# Package 'sharp'

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```
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Description In stability selection (N Meinshausen, P Bühlmann (2010) <doi:10.1111/j.1467-
     9868.2010.00740.x>) and consensus cluster-
     ing (S Monti et al (2003) <doi:10.1023/A:1023949509487>), resampling tech-
     niques are used to enhance the reliability of the results. In this package (B Bod-
     inier et al (2025) <doi:10.18637/jss.v112.i05>), hyper-parameters are calibrated by maximis-
     ing model stability, which is measured under the null hypothesis that all selection (or co-
     membership) probabilities are identical (B Bod-
     inier et al (2023a) <doi:10.1093/jrsssc/qlad058> and B Bod-
     inier et al (2023b) <doi:10.1093/bioinformatics/btad635>). Functions are readily imple-
     mented for the use of LASSO regression, sparse PCA, sparse (group) PLS or graphi-
     cal LASSO in stability selection, and hierarchical clustering, partition-
     ing around medoids, K means or Gaussian mixture models in consensus clustering.
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Suggests cluster, corpcor, dbscan, elasticnet, gglasso, mixOmics,
     nnet, OpenMx, RCy3, randomcoloR, rCOSA, rmarkdown, rpart,
     sgPLS, sparcl, survival (>= 3.2.13), testthat (>= 3.0.0),
     visNetwork
```

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${\bf Additional\_repositories}\   {\tt https://barbarabodinier.github.io/drat}$
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# **Description**

sharp-package

In stability selection and consensus clustering, resampling techniques are used to enhance the reliability of the results. In this package, hyper-parameters are calibrated by maximising model stability, which is measured under the null hypothesis that all selection (or co-membership) probabilities are identical. Functions are readily implemented for the use of LASSO regression, sparse PCA, sparse (group) PLS or graphical LASSO in stability selection, and hierarchical clustering, partitioning around medoids, K means or Gaussian mixture models in consensus clustering.

sharp: Stability-enHanced Approaches using Resampling Procedures

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#### **Details**

Package: sharp
Type: Package
Version: 1.4.6
Date: 2025-03-24
License: GPL (>= 3)

#### References

Bodinier B, Rodrigues S, Karimi M, Filippi S, Chiquet J, Chadeau-Hyam M (2025). "Stability Selection and Consensus Clustering in R: The R Package sharp." *Journal of Statistical Software*, **112**(5), btad635. doi:10.18637/jss.v112.i05.

Bodinier B, Filippi S, Nøst TH, Chiquet J, Chadeau-Hyam M (2023). "Automated calibration for stability selection in penalised regression and graphical models." *Journal of the Royal Statistical Society Series C: Applied Statistics*, qlad058. ISSN 0035-9254, doi:10.1093/jrsssc/qlad058, https://academic.oup.com/jrsssc/advance-article-pdf/doi/10.1093/jrsssc/qlad058/50878777/qlad058.pdf.

Meinshausen N, Bühlmann P (2010). "Stability selection." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **72**(4), 417-473. doi:10.1111/j.14679868.2010.00740.x.

Monti S, Tamayo P, Mesirov J, Golub T (2003). "Consensus Clustering: A Resampling-Based Method for Class Discovery and Visualization of Gene Expression Microarray Data." *Machine Learning*, **52**(1), 91–118. doi:10.1023/A:1023949509487.

#### **Examples**

```
oldpar <- par(no.readonly = TRUE)
par(mar = c(5, 5, 5, 5))
## Regression models
# Data simulation
set.seed(1)
simul <- SimulateRegression(n = 100, pk = 50)</pre>
# Stability selection
stab <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata)</pre>
CalibrationPlot(stab)
summary(stab)
SelectedVariables(stab)
## Graphical models
# Data simulation
set.seed(1)
simul <- SimulateGraphical(n = 100, pk = 20, topology = "scale-free")</pre>
# Stability selection
```

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```
stab <- GraphicalModel(xdata = simul$data)</pre>
CalibrationPlot(stab)
summary(stab)
plot(stab)
## PCA models
if (requireNamespace("elasticnet", quietly = TRUE)) {
  # Data simulation
  set.seed(1)
  simul <- SimulateComponents(pk = c(5, 3, 4))</pre>
  plot(simul)
  # Stability selection
  stab <- BiSelection(</pre>
    xdata = simul$data,
    ncomp = 3,
    implementation = SparsePCA
  CalibrationPlot(stab)
  summary(stab)
  SelectedVariables(stab)
}
## PLS models
if (requireNamespace("sgPLS", quietly = TRUE)) {
  # Data simulation
  set.seed(1)
  simul <- SimulateRegression(n = 50, pk = c(10, 20, 30), family = "gaussian")</pre>
  # Stability selection
  stab <- BiSelection(</pre>
    xdata = simul$xdata, ydata = simul$ydata,
    family = "gaussian", ncomp = 3,
    implementation = SparsePLS
  CalibrationPlot(stab)
  summary(stab)
  plot(stab)
par(oldpar)
```

6 AggregatedEffects

#### **Description**

Computes descriptive statistics (defined by FUN) for coefficients of the (calibrated) models conditionally on selection across resampling iterations.

#### Usage

```
AggregatedEffects(
  stability,
  lambda_id = NULL,
  side = "X",
  comp = 1,
  FUN = stats::median,
  ...
)
```

# **Arguments**

stability	output of VariableSelection or BiSelection.
lambda_id	parameter ID with respect to the grid Lambda. If NULL, aggregated coefficients across the models run with the calibrated parameter are returned.
side	character string indicating if coefficients of predictors ( $side="X"$ ) or outcomes ( $side="Y"$ ) should be returned. Only applicable to PLS models.
comp	component ID. Only applicable to PLS models.
FUN	function to use to aggregate coefficients of visited models over resampling iterations. Recommended functions include median or mean.
	additional arguments to be passed to FUN.

#### Value

A matrix of summarised coefficients conditionally on selection across resampling iterations. Missing values (NA) are returned for variables that are never selected.

#### See Also

```
VariableSelection, BiSelection, Refit
```

# **Examples**

```
# Example with univariate outcome
set.seed(1)
simul <- SimulateRegression(n = 100, pk = 50, family = "gaussian")
stab <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata, family = "gaussian")
median_betas <- AggregatedEffects(stab)

# Comparison with refitted model
refitted <- Refit(xdata = simul$xdata, ydata = simul$ydata, stability = stab)
refitted_betas <- coef(refitted)[-1, 1]
plot(median_betas[names(refitted_betas), ], refitted_betas,</pre>
```

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```
panel.first = abline(0, 1, lty = 2)
# Extracting mean betas conditionally on selection
mean_betas <- AggregatedEffects(stab, FUN = mean)</pre>
plot(median_betas, mean_betas)
# Regression with multivariate outcomes
set.seed(1)
simul <- SimulateRegression(n = 100, pk = 50, q = 2, family = "gaussian")</pre>
stab <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata, family = "mgaussian")</pre>
median_betas <- AggregatedEffects(stab)</pre>
dim(median_betas)
# Sparse PLS with multivariate outcome
if (requireNamespace("sgPLS", quietly = TRUE)) {
 set.seed(1)
 simul <- SimulateRegression(n = 50, pk = 15, q = 3, family = "gaussian")</pre>
 x <- simul$xdata
 y <- simul$ydata
 stab <- BiSelection(</pre>
    xdata = x, ydata = y,
    family = "gaussian", ncomp = 3,
   LambdaX = seq_len(ncol(x) - 1),
    implementation = SparsePLS
 median_betas <- AggregatedEffects(stab)</pre>
 dim(median_betas)
 median_betas <- AggregatedEffects(stab, side = "Y")</pre>
 dim(median_betas)
}
```

ArgmaxId

*Calibrated hyper-parameter(s)* 

## **Description**

Extracts the calibrated hyper-parameters (or their indices for ArgmaxId) with respect to the grids provided in Lambda and  $pi_list$  in argument stability.

# Usage

```
ArgmaxId(stability = NULL, S = NULL)
Argmax(stability)
```

# **Arguments**

stability output of VariableSelection or GraphicalModel.

S

matrix of stability scores obtained with different combinations of parameters where rows correspond to different values of the parameter controlling the level of sparsity in the underlying feature selection algorithm and columns correspond to different values of the threshold in selection proportions. If S=NULL, argument stability must be provided.

#### Value

A matrix of hyper-parameters (Argmax) or indices (ArgmaxId). For multi-block graphical models, rows correspond to different blocks.

#### See Also

VariableSelection, GraphicalModel

#### **Examples**

```
# Data simulation
set.seed(1)
simul <- SimulateGraphical(pk = 20)

# Stability selection
stab <- GraphicalModel(xdata = simul$data)

# Extracting calibrated hyper-parameters
Argmax(stab)

# Extracting calibrated hyper-parameters IDs
ids <- ArgmaxId(stab)
ids

# Relationship between the two functions
stab$Lambda[ids[1], 1]
stab$params$pi_list[ids[2]]</pre>
```

BiSelection

Stability selection of predictors and/or outcomes

# **Description**

Performs stability selection for dimensionality reduction. The underlying variable selection algorithm (e.g. sparse PLS) is run with different combinations of parameters controlling the sparsity (e.g. number of selected variables per component) and thresholds in selection proportions. These hyper-parameters are jointly calibrated by maximisation of the stability score.

# Usage

