOW <- snowSuperLearner(cluster = cl, Y = Y, X = X, newX = newX,</pre>
  SL.library = SL.library, method = "method.NNLS")
testSNOW
stopCluster(cl)
```

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```
## 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)
clusterExport(cl, c("my.SL.wrapper")) # copy the function to all clusters
testSNOW <- snowSuperLearner(cluster = cl, Y = Y, X = X, newX = newX,
 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>
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, trimLogit = 0.001)
```

#### **Arguments**

```
saveFitLibrary Logical. Should the fit 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.

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#### 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)
```

# Arguments

V	Integer.	Number o	of splits for the	V-fold cross-validation ster	o. The default is 10.
V	micgei.	Number o	n spins for the	v-1010 C1055-validation Step	). The uclaun is io.

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 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', ...)
```

trimLogit 27

# **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

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

28 write.method.template

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_ls()
method.AUC(optim_method = "Nelder-Mead")
```

#### **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.

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 <eric.polley@nih.gov>

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#### See Also

SuperLearner

# **Examples**

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

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 <eric.polley@nih.gov>
```

#### See Also

```
SuperLearner
```

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

30 write.SL.template

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 <eric.polley@nih.gov>
```

#### See Also

```
SuperLearner
```

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

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