```
BiSelection(
  xdata,
  ydata = NULL,
 group_x = NULL,
 group_y = NULL,
 LambdaX = NULL,
 LambdaY = NULL,
 AlphaX = NULL,
 AlphaY = NULL,
  ncomp = 1,
  scale = TRUE,
 pi_list = seq(0.01, 0.99, by = 0.01),
 K = 100,
  tau = 0.5,
  seed = 1,
  n_cat = NULL,
  family = "gaussian",
  implementation = SparsePLS,
  resampling = "subsampling",
  cpss = FALSE,
  PFER_method = "MB",
 PFER_thr = Inf,
 FDP_thr = Inf,
 n_{cores} = 1,
  output_data = FALSE,
  verbose = TRUE,
 beep = NULL,
)
```

#### **Arguments**

xdata	matrix of predictors with observations as rows and variables as columns.
ydata	optional vector or matrix of outcome(s). If family is set to "binomial" or "multinomial", ydata can be a vector with character/numeric values or a factor.
group_x	vector encoding the grouping structure among predictors. This argument indicates the number of variables in each group. Only used for models with group penalisation (e.g. implementation=GroupPLS or implementation=SparseGroupPLS).
group_y	optional vector encoding the grouping structure among outcomes. This argument indicates the number of variables in each group. Only used if implementation=GroupPLS or implementation=SparseGroupPLS.
LambdaX	matrix of parameters controlling the number of selected variables (for sparse PCA/PLS) or groups (for group and sparse group PLS) in X.
LambdaY	matrix of parameters controlling the number of selected variables (for sparse

PLS) or groups (for group or sparse group PLS) in Y. Only used if family="gaussian".

AlphaX matrix of parameters controlling the level of sparsity within groups in X. Only used if implementation=SparseGroupPLS. AlphaY matrix of parameters controlling the level of sparsity within groups in X. Only used if implementation=SparseGroupPLS and family="gaussian". ncomp number of components. logical indicating if the data should be scaled (i.e. transformed so that all variscale ables have a standard deviation of one). vector of thresholds in selection proportions. If n\_cat=NULL or n\_cat=2, these pi\_list values must be >0 and <1. If  $n_{cat}=3$ , these values must be >0.5 and <1. K number of resampling iterations. subsample size. Only used if resampling="subsampling" and cpss=FALSE. tau seed value of the seed to initialise the random number generator and ensure reproducibility of the results (see set.seed). n\_cat computation options for the stability score. Default is NULL to use the score based on a z test. Other possible values are 2 or 3 to use the score based on the negative log-likelihood. family type of PLS model. This parameter must be set to family="gaussian" for continuous outcomes, or to family="binomial" for categorical outcomes. Only used if ydata is provided. implementation function to use for feature selection. Possible functions are: SparsePCA, SparsePLS, GroupPLS, SparseGroupPLS. resampling approach. Possible values are: "subsampling" for sampling withresampling out replacement of a proportion tau of the observations, or "bootstrap" for sampling with replacement generating a resampled dataset with as many observations as in the full sample. Alternatively, this argument can be a function to use for resampling. This function must use arguments named data and tau and return the IDs of observations to be included in the resampled dataset. cpss logical indicating if complementary pair stability selection should be done. For this, the algorithm is applied on two non-overlapping subsets of half of the observations. A feature is considered as selected if it is selected for both subsamples. With this method, the data is split K/2 times (K models are fitted). Only used if PFER\_method="MB". PFER\_method method used to compute the upper-bound of the expected number of False Positives (or Per Family Error Rate, PFER). If PFER\_method="MB", the method proposed by Meinshausen and Bühlmann (2010) is used. If PFER\_method="SS", the method proposed by Shah and Samworth (2013) under the assumption of unimodality is used. threshold in PFER for constrained calibration by error control. If PFER\_thr=Inf PFER\_thr and FDP\_thr=Inf, unconstrained calibration is used (the default). FDP\_thr threshold in the expected proportion of falsely selected features (or False Discovery Proportion) for constrained calibration by error control. If PFER\_thr=Inf and FDP\_thr=Inf, unconstrained calibration is used (the default). number of cores to use for parallel computing (see argument workers in multisession). n\_cores

Using n\_cores>1 is only supported with optimisation="grid\_search".

output\_data logical indicating if the input datasets xdata and ydata should be included in

the output.

verbose logical indicating if a loading bar and messages should be printed.

beep sound indicating the end of the run. Possible values are: NULL (no sound) or an

integer between 1 and 11 (see argument sound in beep).

... additional parameters passed to the functions provided in implementation or

resampling.

#### **Details**

In stability selection, a feature selection algorithm is fitted on K subsamples (or bootstrap samples) of the data with different parameters controlling the sparsity (LambdaX, LambdaY, AlphaX, and/or AlphaY). For a given (set of) sparsity parameter(s), the proportion out of the K models in which each feature is selected is calculated. Features with selection proportions above a threshold pi are considered stably selected. The stability selection model is controlled by the sparsity parameter(s) (denoted by  $\lambda$ ) for the underlying algorithm, and the threshold in selection proportion:

$$V_{\lambda,\pi} = \{j : p_{\lambda}(j) \ge \pi\}$$

For sparse and sparse group dimensionality reduction, "feature" refers to variable (variable selection model). For group PLS, "feature" refers to group (group selection model). For (sparse) group PLS, groups need to be defined *a priori* and specified in arguments group\_x and/or group\_y.

These parameters can be calibrated by maximisation of a stability score (see ConsensusScore if n\_cat=NULL or StabilityScore otherwise) calculated under the null hypothesis of equiprobability of selection.

It is strongly recommended to examine the calibration plot carefully to check that the grids of parameters Lambda and pi\_list do not restrict the calibration to a region that would not include the global maximum (see CalibrationPlot). In particular, the grid Lambda may need to be extended when the maximum stability is observed on the left or right edges of the calibration heatmap. In some instances, multiple peaks of stability score can be observed. Simulation studies suggest that the peak corresponding to the largest number of selected features tend to give better selection performances. This is not necessarily the highest peak (which is automatically retained by the functions in this package). The user can decide to manually choose another peak.

To control the expected number of False Positives (Per Family Error Rate) in the results, a threshold PFER\_thr can be specified. The optimisation problem is then constrained to sets of parameters that generate models with an upper-bound in PFER below PFER\_thr (see Meinshausen and Bühlmann (2010) and Shah and Samworth (2013)).

Possible resampling procedures include defining (i) K subsamples of a proportion tau of the observations, (ii) K bootstrap samples with the full sample size (obtained with replacement), and (iii) K/2 splits of the data in half for complementary pair stability selection (see arguments resampling and cpss). In complementary pair stability selection, a feature is considered selected at a given resampling iteration if it is selected in the two complementary subsamples.

For categorical outcomes (argument family is "binomial" or "multinomial"), the proportions of observations from each category in all subsamples or bootstrap samples are the same as in the full sample.

To ensure reproducibility of the results, the starting number of the random number generator is set to seed.

For parallelisation, stability selection with different sets of parameters can be run on n\_cores cores. Using n\_cores > 1 creates a multisession.

#### Value

An object of class bi\_selection. A list with:

summary a matrix of the best stability scores and corresponding parameters controlling

the level of sparsity in the underlying algorithm for different numbers of components. Possible columns include: comp (component index), nx (number of predictors to include, parameter of the underlying algorithm), alphax (sparsity within the predictor groups, parameter of the underlying algorithm), pix (threshold in selection proportion for predictors), ny (number of outcomes to include, parameter of the underlying algorithm), alphay (sparsity within the outcome groups, parameter of the underlying algorithm), piy (threshold in selection proportion for outcomes), S (stability score). Columns that are not relevant to the model are not reported (e.g. alpha\_x and alpha\_y are not returned for sparse

PLS models).

summary\_full a matrix of the best stability scores for different combinations of parameters

controlling the sparsity and components.

selectedX a binary matrix encoding stably selected predictors.

selpropX a matrix of calibrated selection proportions for predictors.

selectedY a binary matrix encoding stably selected outcomes. Only returned for PLS mod-

els.

selpropY a matrix of calibrated selection proportions for outcomes. Only returned for PLS

models.

selected a binary matrix encoding stable relationships between predictor and outcome

variables. Only returned for PLS models.

selectedX\_full a binary matrix encoding stably selected predictors.

selpropX\_full a matrix of selection proportions for predictors.

selectedY\_full a binary matrix encoding stably selected outcomes. Only returned for PLS mod-

els.

selpropY\_full a matrix of selection proportions for outcomes. Only returned for PLS models.

coefX an array of estimated loadings coefficients for the different components (rows),

for the predictors (columns), as obtained across the K visited models (along the

third dimension).

coefY an array of estimated loadings coefficients for the different components (rows),

for the outcomes (columns), as obtained across the K visited models (along the

third dimension). Only returned for PLS models.

method a list with type="bi\_selection" and values used for arguments implementation,

family, scale, resampling, cpss and PFER\_method.

params a list with values used for arguments K, group\_x, group\_y, LambdaX, LambdaY,

AlphaX, AlphaY, pi\_list, tau, n\_cat, pk, n (number of observations), PFER\_thr,

FDP\_thr and seed. The datasets xdata and ydata are also included if output\_data=TRUE.

The rows of summary and columns of selectedX, selectedY, selpropX, selpropY, selected, coefX and coefY are ordered in the same way and correspond to components and parameter values stored in summary. The rows of summary\_full and columns of selectedX\_full, selectedY\_full, selpropX\_full and selpropY\_full are ordered in the same way and correspond to components and parameter values stored in summary\_full.

#### References

Bodinier B, Filippi S, Nøst TH, Chiquet J, Chadeau-Hyam M (2023). "Automated calibration for stability selection in penalised regression and graphical models." *Journal of the Royal Statistical Society Series C: Applied Statistics*, qlad058. ISSN 0035-9254, doi:10.1093/jrsssc/qlad058, https://academic.oup.com/jrsssc/advance-article-pdf/doi/10.1093/jrsssc/qlad058/50878777/qlad058.pdf.

Shah RD, Samworth RJ (2013). "Variable selection with error control: another look at stability selection." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **75**(1), 55-80. doi:10.1111/j.14679868.2011.01034.x.

Meinshausen N, Bühlmann P (2010). "Stability selection." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **72**(4), 417-473. doi:10.1111/j.14679868.2010.00740.x.

Liquet B, de Micheaux PL, Hejblum BP, Thiébaut R (2016). "Group and sparse group partial least square approaches applied in genomics context." *Bioinformatics*, **32**(1), 35-42. ISSN 1367-4803, doi:10.1093/bioinformatics/btv535.

KA LC, Rossouw D, Robert-Granié C, Besse P (2008). "A sparse PLS for variable selection when integrating omics data." *Stat Appl Genet Mol Biol*, **7**(1), Article 35. ISSN 1544-6115, doi:10.2202/15446115.1390.

Shen H, Huang JZ (2008). "Sparse principal component analysis via regularized low rank matrix approximation." *Journal of Multivariate Analysis*, **99**(6), 1015-1034. ISSN 0047-259X, doi:10.1016/j.jmva.2007.06.007.

Zou H, Hastie T, Tibshirani R (2006). "Sparse Principal Component Analysis." *Journal of Computational and Graphical Statistics*, **15**(2), 265-286. doi:10.1198/106186006X113430.

#### See Also

SparsePCA, SparsePLS, GroupPLS, SparseGroupPLS, VariableSelection, Resample, StabilityScore Other stability functions: Clustering(), GraphicalModel(), StructuralModel(), VariableSelection()

#### **Examples**

```
if (requireNamespace("sgPLS", quietly = TRUE)) {
  oldpar <- par(no.readonly = TRUE)
  par(mar = c(12, 5, 1, 1))

## Sparse Principal Component Analysis

# Data simulation
  set.seed(1)
  simul <- SimulateComponents(pk = c(5, 3, 4))

# sPCA: sparsity on X (unsupervised)
  stab <- BiSelection(</pre>
```

```
xdata = simul$data,
  ncomp = 2,
 LambdaX = seq_len(ncol(simul$data) - 1),
  implementation = SparsePCA
)
print(stab)
# Calibration plot
CalibrationPlot(stab)
# Visualisation of the results
summary(stab)
plot(stab)
SelectedVariables(stab)
## Sparse (Group) Partial Least Squares
# Data simulation (continuous outcomes)
simul <- SimulateRegression(n = 100, pk = 15, q = 3, family = "gaussian")</pre>
x <- simul$xdata
y <- simul$ydata
\# sPLS: sparsity on X
stab <- BiSelection(</pre>
  xdata = x, ydata = y,
  family = "gaussian", ncomp = 3,
 LambdaX = seq_len(ncol(x) - 1),
  implementation = SparsePLS
CalibrationPlot(stab)
summary(stab)
plot(stab)
# sPLS: sparsity on both X and Y
stab <- BiSelection(</pre>
 xdata = x, ydata = y,
  family = "gaussian", ncomp = 3,
 LambdaX = seq_len(ncol(x) - 1),
 LambdaY = seq_len(ncol(y) - 1),
  implementation = SparsePLS,
 n_cat = 2
)
CalibrationPlot(stab)
summary(stab)
plot(stab)
\# sgPLS: sparsity on X
stab <- BiSelection(</pre>
 xdata = x, ydata = y, K = 10,
  group_x = c(2, 8, 5),
  family = "gaussian", ncomp = 3,
```

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```
LambdaX = seq_len(2), AlphaX = seq(0.1, 0.9, by = 0.1),
   implementation = SparseGroupPLS
)
CalibrationPlot(stab)
summary(stab)
par(oldpar)
}
```

BlockLambdaGrid

Multi-block grid

## **Description**

Generates a matrix of parameters controlling the sparsity of the underlying selection algorithm for multi-block calibration.

# Usage

```
BlockLambdaGrid(Lambda, lambda_other_blocks = NULL)
```

#### **Arguments**

Lambda

vector or matrix of penalty parameters.

lambda\_other\_blocks

optional vector of penalty parameters to use for other blocks in the iterative multi-block procedure.

#### Value

A list with:

Lambda

a matrix of (block-specific) penalty parameters. In multi-block stability selection, rows correspond to sets of penalty parameters and columns correspond to different blocks.

Sequential\_template

logical matrix encoding the type of procedure for data with multiple blocks in stability selection graphical modelling. For multi-block estimation, each block is calibrated separately while others blocks are weakly penalised (TRUE only for the block currently being calibrated and FALSE for other blocks). Other approaches with joint calibration of the blocks are allowed (all entries are set to TRUE).

#### See Also

GraphicalModel

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#### **Examples**

```
# Multi-block grid
Lambda <- matrix(</pre>
  c(
    0.8, 0.6, 0.3,
    0.5, 0.4, 0.2,
    0.7, 0.5, 0.1
  ncol = 3, byrow = TRUE
mygrid <- BlockLambdaGrid(Lambda, lambda_other_blocks = 0.1)</pre>
# Multi-parameter grid (not recommended)
Lambda <- matrix(</pre>
  c(
    0.8, 0.6, 0.3,
    0.5, 0.4, 0.2,
    0.7, 0.5, 0.1
  ),
  ncol = 3, byrow = TRUE
)
mygrid <- BlockLambdaGrid(Lambda, lambda_other_blocks = NULL)</pre>
```

CalibrationPlot

Calibration plot

# **Description**

Creates a plot showing the stability score as a function of the parameter(s) controlling the level of sparsity in the underlying feature selection algorithm and/or the threshold in selection proportions. See examples in VariableSelection, GraphicalModel, Clustering and BiSelection.

# Usage

```
CalibrationPlot(
   stability,
   block_id = NULL,
   col = NULL,
   pch = 19,
   cex = 0.7,
   xlim = NULL,
   ylim = NULL,
   bty = "o",
   lines = TRUE,
   lty = 3,
   lwd = 2,
   show_argmax = TRUE,
   show_pix = FALSE,
```

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```
show_piy = FALSE,
 offset = 0.3,
 legend = TRUE,
 legend_length = NULL,
 legend_range = NULL,
 ncol = 1,
 xlab = NULL,
 ylab = NULL,
 zlab = expression(italic(q)),
 xlas = 2,
 ylas = NULL,
 zlas = 2,
 cex.lab = 1.5,
 cex.axis = 1,
 cex.legend = 1.2,
 xgrid = FALSE,
 ygrid = FALSE,
 params = c("ny", "alphay", "nx", "alphax")
)
```

# Arguments

stability	output of VariableSelection, GraphicalModel or BiSelection.
block_id	ID of the block to visualise. Only used for multi-block stability selection graphical models. If block_id=NULL, all blocks are represented in separate panels.
col	vector of colours.
pch	type of point, as in points.
cex	size of point.
xlim	displayed range along the x-axis. Only used if stability is the output of BiSelection.
ylim	displayed range along the y-axis. Only used if stability is the output of BiSelection.
bty	character string indicating if the box around the plot should be drawn. Possible values include: "o" (default, the box is drawn), or "n" (no box).
lines	logical indicating if the points should be linked by lines. Only used if stability is the output of BiSelection or Clustering.
lty	line type, as in par. Only used if stability is the output of BiSelection.
lwd	line width, as in par. Only used if stability is the output of BiSelection.
show_argmax	logical indicating if the calibrated parameter(s) should be indicated by lines.
show_pix	logical indicating if the calibrated threshold in selection proportion in X should be written for each point. Only used if stability is the output of BiSelection.
show_piy	logical indicating if the calibrated threshold in selection proportion in Y should be written for each point. Only used if stability is the output of BiSelection with penalisation of the outcomes.

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distance between the point and the text, as in text. Only used if show\_pix=TRUE offset or show\_piy=TRUE. legend logical indicating if the legend should be included. length of the colour bar. Only used if stability is the output of VariableSelection legend\_length or Graphical Model. legend\_range range of the colour bar. Only used if stability is the output of VariableSelection or Graphical Model. ncol integer indicating the number of columns in the legend. xlab label of the x-axis. ylab label of the y-axis. zlab label of the z-axis. Only used if stability is the output of VariableSelection or Graphical Model. xlas orientation of labels on the x-axis, as las in par. ylas orientation of labels on the y-axis, as las in par. zlas orientation of labels on the z-axis, as las in par. cex.lab font size for labels. cex.axis font size for axes. cex.legend font size for text legend entries. logical indicating if a vertical grid should be drawn. Only used if stability is xgrid the output of BiSelection.

logical indicating if a horizontal grid should be drawn. Only used if stability

vector of possible parameters if stability is of class bi\_selection. The order

of these parameters defines the order in which they are represented. Only used

# Value

ygrid

params

A calibration plot.

#### See Also

VariableSelection, GraphicalModel, Clustering, BiSelection

is the output of BiSelection.

if stability is the output of BiSelection.

CART Classification And Regression Trees	CART	Classification And Regression Trees	
--	------	-------------------------------------	--

# **Description**

Runs decision trees using implementation from rpart. This function is not using stability.

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#### Usage

```
CART(xdata, ydata, Lambda = NULL, family, ...)
```

# **Arguments**

xdata matrix of predictors with observations as rows and variables as columns.

ydata optional vector or matrix of outcome(s). If family is set to "binomial" or

"multinomial", ydata can be a vector with character/numeric values or a fac-

tor.

Lambda matrix of parameters controlling the number of splits in the decision tree.

family type of regression model. This argument is defined as in glmnet. Possible val-

ues include "gaussian" (linear regression), "binomial" (logistic regression), "multinomial" (multinomial regression), and "cox" (survival analysis).

. additional parameters passed to rpart.

#### Value

A list with:

selected matrix of binary selection status. Rows correspond to different model parame-

ters. Columns correspond to predictors.

beta\_full array of model coefficients. Rows correspond to different model parameters.

Columns correspond to predictors. Indices along the third dimension correspond

to outcome variable(s).

#### References

Breiman L, Friedman JH, Olshen R, Stone CJ (1984). Classification and Regression Trees. Wadsworth.

#### See Also

```
SelectionAlgo, VariableSelection
```

Other underlying algorithm functions: ClusteringAlgo(), PenalisedGraphical(), PenalisedOpenMx(), PenalisedRegression()

# **Examples**

```
if (requireNamespace("rpart", quietly = TRUE)) {
    # Data simulation
    set.seed(1)
    simul <- SimulateRegression(pk = 50)

# Running the LASSO
    mycart <- CART(
        xdata = simul$xdata,
        ydata = simul$ydata,
        family = "gaussian"
)</pre>
```

```
head(mycart$selected)
}
```

Clustering

Consensus clustering

# **Description**

Performs consensus (weighted) clustering. The underlying algorithm (e.g. hierarchical clustering) is run with different number of clusters nc. In consensus weighted clustering, weighted distances are calculated using the cosa2 algorithm with different penalty parameters Lambda. The hyperparameters are calibrated by maximisation of the consensus score.

# Usage

```
Clustering(
  xdata,
  nc = NULL,
  eps = NULL,
  Lambda = NULL,
  K = 100,
  tau = 0.5,
  seed = 1,
  n_cat = 3,
  implementation = HierarchicalClustering,
  scale = TRUE,
  linkage = "complete",
  row = TRUE,
  optimisation = c("grid_search", "nloptr"),
  n_{cores} = 1,
  output_data = FALSE,
  verbose = TRUE,
  beep = NULL,
)
```

# **Arguments**

xdata	data matrix with observations as rows and variables as columns.
nc	matrix of parameters controlling the number of clusters in the underlying algorithm specified in implementation. If nc is not provided, it is set to seq(1, tau*nrow(xdata)).
eps	$radius\ in\ density-based\ clustering,\ see\ dbscan.\ Only\ used\ if\ implementation=DBSCANClustering.$
Lambda	vector of penalty parameters for weighted distance calculation. Only used for distance-based clustering, including for example implementation=HierarchicalClustering,

implementation=PAMClustering, or implementation=DBSCANClustering.

K number of resampling iterations. tau subsample size. seed value of the seed to initialise the random number generator and ensure reproducibility of the results (see set.seed). computation options for the stability score. Default is NULL to use the score n\_cat based on a z test. Other possible values are 2 or 3 to use the score based on the negative log-likelihood. implementation function to use for clustering. Possible functions include HierarchicalClustering (hierarchical clustering), PAMClustering (Partitioning Around Medoids), KMeansClustering (k-means) and GMMClustering (Gaussian Mixture Models). Alternatively, a user-defined function taking xdata and Lambda as arguments and returning a binary and symmetric matrix for which diagonal elements are equal to zero can be used. scale logical indicating if the data should be scaled to ensure that all variables contribute equally to the clustering of the observations. linkage character string indicating the type of linkage used in hierarchical clustering to define the stable clusters. Possible values include "complete", "single" and "average" (see argument "method" in hclust for a full list). Only used if implementation=HierarchicalClustering. logical indicating if rows (if row=TRUE) or columns (if row=FALSE) contain the row items to cluster. optimisation character string indicating the type of optimisation method to calibrate the regularisation parameter (only used if Lambda is not NULL). With optimisation="grid\_search" (the default), all values in Lambda are visited. Alternatively, optimisation algorithms implemented in nloptr can be used with optimisation="nloptr". By default, we use "algorithm"="NLOPT\_GN\_DIRECT\_L", "xtol\_abs"=0.1, "ftol\_abs"=0.1 and "maxeval" defined as length(Lambda). These values can be changed by providing the argument opts (see nloptr). number of cores to use for parallel computing (see argument workers in multisession). n cores Using n\_cores>1 is only supported with optimisation="grid\_search". output\_data logical indicating if the input datasets xdata and ydata should be included in the output. verbose logical indicating if a loading bar and messages should be printed.

beep

sound indicating the end of the run. Possible values are: NULL (no sound) or an

integer between 1 and 11 (see argument sound in beep).

additional parameters passed to the functions provided in implementation or

resampling.

# **Details**

In consensus clustering, a clustering algorithm is applied on K subsamples of the observations with different numbers of clusters provided in nc. If row=TRUE (the default), the observations (rows) are the items to cluster. If row=FALSE, the variables (columns) are the items to cluster. For a given number of clusters, the consensus matrix coprop stores the proportion of iterations where

two items were in the same estimated cluster, out of all iterations where both items were drawn in the subsample.

Stable cluster membership is obtained by applying a distance-based clustering method using (1-coprop) as distance (see Clusters).

These parameters can be calibrated by maximisation of a stability score (see ConsensusScore) calculated under the null hypothesis of equiprobability of co-membership.

It is strongly recommended to examine the calibration plot (see CalibrationPlot) to check that there is a clear maximum. The absence of a clear maximum suggests that the clustering is not stable, consensus clustering outputs should not be trusted in that case.

To ensure reproducibility of the results, the starting number of the random number generator is set to seed.

For parallelisation, stability selection with different sets of parameters can be run on n\_cores cores. Using n\_cores > 1 creates a multisession.

#### Value

An object of class clustering. A list with:

Sc	a matrix of the best stability	scores for different	(sets of) r	parameters controlling
30	a matrix of the best stability	scores for different	(SCIS OI) I	Jarameters controlling

the number of clusters and penalisation of attribute weights.

nc a matrix of numbers of clusters.

Lambda a matrix of regularisation parameters for attribute weights.

Q a matrix of the average number of selected attributes by the underlying algorithm

with different regularisation parameters.

coprop an array of consensus matrices. Rows and columns correspond to items. In-

dices along the third dimension correspond to different parameters controlling

the number of clusters and penalisation of attribute weights.

selprop an array of selection proportions. Columns correspond to attributes. Rows corre-

spond to different parameters controlling the number of clusters and penalisation

of attribute weights.

method a list with type="clustering" and values used for arguments implementation,

linkage, and resampling.

params a list with values used for arguments K, tau, pk, n (number of observations in

xdata), and seed.

The rows of Sc, nc, Lambda, Q, selprop and indices along the third dimension of coprop are ordered in the same way and correspond to parameter values stored in nc and Lambda.

#### References

Bodinier B, Rodrigues S, Karimi M, Filippi S, Chiquet J, Chadeau-Hyam M (2025). "Stability Selection and Consensus Clustering in R: The R Package sharp." *Journal of Statistical Software*, **112**(5), btad635. doi:10.18637/jss.v112.i05.

Bodinier B, Vuckovic D, Rodrigues S, Filippi S, Chiquet J, Chadeau-Hyam M (2023). "Automated calibration of consensus weighted distance-based clustering approaches using sharp." *Bioinformatics*, btad635. ISSN 1367-4811, doi:10.1093/bioinformatics/btad635, https://academic.oup.com/bioinformatics/advance-article-pdf/doi/10.1093/bioinformatics/btad635/52191190/btad635.pdf.

Kampert MM, Meulman JJ, Friedman JH (2017). "rCOSA: A Software Package for Clustering Objects on Subsets of Attributes." *Journal of Classification*, **34**(3), 514–547. doi:10.1007/s00357-0179240z.

Friedman JH, Meulman JJ (2004). "Clustering objects on subsets of attributes (with discussion)." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **66**(4), 815-849. doi:10.1111/j.14679868.2004.02059.x, https://rss.onlinelibrary.wiley.com/doi/pdf/10.1111/j.1467-9868.2004.02059.x, https://rss.onlinelibrary.wiley.com/doi/abs/10.1111/j.1467-9868.2004.02059.x.

Monti S, Tamayo P, Mesirov J, Golub T (2003). "Consensus Clustering: A Resampling-Based Method for Class Discovery and Visualization of Gene Expression Microarray Data." *Machine Learning*, **52**(1), 91–118. doi:10.1023/A:1023949509487.

#### See Also

Resample, ConsensusScore, HierarchicalClustering, PAMClustering, KMeansClustering, GMMClustering

Other stability functions: BiSelection(), GraphicalModel(), StructuralModel(), VariableSelection()

# **Examples**

```
# Consensus clustering
set.seed(1)
simul <- SimulateClustering(</pre>
  n = c(30, 30, 30), nu_xc = 1, ev_xc = 0.5
stab <- Clustering(xdata = simul$data)</pre>
print(stab)
CalibrationPlot(stab)
summary(stab)
Clusters(stab)
plot(stab)
# Consensus weighted clustering
if (requireNamespace("rCOSA", quietly = TRUE)) {
  set.seed(1)
  simul <- SimulateClustering(</pre>
    n = c(30, 30, 30), pk = 20,
    theta_xc = c(rep(1, 10), rep(0, 10)),
    ev_xc = 0.9
  )
  stab <- Clustering(</pre>
    xdata = simul$data,
    Lambda = LambdaSequence(lmin = 0.1, lmax = 10, cardinal = 10),
    noit = 20, niter = 10
  print(stab)
  CalibrationPlot(stab)
  summary(stab)
  Clusters(stab)
  plot(stab)
  WeightBoxplot(stab)
}
```

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ClusteringAlgo	(Weighted) clustering algorithm
CIUSCELINGALEO	(weighted) clustering digorium

# Description

Runs the (weighted) clustering algorithm specified in the argument implementation and returns matrices of variable weights, and the co-membership structure. This function is not using stability.

# Usage

```
ClusteringAlgo(
  xdata,
  nc = NULL,
  eps = NULL,
  Lambda = NULL,
  scale = TRUE,
  row = TRUE,
  implementation = HierarchicalClustering,
  ...
)
```

# Arguments

xdata	data matrix with observations as rows and variables as columns.
nc	matrix of parameters controlling the number of clusters in the underlying algorithm specified in implementation. If nc is not provided, it is set to seq(1, nrow(xdata)).
eps	$radius\ in\ density-based\ clustering,\ see\ dbscan.\ Only\ used\ if\ implementation=DBSCANClustering.$
Lambda	vector of penalty parameters.
scale	logical indicating if the data should be scaled to ensure that all variables contribute equally to the clustering of the observations.
row	logical indicating if rows (if row=TRUE) or columns (if row=FALSE) contain the items to cluster.
implementation	function to use for clustering. Possible functions include HierarchicalClustering (hierarchical clustering), PAMClustering (Partitioning Around Medoids), KMeansClustering (k-means) and GMMClustering (Gaussian Mixture Models). Alternatively, a user-defined function taking xdata and Lambda as arguments and returning a binary and symmetric matrix for which diagonal elements are equal to zero can be used.

additional parameters passed to the function provided in implementation.

#### Value

A list with:

selected matrix of binary selection status. Rows correspond to different model parame-

ters. Columns correspond to predictors.

weight array of model coefficients. Rows correspond to different model parameters.

Columns correspond to predictors. Indices along the third dimension correspond

to outcome variable(s).

comembership array of model coefficients. Rows correspond to different model parameters.

Columns correspond to predictors. Indices along the third dimension correspond

to outcome variable(s).

#### See Also

```
VariableSelection
```

```
Other underlying algorithm functions: CART(), PenalisedGraphical(), PenalisedOpenMx(), PenalisedRegression()
```

#### **Examples**

```
# Simulation of 15 observations belonging to 3 groups
set.seed(1)
simul <- SimulateClustering(
   n = c(5, 5, 5), pk = 100
)

# Running hierarchical clustering
myclust <- ClusteringAlgo(
   xdata = simul$data, nc = 2:5,
   implementation = HierarchicalClustering
)</pre>
```

ClusteringPerformance Clustering performance

#### **Description**

Computes different metrics of clustering performance by comparing true and predicted co-membership. This function can only be used in simulation studies (i.e. when the true cluster membership is known).

#### Usage

```
ClusteringPerformance(theta, theta_star, ...)
```

#### **Arguments**

output from Clustering. Alternatively, it can be the estimated co-membership matrix (see CoMembership).
 output from SimulateClustering. Alternatively, it can be the true co-membership matrix (see CoMembership).
 additional arguments to be passed to Clusters.

#### Value

A matrix of selection metrics including:

```
number of True Positives (TP)
FΝ
                 number of False Negatives (TN)
FP
                 number of False Positives (FP)
ΤN
                 number of True Negatives (TN)
                 sensitivity, i.e. TP/(TP+FN)
sensitivity
                 specificity, i.e. TN/(TN+FP)
specificity
                 accuracy, i.e. (TP+TN)/(TP+TN+FP+FN)
accuracy
precision
                 precision (p), i.e. TP/(TP+FP)
                 recall (r), i.e. TP/(TP+FN)
recall
                 F1-score, i.e. 2*p*r/(p+r)
F1_score
                 Rand Index, i.e. (TP+TN)/(TP+FP+TN+FN)
rand
                 Adjusted Rand Index (ARI), i.e. 2*(TP*TN-FP*FN)/((TP+FP)*(TN+FP)+(TP+FN)*(TN+FN))
ari
                 Jaccard index, i.e. TP/(TP+FP+FN)
jaccard
```

#### See Also

Other functions for model performance: SelectionPerformance(), SelectionPerformanceGraph()

# **Examples**

```
# Data simulation
set.seed(1)
simul <- SimulateClustering(
   n = c(30, 30, 30), nu_xc = 1
)
plot(simul)

# Consensus clustering
stab <- Clustering(
   xdata = simul$data, nc = seq_len(5)
)

# Clustering performance
ClusteringPerformance(stab, simul)</pre>
```

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```
# Alternative formulation
ClusteringPerformance(
  theta = CoMembership(Clusters(stab)),
  theta_star = simul$theta
)
```

Combine

Merging stability selection outputs

# **Description**

Merges the outputs from two runs of VariableSelection, GraphicalModel or Clustering. The two runs must have been done using the same methods and the same params but with different seeds. The combined output will contain results based on iterations from both stability1 and stability2. This function can be used for parallelisation.

#### Usage

```
Combine(stability1, stability2, include_beta = TRUE)
```

#### **Arguments**

```
stability1 output from a first run of VariableSelection, GraphicalModel, or Clustering.
stability2 output from a second run of VariableSelection, GraphicalModel, or Clustering.
include_beta logical indicating if the beta coefficients of visited models should be concatenated. Only applicable to variable selection or clustering.
```

#### Value

A single output of the same format.

## See Also

VariableSelection, GraphicalModel

# **Examples**

```
## Variable selection

# Data simulation
set.seed(1)
simul <- SimulateRegression(n = 100, pk = 50, family = "gaussian")

# Two runs
stab1 <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata, seed = 1, K = 10)
stab2 <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata, seed = 2, K = 10)</pre>
```

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```
# Merging the outputs
stab <- Combine(stability1 = stab1, stability2 = stab2, include_beta = FALSE)</pre>
str(stab)
## Graphical modelling
# Data simulation
simul <- SimulateGraphical(pk = 20)</pre>
# Two runs
stab1 <- GraphicalModel(xdata = simul$data, seed = 1, K = 10)</pre>
stab2 <- GraphicalModel(xdata = simul$data, seed = 2, K = 10)</pre>
# Merging the outputs
stab <- Combine(stability1 = stab1, stability2 = stab2)</pre>
str(stab)
## Clustering
# Data simulation
simul \leftarrow SimulateClustering(n = c(15, 15, 15))
# Two runs
stab1 <- Clustering(xdata = simul$data, seed = 1)</pre>
stab2 <- Clustering(xdata = simul$data, seed = 2)</pre>
# Merging the outputs
stab <- Combine(stability1 = stab1, stability2 = stab2)</pre>
str(stab)
```

CoMembership

Pairwise co-membership

#### **Description**

Generates a symmetric and binary matrix indicating, if two items are co-members, i.e. belong to the same cluster.

# Usage

```
CoMembership(groups)
```

# **Arguments**

groups

vector of group membership.

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#### Value

A symmetric and binary matrix.

#### **Examples**

```
# Simulated grouping structure
mygroups <- c(rep(1, 3), rep(2, 5), rep(3, 2))
# Co-membership matrix
CoMembership(mygroups)</pre>
```

ConsensusScore

Consensus score

# Description

Computes the consensus score from the consensus matrix, matrix of co-sampling counts and consensus clusters. The score is a z statistic for the comparison of the co-membership proportions observed within and between the consensus clusters.

# Usage

```
ConsensusScore(prop, K, theta)
```

# **Arguments**

prop consensus matrix.

K matrix of co-sampling counts. theta consensus co-membership matrix.

#### **Details**

To calculate the consensus score, the features are classified as being stably selected or not (in selection) or as being in the same consensus cluster or not (in clustering). In selection, the quantities  $X_w$  and  $X_b$  are defined as the sum of the selection counts for features that are stably selected or not, respectively. In clustering, the quantities  $X_w$  and  $X_b$  are defined as the sum of the co-membership counts for pairs of items in the same consensus cluster or in different consensus clusters, respectively.

Conditionally on this classification, and under the assumption that the selection (or co-membership) probabilities are the same for all features (or item pairs) in each of these two categories, the quantities  $X_w$  and  $X_b$  follow binomial distributions with probabilities  $p_w$  and  $p_b$ , respectively.

In the most unstable situation, we suppose that all features (or item pairs) would have the same probability of being selected (or co-members). The consensus score is the z statistic from a z test where the null hypothesis is  $p_w \le p_b$ .

The consensus score increases with stability.

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#### Value

A consensus score.

#### See Also

Other stability metric functions: FDP(), PFER(), StabilityMetrics(), StabilityScore()

#### **Examples**

```
# Data simulation
set.seed(2)
simul <- SimulateClustering(</pre>
 n = c(30, 30, 30),
 nu\_xc = 1
plot(simul)
# Consensus clustering
stab <- Clustering(</pre>
 xdata = simul$data
stab$Sc[3]
# Calculating the consensus score
theta <- CoMembership(Clusters(stab, argmax_id = 3))</pre>
ConsensusScore(
 prop = (stab$coprop[, , 3])[upper.tri(stab$coprop[, , 3])],
 K = stab$sampled_pairs[upper.tri(stab$sampled_pairs)],
 theta = theta[upper.tri(theta)]
```

DBSCANClustering

(Weighted) density-based clustering

# Description

Runs Density-Based Spatial Clustering of Applications with Noise (DBSCAN) clustering using implementation from dbscan. This is also known as the k-medoids algorithm. If Lambda is provided, clustering is applied on the weighted distance matrix calculated using the COSA algorithm as implemented in cosa2. Otherwise, distances are calculated using dist. This function is not using stability.

# Usage

```
DBSCANClustering(
  xdata,
  nc = NULL,
  eps = NULL,
```

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```
Lambda = NULL,
distance = "euclidean",
...
)
```

#### **Arguments**

xdata data matrix with observations as rows and variables as columns.

nc matrix of parameters controlling the number of clusters in the underlying algo-

rithm specified in implementation. If nc is not provided, it is set to seq(1,

tau\*nrow(xdata)).

eps radius in density-based clustering, see dbscan.

Lambda vector of penalty parameters (see argument lambda in cosa2). Unweighted dis-

tance matrices are used if Lambda=NULL.

distance character string indicating the type of distance to use. If Lambda=NULL, pos-

sible values include "euclidean", "maximum", "canberra", "binary", and "minkowski" (see argument method in dist). Otherwise, possible values include "euclidean" (pwr=2) or "absolute" (pwr=1) (see argument pwr in cosa2).

... additional parameters passed to dbscan (except for minPts which is fixed to 2),

dist, or cosa2. If weighted=TRUE, parameters niter (default to 1) and noit (default to 100) correspond to the number of iterations in cosa2 to calculate

weights and may need to be modified.

#### Value

A list with:

comembership an array of binary and symmetric co-membership matrices.

weights a matrix of median weights by feature.

#### References

Kampert MM, Meulman JJ, Friedman JH (2017). "rCOSA: A Software Package for Clustering Objects on Subsets of Attributes." *Journal of Classification*, **34**(3), 514–547. doi:10.1007/s00357-0179240z.

Friedman JH, Meulman JJ (2004). "Clustering objects on subsets of attributes (with discussion)." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **66**(4), 815-849. doi:10.1111/j.14679868.2004.02059.x, https://rss.onlinelibrary.wiley.com/doi/pdf/10.1111/j.1467-9868.2004.02059.x, https://rss.onlinelibrary.wiley.com/doi/abs/10.1111/j.1467-9868.2004.02059.x.

#### See Also

Other clustering algorithms: GMMClustering(), HierarchicalClustering(), KMeansClustering(), PAMClustering()

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#### **Examples**

```
if (requireNamespace("dbscan", quietly = TRUE)) {
 # Data simulation
 set.seed(1)
 simul \leftarrow SimulateClustering(n = c(10, 10), pk = 50)
 plot(simul)
 # DBSCAN clustering
 myclust <- DBSCANClustering(</pre>
   xdata = simul$data,
   eps = seq(0, 2 * sqrt(ncol(simul$data) - 1), by = 0.1)
 # Weighted PAM clustering (using COSA)
 if (requireNamespace("rCOSA", quietly = TRUE)) {
   myclust <- DBSCANClustering(</pre>
      xdata = simul$data,
      eps = c(0.25, 0.5, 0.75),
      Lambda = c(0.2, 0.5)
   )
 }
}
```

Ensemble

Ensemble model

## **Description**

Creates an ensemble predictive model from VariableSelection outputs.

# Usage

```
Ensemble(stability, xdata, ydata)
```

# Arguments

stability output of VariableSelection.

xdata matrix of predictors with observations as rows and variables as columns.

ydata optional vector or matrix of outcome(s). If family is set to "binomial" or

"multinomial", ydata can be a vector with character/numeric values or a fac-

tor.

#### Value

An object of class ensemble\_model. A list with:

intercept a vector of refitted intercepts for the K calibrated models.

beta a matrix of beta coefficients from the K calibrated models.

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models	a list of K models that can be used for prediction. These models are of class "lm" if family="gaussian" or "glm" if family="binomial".
family	type of regression, extracted from stability. Possible values are "gaussian" or "binomial".

#### See Also

Other ensemble model functions: EnsemblePredictions()

# **Examples**

```
# Linear regression
set.seed(1)
simul <- SimulateRegression(n = 100, pk = 50, family = "gaussian")
stab <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata, family = "gaussian")
ensemble <- Ensemble(stability = stab, xdata = simul$xdata, ydata = simul$ydata)

# Logistic regression
set.seed(1)
simul <- SimulateRegression(n = 200, pk = 20, family = "binomial")
stab <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata, family = "binomial")
ensemble <- Ensemble(stability = stab, xdata = simul$xdata, ydata = simul$ydata)</pre>
```

EnsemblePredictions

Predictions from ensemble model

#### **Description**

Makes predictions using an ensemble model created from VariableSelection outputs. For each observation in xdata, the predictions are calculated as the average predicted values obtained for that observation over the K models fitted in calibrated stability selection.

# Usage

```
EnsemblePredictions(ensemble, xdata, ...)
```

# **Arguments**

```
ensemble output of Ensemble.

xdata matrix of predictors with observations as rows and variables as columns.

... additional parameters passed to predict.
```

#### Value

A matrix of predictions computed from the observations in xdata.

#### See Also

```
predict.variable_selection
```

Other ensemble model functions: Ensemble()

#### **Examples**

```
# Data simulation
set.seed(1)
simul <- SimulateRegression(n = 1000, pk = 50, family = "gaussian")</pre>
# Training/test split
ids <- Split(data = simul$ydata, tau = c(0.8, 0.2))
stab <- VariableSelection(</pre>
  xdata = simul$xdata[ids[[1]], ],
  ydata = simul$ydata[ids[[1]], ]
)
# Constructing the ensemble model
ensemble <- Ensemble(</pre>
  stability = stab,
  xdata = simul$xdata[ids[[1]], ],
  ydata = simul$ydata[ids[[1]], ]
# Making predictions
yhat <- EnsemblePredictions(</pre>
  ensemble = ensemble,
  xdata = simul$xdata[ids[[2]], ]
)
# Calculating Q-squared
cor(simul$ydata[ids[[2]], ], yhat)^2
```

ExplanatoryPerformance

Prediction performance in regression

## **Description**

Calculates model performance for linear (measured by Q-squared), logistic (AUC) or Cox (C-statistic) regression. This is done by (i) refitting the model on a training set including a proportion tau of the observations, and (ii) evaluating the performance on the remaining observations (test set). For more reliable results, the procedure can be repeated K times (default K=1).

# Usage

```
ExplanatoryPerformance(
  xdata,
  ydata,
  new_xdata = NULL,
  new_ydata = NULL,
  stability = NULL,
  family = NULL,
  implementation = NULL,
  prediction = NULL,
  resampling = "subsampling",
  K = 1,
  tau = 0.8,
  seed = 1,
  n_{thr} = NULL,
  time = 1000,
  verbose = FALSE,
)
```

# **Arguments**

xdata	matrix of predictors with observations as rows and variables as columns.
ydata	optional vector or matrix of outcome(s). If family is set to "binomial" or "multinomial", ydata can be a vector with character/numeric values or a factor.
new_xdata	optional test set (predictor data).
new_ydata	optional test set (outcome data).
stability	output of VariableSelection. If stability=NULL (the default), a model including all variables in xdata as predictors is fitted. Argument family must be provided in this case.
family	type of regression model. Possible values include "gaussian" (linear regression), "binomial" (logistic regression), and "cox" (survival analysis). If provided, this argument must be consistent with input stability.
implementation	optional function to refit the model. If implementation=NULL and stability is the output of VariableSelection, lm (linear regression), coxph (Cox regression), glm (logistic regression), or multinom (multinomial regression) is used.
prediction	$optional \ function \ to \ compute \ predicted \ values \ from \ the \ model \ refitted \ with \ implementation.$
resampling	resampling approach to create the training set. The default is "subsampling" for sampling without replacement of a proportion tau of the observations. Alternatively, this argument can be a function to use for resampling. This function must use arguments named data and tau and return the IDs of observations to be included in the resampled dataset.
K	number of training-test splits. Only used if new_xdata and new_ydata are not provided.

tau proportion of observations used in the training set. Only used if new\_xdata and

new\_ydata are not provided.

seed value of the seed to ensure reproducibility of the results. Only used if new\_xdata

and new\_ydata are not provided.

n\_thr number of thresholds to use to construct the ROC curve. If n\_thr=NULL, all

predicted probability values are iteratively used as thresholds. For faster computations on large data, less thresholds can be used. Only applicable to logistic

regression.

time numeric indicating the time for which the survival probabilities are computed.

Only applicable to Cox regression.

verbose logical indicating if a loading bar and messages should be printed.

... additional parameters passed to the function provided in resampling.

#### **Details**

For a fair evaluation of the prediction performance, the data is split into a training set (including a proportion tau of the observations) and test set (remaining observations). The regression model is fitted on the training set and applied on the test set. Performance metrics are computed in the test set by comparing predicted and observed outcomes.

For logistic regression, a Receiver Operating Characteristic (ROC) analysis is performed: the True and False Positive Rates (TPR and FPR), and Area Under the Curve (AUC) are computed for different thresholds in predicted probabilities.

For Cox regression, the Concordance Index (as implemented in concordance) looking at survival probabilities up to a specific time is computed.

For linear regression, the squared correlation between predicted and observed outcome in the test set (Q-squared) is reported.

#### Value

A list with:

TPR True Positive Rate (for logistic regression only).

FPR False Positive Rate (for logistic regression only).

AUC Area Under the Curve (for logistic regression only).

concordance index (for Cox regression only).

Beta matrix of estimated beta coefficients across the K iterations. Coefficients are

extracted using the coef function.

# See Also

#### VariableSelection, Refit

Other prediction performance functions: Incremental()

```
# Data simulation
set.seed(1)
simul <- SimulateRegression(</pre>
  n = 1000, pk = 20,
  family = "binomial", ev_xy = 0.8
# Data split: selection, training and test set
ids <- Split(</pre>
  data = simul$ydata,
  family = "binomial",
  tau = c(0.4, 0.3, 0.3)
)
xselect <- simul$xdata[ids[[1]], ]</pre>
yselect <- simul$ydata[ids[[1]], ]</pre>
xtrain <- simul$xdata[ids[[2]], ]</pre>
ytrain <- simul$ydata[ids[[2]], ]</pre>
xtest <- simul$xdata[ids[[3]], ]</pre>
ytest <- simul$ydata[ids[[3]], ]</pre>
# Stability selection
stab <- VariableSelection(</pre>
  xdata = xselect,
  ydata = yselect,
  family = "binomial"
)
# Performances in test set of model refitted in training set
roc <- ExplanatoryPerformance(</pre>
  xdata = xtrain, ydata = ytrain,
  new_xdata = xtest, new_ydata = ytest,
  stability = stab
plot(roc)
roc$AUC
# Alternative with multiple training/test splits
roc <- ExplanatoryPerformance(</pre>
  xdata = rbind(xtrain, xtest),
  ydata = c(ytrain, ytest),
  stability = stab, K = 100
)
plot(roc)
boxplot(roc$AUC)
# Partial Least Squares Discriminant Analysis
if (requireNamespace("sgPLS", quietly = TRUE)) {
  stab <- VariableSelection(</pre>
    xdata = xselect,
    ydata = yselect,
    implementation = SparsePLS,
```

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```
family = "binomial"
 # Defining wrapping functions for predictions from PLS-DA
 PLSDA <- function(xdata, ydata, family = "binomial") {
   model <- mixOmics::plsda(X = xdata, Y = as.factor(ydata), ncomp = 1)</pre>
    return(model)
 PredictPLSDA <- function(xdata, model) {</pre>
    xdata <- xdata[, rownames(model$loadings$X), drop = FALSE]</pre>
   predicted <- predict(object = model, newdata = xdata)$predict[, 2, 1]</pre>
    return(predicted)
 # Performances with custom models
 roc <- ExplanatoryPerformance(</pre>
    xdata = rbind(xtrain, xtest),
   ydata = c(ytrain, ytest),
    stability = stab, K = 100,
    implementation = PLSDA, prediction = PredictPLSDA
 plot(roc)
}
```

FDP

False Discovery Proportion

# Description

Computes the False Discovery Proportion (upper-bound) as a ratio of the PFER (upper-bound) over the number of stably selected features. In stability selection, the FDP corresponds to the expected proportion of stably selected features that are not relevant to the outcome (i.e. proportion of False Positives among stably selected features).

### Usage

```
FDP(selprop, PFER, pi)
```

# Arguments

selprop matrix or vector of selection proportions.

PFER Per Family Error Rate.

pi threshold in selection proportions.

### Value

The estimated upper-bound in FDP.

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### See Also

Other stability metric functions: ConsensusScore(), PFER(), StabilityMetrics(), StabilityScore()

### **Examples**

```
# Simulating set of selection proportions
selprop <- round(runif(n = 20), digits = 2)
# Computing the FDP with a threshold of 0.8
fdp <- FDP(PFER = 3, selprop = selprop, pi = 0.8)</pre>
```

Folds

Splitting observations into folds

# Description

Generates a list of n\_folds non-overlapping sets of observation IDs (folds).

## Usage

```
Folds(data, family = NULL, n_folds = 5)
```

## **Arguments**

data	vector or matrix of data. In regression, this should be the outcome data.
family	type of regression model. This argument is defined as in glmnet. Possible values include "gaussian" (linear regression), "binomial" (logistic regression), "multinomial" (multinomial regression), and "cox" (survival analysis).
n folds	number of folds.

### **Details**

For categorical outcomes (i.e. family argument is set to "binomial", "multinomial" or "cox"), the split is done such that the proportion of observations from each of the categories in each of the folds is representative of that of the full sample.

## Value

A list of length n\_folds with sets of non-overlapping observation IDs.

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## **Examples**

```
# Splitting into 5 folds
simul <- SimulateRegression()
ids <- Folds(data = simul$ydata)
lapply(ids, length)

# Balanced folds with respect to a binary variable
simul <- SimulateRegression(family = "binomial")
ids <- Folds(data = simul$ydata, family = "binomial")
lapply(ids, FUN = function(x) {
  table(simul$ydata[x, ])
})</pre>
```

GMMClustering

Model-based clustering

### **Description**

Runs clustering with Gaussian Mixture Models (GMM) using implementation from Mclust. This function is not using stability.

### Usage

```
GMMClustering(xdata, nc = NULL, ...)
```

### **Arguments**

xdata data matrix with observations as rows and variables as columns.

nc matrix of parameters controlling the number of clusters in the underlying algo-

rithm specified in implementation. If nc is not provided, it is set to seq(1,

tau\*nrow(xdata)).

... additional parameters passed to Mclust.

## Value

A list with:

comembership an array of binary and symmetric co-membership matrices.

weights a matrix of median weights by feature.

#### See Also

```
Other clustering algorithms: DBSCANClustering(), HierarchicalClustering(), KMeansClustering(), PAMClustering()
```

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## **Examples**

```
# Data simulation
set.seed(1)
simul <- SimulateClustering(n = c(10, 10), pk = 50)
# Clustering using Gaussian Mixture Models
mygmm <- GMMClustering(xdata = simul$data, nc = seq_len(30))</pre>
```

Graph

Graph visualisation

## **Description**

Produces an igraph object from an adjacency matrix.

# Usage

```
Graph(
  adjacency,
  node_label = NULL,
  node_colour = NULL,
  node_shape = NULL,
  edge_colour = "grey60",
  label_colour = "grey20",
  mode = "undirected",
  weighted = FALSE,
  satellites = FALSE
)
```

## **Arguments**

adjacency	adjacency matrix or output of GraphicalModel.
node_label	optional vector of node labels. This vector must contain as many entries as there are rows/columns in the adjacency matrix and must be in the same order (the order is used to assign labels to nodes).
node_colour	optional vector of node colours. This vector must contain as many entries as there are rows/columns in the adjacency matrix and must be in the same order (the order is used to assign colours to nodes). Integers, named colours or RGB values can be used.
node_shape	optional vector of node shapes. This vector must contain as many entries as there are rows/columns in the adjacency matrix and must be in the same order (the order is used to assign shapes to nodes). Possible values are "circle", "square", "triangle" or "star".
edge_colour	optional character string for edge colour. Integers, named colours or RGB values can be used.

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label\_colour optional character string for label colour. Integers, named colours or RGB values

can be used.

mode character string indicating how the adjacency matrix should be interpreted. Pos-

sible values include "undirected" or "directed" (see graph\_from\_adjacency\_matrix).

weighted indicating if entries of the adjacency matrix should define edge width. If weighted=FALSE,

an unweighted igraph object is created, all edges have the same width. If weighted=TRUE,

edge width is defined by the corresponding value in the adjacency matrix. If weighted=NULL, nodes are linked by as many edges as indicated in the adja-

cency matrix (integer values are needed).

satellites logical indicating if unconnected nodes (satellites) should be included in the

igraph object.

### **Details**

All functionalities implemented in igraph can be used on the output. These include cosmetic changes for the visualisation, but also various tools for network analysis (including topological properties and community detection).

The R package visNetwork offers interactive network visualisation tools. An igraph object can easily be converted to a visNetwork object (see example below).

For Cytoscape users, the RCy3 package can be used to open the network in Cytoscape.

#### Value

An igraph object.

### See Also

Adjacency, Graphical Model, igraph manual, vis Network manual, Cytoscape

```
## From adjacency matrix

# Un-weighted
adjacency <- SimulateAdjacency(pk = 20, topology = "scale-free")
plot(Graph(adjacency))

# Weighted
adjacency <- adjacency * runif(prod(dim(adjacency)))
adjacency <- adjacency + t(adjacency)
plot(Graph(adjacency, weighted = TRUE))

# Node colours and shapes
plot(Graph(adjacency, weighted = TRUE, node_shape = "star", node_colour = "red"))

## From stability selection outputs

# Graphical model</pre>
```

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```
set.seed(1)
simul <- SimulateGraphical(pk = 20)</pre>
stab <- GraphicalModel(xdata = simul$data)</pre>
plot(Graph(stab))
# Sparse PLS
if (requireNamespace("sgPLS", quietly = TRUE)) {
 set.seed(1)
 simul <- SimulateRegression(n = 50, pk = c(5, 5, 5), family = "gaussian")
 x <- simul$xdata
 y <- simul$ydata
 stab <- BiSelection(</pre>
    xdata = simul$xdata, ydata = simul$ydata,
    family = "gaussian", ncomp = 3,
   LambdaX = seq_len(ncol(x) - 1),
    implementation = SparsePLS
 )
 plot(Graph(stab))
}
## Tools from other packages
# Applying some igraph functionalities
adjacency <- SimulateAdjacency(pk = 20, topology = "scale-free")</pre>
mygraph <- Graph(adjacency)</pre>
igraph::degree(mygraph)
igraph::betweenness(mygraph)
igraph::shortest_paths(mygraph, from = 1, to = 2)
igraph::walktrap.community(mygraph)
# Interactive view using visNetwork
if (requireNamespace("visNetwork", quietly = TRUE)) {
 vgraph <- mygraph
 igraph::V(vgraph)$shape <- rep("dot", length(igraph::V(vgraph)))</pre>
 v <- visNetwork::visIgraph(vgraph)</pre>
 mylayout <- as.matrix(v$x$nodes[, c("x", "y")])</pre>
 mylayout[, 2] <- -mylayout[, 2]</pre>
 plot(mygraph, layout = mylayout)
}
# Opening in Cytoscape using RCy3
if (requireNamespace("RCy3", quietly = TRUE)) {
 # Make sure that Cytoscape is open before running the following line
 # RCy3::createNetworkFromIgraph(mygraph)
}
```

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### **Description**

Generates an igraph object representing the common and graph-specific edges.

### Usage

```
GraphComparison(
  graph1,
  graph2,
  col = c("tomato", "forestgreen", "navy"),
  lty = c(2, 3, 1),
  node_colour = NULL,
  show_labels = TRUE,
  ...
)
```

## Arguments

graph1 first graph. Possible inputs are: adjacency matrix, or igraph object, or output of

GraphicalModel, VariableSelection, BiSelection, or output of SimulateGraphical,

SimulateRegression.

graph2 second graph.

col vector of edge colours. The first entry of the vector defines the colour of edges

in graph1 only, second entry is for edges in graph2 only and third entry is for

common edges.

1ty vector of line types for edges. The order is defined as for argument col.

node\_colour optional vector of node colours. This vector must contain as many entries as

there are rows/columns in the adjacency matrix and must be in the same order (the order is used to assign colours to nodes). Integers, named colours or RGB

values can be used.

show\_labels logical indicating if the node labels should be displayed.

... additional arguments to be passed to Graph.

#### Value

An igraph object.

## See Also

SelectionPerformanceGraph

```
# Data simulation
set.seed(1)
simul1 <- SimulateGraphical(pk = 30)
set.seed(2)
simul2 <- SimulateGraphical(pk = 30)</pre>
```

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```
# Edge-wise comparison of the two graphs
mygraph <- GraphComparison(
  graph1 = simul1,
  graph2 = simul2
)
plot(mygraph, layout = igraph::layout_with_kk(mygraph))</pre>
```

GraphicalAlgo

Graphical model algorithm

# Description

Runs the algorithm specified in the argument implementation and returns the estimated adjacency matrix. This function is not using stability.

### Usage

```
GraphicalAlgo(
  xdata,
  pk = NULL,
  Lambda,
  Sequential_template = NULL,
  scale = TRUE,
  implementation = PenalisedGraphical,
  start = "cold",
  ...
)
```

### **Arguments**

xdata

matrix with observations as rows and variables as columns.

pk

optional vector encoding the grouping structure. Only used for multi-block stability selection where pk indicates the number of variables in each group. If pk=NULL, single-block stability selection is performed.

Lambda

matrix of parameters controlling the level of sparsity in the underlying feature selection algorithm specified in implementation. If Lambda=NULL and implementation=PenalisedGraphical, LambdaGridGraphical is used to define a relevant grid. Lambda can be provided as a vector or a matrix with length(pk) columns.

### Sequential\_template

logical matrix encoding the type of procedure to use for data with multiple blocks in stability selection graphical modelling. For multi-block estimation, the stability selection model is constructed as the union of block-specific stable edges estimated while the others are weakly penalised (TRUE only for the block currently being calibrated and FALSE for other blocks). Other approaches with joint calibration of the blocks are allowed (all entries are set to TRUE).

scale logical indicating if the correlation (scale=TRUE) or covariance (scale=FALSE) matrix should be used as input of glassoFast if implementation=PenalisedGraphical.

Otherwise, this argument must be used in the function provided in implementation.

Otherwise, this argument must be used in the function provided in implementation.

 $implementation \quad function \ to \ use \ for \ graphical \ modelling. \ If \ implementation = Penalised Graphical,$ 

the algorithm implemented in glassoFast is used for regularised estimation of a conditional independence graph. Alternatively, a user-defined function can be

provided.

start character string indicating if the algorithm should be initialised at the estimated

(inverse) covariance with previous penalty parameters (start="warm") or not (start="cold"). Using start="warm" can speed-up the computations, but could lead to convergence issues (in particular with small Lambda\_cardinal). Only used for implementation=PenalisedGraphical (see argument "start"

in glassoFast).

additional parameters passed to the function provided in implementation.

#### **Details**

. . .

The use of the procedure from Equation (4) or (5) is controlled by the argument "Sequential\_template".

#### Value

An array with binary and symmetric adjacency matrices along the third dimension.

#### See Also

```
GraphicalModel, PenalisedGraphical
Other wrapping functions: SelectionAlgo()
```

### **Examples**

```
# Data simulation
set.seed(1)
simul <- SimulateGraphical()

# Running graphical LASSO
myglasso <- GraphicalAlgo(
    xdata = simul$data,
    Lambda = cbind(c(0.1, 0.2))
)</pre>
```

GraphicalModel

Stability selection graphical model

### **Description**

Performs stability selection for graphical models. The underlying graphical model (e.g. graphical LASSO) is run with different combinations of parameters controlling the sparsity (e.g. penalty parameter) and thresholds in selection proportions. These two hyper-parameters are jointly calibrated by maximisation of the stability score.

### Usage

```
GraphicalModel(
  xdata,
  pk = NULL,
  Lambda = NULL,
  lambda_other_blocks = 0.1,
 pi_list = seq(0.01, 0.99, by = 0.01),
 K = 100,
  tau = 0.5,
  seed = 1,
  n_cat = NULL,
  implementation = PenalisedGraphical,
  start = "warm",
  scale = TRUE,
  resampling = "subsampling",
  cpss = FALSE,
  PFER_method = "MB",
  PFER_thr = Inf,
  FDP_thr = Inf,
  Lambda_cardinal = 50,
  lambda_max = NULL,
  lambda_path_factor = 0.001,
 max_density = 0.5,
  optimisation = c("grid_search", "nloptr"),
  n_{cores} = 1,
  output_data = FALSE,
  verbose = TRUE,
  beep = NULL,
)
```

### Arguments

xdata

data matrix with observations as rows and variables as columns. For multi-block stability selection, the variables in data have to be ordered by group.

pk

optional vector encoding the grouping structure. Only used for multi-block stability selection where pk indicates the number of variables in each group. If pk=NULL, single-block stability selection is performed.

Lambda

matrix of parameters controlling the level of sparsity in the underlying feature selection algorithm specified in implementation. If Lambda=NULL and implementation=PenalisedGraphical, LambdaGridGraphical is used to define a relevant grid. Lambda can be provided as a vector or a matrix with length(pk) columns.

lambda\_other\_blocks

optional vector of parameters controlling the level of sparsity in neighbour blocks for the multi-block procedure. To use jointly a specific set of parameters for each block, lambda\_other\_blocks must be set to NULL (not recommended). Only used for multi-block stability selection, i.e. if length(pk)>1.

pi\_list vector of thresholds in selection proportions. If n\_cat=NULL or n\_cat=2, these

values must be >0 and <1. If  $n_{cat}=3$ , these values must be >0.5 and <1.

K number of resampling iterations.

tau subsample size. Only used if resampling="subsampling" and cpss=FALSE.
seed value of the seed to initialise the random number generator and ensure repro-

ducibility of the results (see set.seed).

n\_cat computation options for the stability score. Default is NULL to use the score

based on a z test. Other possible values are 2 or 3 to use the score based on the

negative log-likelihood.

implementation function to use for graphical modelling. If implementation=PenalisedGraphical,

the algorithm implemented in glassoFast is used for regularised estimation of a conditional independence graph. Alternatively, a user-defined function can be

provided.

start character string indicating if the algorithm should be initialised at the estimated

(inverse) covariance with previous penalty parameters (start="warm") or not (start="cold"). Using start="warm" can speed-up the computations, but could lead to convergence issues (in particular with small Lambda\_cardinal). Only used for implementation=PenalisedGraphical (see argument "start"

in glassoFast).

scale logical indicating if the correlation (scale=TRUE) or covariance (scale=FALSE)

 $matrix\ should\ be\ used\ as\ input\ of\ {\tt glassoFast}\ if\ {\tt implementation=PenalisedGraphical}.$ 

Otherwise, this argument must be used in the function provided in implementation.

resampling resampling approach. Possible values are: "subsampling" for sampling with-

out replacement of a proportion tau of the observations, or "bootstrap" for sampling with replacement generating a resampled dataset with as many observations as in the full sample. Alternatively, this argument can be a function to use for resampling. This function must use arguments named data and tau and

return the IDs of observations to be included in the resampled dataset.

cpss logical indicating if complementary pair stability selection should be done. For

this, the algorithm is applied on two non-overlapping subsets of half of the observations. A feature is considered as selected if it is selected for both subsamples. With this method, the data is split K/2 times (K models are fitted). Only used if

PFER\_method="MB".

PFER\_method method used to compute the upper-bound of the expected number of False Posi-

tives (or Per Family Error Rate, PFER). If PFER\_method="MB", the method proposed by Meinshausen and Bühlmann (2010) is used. If PFER\_method="SS", the method proposed by Shah and Samworth (2013) under the assumption of

unimodality is used.

PFER\_thr threshold in PFER for constrained calibration by error control. If PFER\_thr=Inf

and FDP\_thr=Inf, unconstrained calibration is used (the default).

FDP\_thr threshold in the expected proportion of falsely selected features (or False Dis-

covery Proportion) for constrained calibration by error control. If PFER\_thr=Inf

and FDP\_thr=Inf, unconstrained calibration is used (the default).

Lambda\_cardinal

number of values in the grid of parameters controlling the level of sparsity in the underlying algorithm. Only used if Lambda=NULL.

lambda\_max optional maximum value for the grid in penalty parameters. If lambda\_max=NULL,

the maximum value is set to the maximum covariance in absolute value. Only

used if implementation=PenalisedGraphical and Lambda=NULL.

lambda\_path\_factor

multiplicative factor used to define the minimum value in the grid.

max\_density threshold on the density. The grid is defined such that the density of the esti-

mated graph does not exceed max\_density.

optimisation character string indicating the type of optimisation method. With optimisation="grid\_search"

(the default), all values in Lambda are visited. Alternatively, optimisation algorithms implemented in nloptr can be used with optimisation="nloptr". By default, we use "algorithm"="NLOPT\_GN\_DIRECT\_L", "xtol\_abs"=0.1, "ftol\_abs"=0.1 and "maxeval"=Lambda\_cardinal. These values can be changed by providing the argument opts (see nloptr). For stability selection using penalised regression, optimisation="grid\_search" may be faster as it allows

for warm start.

n\_cores number of cores to use for parallel computing (see argument workers in multisession).

Using n\_cores>1 is only supported with optimisation="grid\_search".

output\_data logical indicating if the input datasets xdata and ydata should be included in

the output.

verbose logical indicating if a loading bar and messages should be printed.

beep sound indicating the end of the run. Possible values are: NULL (no sound) or an

integer between 1 and 11 (see argument sound in beep).

... additional parameters passed to the functions provided in implementation or

resampling.

### Details

In stability selection, a feature selection algorithm is fitted on K subsamples (or bootstrap samples) of the data with different parameters controlling the sparsity (Lambda). For a given (set of) sparsity parameter(s), the proportion out of the K models in which each feature is selected is calculated. Features with selection proportions above a threshold pi are considered stably selected. The stability selection model is controlled by the sparsity parameter(s) for the underlying algorithm, and the threshold in selection proportion:

$$V_{\lambda,\pi} = \{j : p_{\lambda}(j) \ge \pi\}$$

These parameters can be calibrated by maximisation of a stability score (see ConsensusScore if n\_cat=NULL or StabilityScore otherwise) calculated under the null hypothesis of equiprobability of selection.

It is strongly recommended to examine the calibration plot carefully to check that the grids of parameters Lambda and pi\_list do not restrict the calibration to a region that would not include the global maximum (see CalibrationPlot). In particular, the grid Lambda may need to be extended when the maximum stability is observed on the left or right edges of the calibration heatmap. In some instances, multiple peaks of stability score can be observed. Simulation studies suggest that the peak corresponding to the largest number of selected features tend to give better selection performances. This is not necessarily the highest peak (which is automatically retained by the functions in this package). The user can decide to manually choose another peak.

To control the expected number of False Positives (Per Family Error Rate) in the results, a threshold PFER\_thr can be specified. The optimisation problem is then constrained to sets of parameters that generate models with an upper-bound in PFER below PFER\_thr (see Meinshausen and Bühlmann (2010) and Shah and Samworth (2013)).

Possible resampling procedures include defining (i) K subsamples of a proportion tau of the observations, (ii) K bootstrap samples with the full sample size (obtained with replacement), and (iii) K/2 splits of the data in half for complementary pair stability selection (see arguments resampling and cpss). In complementary pair stability selection, a feature is considered selected at a given resampling iteration if it is selected in the two complementary subsamples.

To ensure reproducibility of the results, the starting number of the random number generator is set to seed.

For parallelisation, stability selection with different sets of parameters can be run on n\_cores cores. Using n\_cores > 1 creates a multisession. Alternatively, the function can be run manually with different seeds and all other parameters equal. The results can then be combined using Combine.

The generated network can be converted into igraph object using Graph. The R package visNetwork can be used for interactive network visualisation (see examples in Graph).

### Value

An object of class graphical\_model. A list with:

S	a matrix of the best stability scores for different (sets of) parameters controlling the level of sparsity in the underlying algorithm.
Lambda	a matrix of parameters controlling the level of sparsity in the underlying algorithm.
Q	a matrix of the average number of selected features by the underlying algorithm with different parameters controlling the level of sparsity.
Q_s	a matrix of the calibrated number of stably selected features with different parameters controlling the level of sparsity.
P	a matrix of calibrated thresholds in selection proportions for different parameters controlling the level of sparsity in the underlying algorithm.
PFER	a matrix of upper-bounds in PFER of calibrated stability selection models with different parameters controlling the level of sparsity.
FDP	a matrix of upper-bounds in FDP of calibrated stability selection models with different parameters controlling the level of sparsity.
S_2d	a matrix of stability scores obtained with different combinations of parameters. Columns correspond to different thresholds in selection proportions.
PFER_2d	a matrix of upper-bounds in FDP obtained with different combinations of parameters. Columns correspond to different thresholds in selection proportions. Only returned if length(pk)=1.
FDP_2d	a matrix of upper-bounds in PFER obtained with different combinations of parameters. Columns correspond to different thresholds in selection proportions. Only returned if length(pk)=1.
selprop	an array of selection proportions. Rows and columns correspond to nodes in the graph. Indices along the third dimension correspond to different parameters controlling the level of sparsity in the underlying algorithm.

sign a matrix of signs of Pearson's correlations estimated from xdata.

method a list with type="graphical\_model" and values used for arguments implementation,

start, resampling, cpss and PFER\_method.

params a list with values used for arguments K, pi\_list, tau, n\_cat, pk, n (number

of observations in xdata), PFER\_thr, FDP\_thr, seed, lambda\_other\_blocks,

and Sequential\_template.

The rows of S, Lambda, Q, Q\_s, P, PFER, FDP, S\_2d, PFER\_2d and FDP\_2d, and indices along the third dimension of selprop are ordered in the same way and correspond to parameter values stored in Lambda. For multi-block inference, the columns of S, Lambda, Q, Q\_s, P, PFER and FDP, and indices along the third dimension of S\_2d correspond to the different blocks.

#### References

Bodinier B, Rodrigues S, Karimi M, Filippi S, Chiquet J, Chadeau-Hyam M (2025). "Stability Selection and Consensus Clustering in R: The R Package sharp." *Journal of Statistical Software*, **112**(5), btad635. doi:10.18637/jss.v112.i05.

Bodinier B, Filippi S, Nøst TH, Chiquet J, Chadeau-Hyam M (2023). "Automated calibration for stability selection in penalised regression and graphical models." *Journal of the Royal Statistical Society Series C: Applied Statistics*, qlad058. ISSN 0035-9254, doi:10.1093/jrsssc/qlad058, https://academic.oup.com/jrsssc/advance-article-pdf/doi/10.1093/jrsssc/qlad058/50878777/qlad058.pdf.

Shah RD, Samworth RJ (2013). "Variable selection with error control: another look at stability selection." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **75**(1), 55-80. doi:10.1111/j.14679868.2011.01034.x.

Meinshausen N, Bühlmann P (2010). "Stability selection." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **72**(4), 417-473. doi:10.1111/j.14679868.2010.00740.x.

Friedman J, Hastie T, Tibshirani R (2008). "Sparse inverse covariance estimation with the graphical lasso." *Biostatistics*, **9**(3), 432–441.

#### See Also

PenalisedGraphical, GraphicalAlgo, LambdaGridGraphical, Resample, StabilityScore Graph, Adjacency,

Other stability functions: BiSelection(), Clustering(), StructuralModel(), VariableSelection()

```
oldpar <- par(no.readonly = TRUE)
par(mar = rep(7, 4))

## Single-block stability selection

# Data simulation
set.seed(1)
simul <- SimulateGraphical(n = 100, pk = 20, nu_within = 0.1)

# Stability selection
stab <- GraphicalModel(xdata = simul$data)</pre>
```

```
print(stab)
# Calibration heatmap
CalibrationPlot(stab)
# Visualisation of the results
summary(stab)
plot(stab)
# Extraction of adjacency matrix or igraph object
Adjacency(stab)
Graph(stab)
## Multi-block stability selection
# Data simulation
set.seed(1)
simul <- SimulateGraphical(pk = c(10, 10))
# Stability selection
stab \leftarrow GraphicalModel(xdata = simul*data, pk = c(10, 10), Lambda_cardinal = 10)
print(stab)
# Calibration heatmap
\# par(mfrow = c(1, 3))
CalibrationPlot(stab) # Producing three plots
# Visualisation of the results
summary(stab)
plot(stab)
# Multi-parameter stability selection (not recommended)
Lambda <- matrix(c(0.8, 0.6, 0.3, 0.5, 0.4, 0.3, 0.7, 0.5, 0.1), ncol = 3)
stab <- GraphicalModel(</pre>
  xdata = simul data, pk = c(10, 10),
  Lambda = Lambda, lambda_other_blocks = NULL
)
stab$Lambda
## Example with user-defined function: shrinkage estimation and selection
# Data simulation
set.seed(1)
simul <- SimulateGraphical(n = 100, pk = 20, nu_within = 0.1)</pre>
if (requireNamespace("corpcor", quietly = TRUE)) {
  # Writing user-defined algorithm in a portable function
  ShrinkageSelection <- function(xdata, Lambda, ...) {</pre>
    mypcor <- corpcor::pcor.shrink(xdata, verbose = FALSE)</pre>
    adjacency <- array(NA, dim = c(nrow(mypcor), ncol(mypcor), nrow(Lambda)))</pre>
    for (k in seq_len(nrow(Lambda))) {
```

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```
A <- ifelse(abs(mypcor) >= Lambda[k, 1], yes = 1, no = 0)
      diag(A) <- 0
      adjacency[, , k] <- A
    }
    return(list(adjacency = adjacency))
  }
  # Running the algorithm without stability
  myglasso <- GraphicalAlgo(</pre>
    xdata = simul$data,
    Lambda = matrix(c(0.05, 0.1), ncol = 1), implementation = ShrinkageSelection
  # Stability selection using shrinkage estimation and selection
  stab <- GraphicalModel(</pre>
    xdata = simul$data, Lambda = matrix(c(0.01, 0.05, 0.1), ncol = 1),
    implementation = ShrinkageSelection
  CalibrationPlot(stab)
  stable_adjacency <- Adjacency(stab)</pre>
}
par(oldpar)
```

GroupPLS

Group Partial Least Squares

## **Description**

Runs a group Partial Least Squares model using implementation from sgPLS-package. This function is not using stability.

#### Usage

```
GroupPLS(
  xdata,
  ydata,
  family = "gaussian",
  group_x,
  group_y = NULL,
  Lambda,
  keepX_previous = NULL,
  keepY = NULL,
  ncomp = 1,
  scale = TRUE,
  ...
)
```

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### **Arguments**

matrix of predictors with observations as rows and variables as columns. xdata optional vector or matrix of outcome(s). If family is set to "binomial" or ydata "multinomial", ydata can be a vector with character/numeric values or a facfamily type of PLS model. If family="gaussian", a group PLS model as defined in gPLS is run (for continuous outcomes). If family="binomial", a PLS-DA model as defined in gPLSda is run (for categorical outcomes). vector encoding the grouping structure among predictors. This argument indigroup\_x cates the number of variables in each group. optional vector encoding the grouping structure among outcomes. This argugroup\_y ment indicates the number of variables in each group. Lambda matrix of parameters controlling the number of selected groups at current component, as defined by ncomp. number of selected groups in previous components. Only used if ncomp > 1. keepX\_previous The argument keepX in sgPLS is obtained by concatenating keepX\_previous and Lambda. keepY number of selected groups of outcome variables. This argument is defined as in sgPLS. Only used if family="gaussian". number of components. ncomp scale logical indicating if the data should be scaled (i.e. transformed so that all variables have a standard deviation of one). Only used if family="gaussian". additional arguments to be passed to gPLS or gPLSda.

#### Value

A list with:

selected matrix of binary selection status. Rows correspond to different model parame-

ters. Columns correspond to predictors.

beta\_full array of model coefficients. Rows correspond to different model parameters.

Columns correspond to predictors (starting with "X") or outcomes (starting with

"Y") variables for different components (denoted by "PC").

#### References

Liquet B, de Micheaux PL, Hejblum BP, Thiébaut R (2016). "Group and sparse group partial least square approaches applied in genomics context." *Bioinformatics*, **32**(1), 35-42. ISSN 1367-4803, doi:10.1093/bioinformatics/btv535.

#### See Also

VariableSelection, BiSelection

Other penalised dimensionality reduction functions: SparseGroupPLS(), SparsePCA(), SparsePLS()

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### **Examples**

```
if (requireNamespace("sgPLS", quietly = TRUE)) {
 ## Group PLS
 # Data simulation
 set.seed(1)
 simul <- SimulateRegression(n = 100, pk = 50, q = 3, family = "gaussian")</pre>
 x <- simul$xdata
 y <- simul$ydata
 # Running gPLS with 1 group and sparsity of 0.5
 mypls <- GroupPLS(</pre>
   xdata = x, ydata = y, Lambda = 1, family = "gaussian",
   group_x = c(10, 15, 25),
 )
 # Running gPLS with groups on outcomes
 mypls <- GroupPLS(</pre>
   xdata = x, ydata = y, Lambda = 1, family = "gaussian",
   group_x = c(10, 15, 25),
   group_y = c(2, 1), keepY = 1
}
```

**HierarchicalClustering** 

(Weighted) hierarchical clustering

## **Description**

Runs hierarchical clustering using implementation from hclust. If Lambda is provided, clustering is applied on the weighted distance matrix calculated using the cosa2 algorithm. Otherwise, distances are calculated using dist. This function is not using stability.

## Usage

```
HierarchicalClustering(
  xdata,
  nc = NULL,
  Lambda = NULL,
  distance = "euclidean",
  linkage = "complete",
  ...
)
```

## **Arguments**

xdata

data matrix with observations as rows and variables as columns.

nc matrix of parameters controlling the number of clusters in the underlying algo-

rithm specified in implementation. If nc is not provided, it is set to seq(1,

tau\*nrow(xdata)).

Lambda vector of penalty parameters (see argument lambda in cosa2). Unweighted dis-

tance matrices are used if Lambda=NULL.

distance character string indicating the type of distance to use. If Lambda=NULL, pos-

sible values include "euclidean", "maximum", "canberra", "binary", and "minkowski" (see argument method in dist). Otherwise, possible values include "euclidean" (pwr=2) or "absolute" (pwr=1) (see argument pwr in cosa2).

linkage character string indicating the type of linkage used in hierarchical clustering to

define the stable clusters. Possible values include "complete", "single" and "average" (see argument "method" in hclust for a full list). Only used if

implementation=HierarchicalClustering.

... additional parameters passed to hclust, dist, or cosa2. Parameters niter

(default to 1) and noit (default to 100) correspond to the number of iterations in cosa2 to calculate weights and may need to be modified. Argument pwr in

cosa2 is ignored, please provide distance instead.

#### Value

A list with:

comembership an array of binary and symmetric co-membership matrices.

weights a matrix of median weights by feature.

### References

Kampert MM, Meulman JJ, Friedman JH (2017). "rCOSA: A Software Package for Clustering Objects on Subsets of Attributes." *Journal of Classification*, **34**(3), 514–547. doi:10.1007/s00357-0179240z.

Friedman JH, Meulman JJ (2004). "Clustering objects on subsets of attributes (with discussion)." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **66**(4), 815-849. doi:10.1111/j.14679868.2004.02059.x, https://rss.onlinelibrary.wiley.com/doi/pdf/10.1111/j.1467-9868.2004.02059.x, https://rss.onlinelibrary.wiley.com/doi/abs/10.1111/j.1467-9868.2004.02059.x.

#### See Also

Other clustering algorithms: DBSCANClustering(), GMMClustering(), KMeansClustering(), PAMClustering()

```
# Data simulation
set.seed(1)
simul <- SimulateClustering(n = c(10, 10), pk = 50)
# Hierarchical clustering
myhclust <- HierarchicalClustering(</pre>
```

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```
xdata = simul$data,
nc = seq_len(20)
)

# Weighted Hierarchical clustering (using COSA)
if (requireNamespace("rCOSA", quietly = TRUE)) {
  myhclust <- HierarchicalClustering(
    xdata = simul$data,
    weighted = TRUE,
    nc = seq_len(20),
    Lambda = c(0.2, 0.5)
)
}</pre>
```

Incremental

Incremental prediction performance in regression

## **Description**

Computes the prediction performance of regression models where predictors are sequentially added by order of decreasing selection proportion. This function can be used to evaluate the marginal contribution of each of the selected predictors over and above more stable predictors. Performances are evaluated as in ExplanatoryPerformance.

## Usage

```
Incremental(
  xdata,
 ydata,
 new_xdata = NULL,
 new_ydata = NULL,
  stability = NULL,
  family = NULL,
  implementation = NULL,
  prediction = NULL,
  resampling = "subsampling",
  n_predictors = NULL,
 K = 100,
  tau = 0.8,
  seed = 1,
 n_{thr} = NULL
  time = 1000,
  verbose = TRUE,
)
```

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#### **Arguments**

xdata matrix of predictors with observations as rows and variables as columns.

ydata optional vector or matrix of outcome(s). If family is set to "binomial" or

"multinomial", ydata can be a vector with character/numeric values or a fac-

tor.

new\_xdata optional test set (predictor data).
new\_ydata optional test set (outcome data).

stability output of VariableSelection. If stability=NULL (the default), a model in-

cluding all variables in xdata as predictors is fitted. Argument family must be

provided in this case.

family type of regression model. Possible values include "gaussian" (linear regres-

sion), "binomial" (logistic regression), and "cox" (survival analysis). If pro-

vided, this argument must be consistent with input stability.

implementation optional function to refit the model. If implementation=NULL and stability

is the output of VariableSelection, lm (linear regression), coxph (Cox regression), glm (logistic regression), or multinom (multinomial regression) is used.

prediction optional function to compute predicted values from the model refitted with implementation.

resampling resampling approach to create the training set. The default is "subsampling"

for sampling without replacement of a proportion tau of the observations. Alternatively, this argument can be a function to use for resampling. This function must use arguments named data and tau and return the IDs of observations to

be included in the resampled dataset.

n\_predictors number of predictors to consider.

K number of training-test splits. Only used if new\_xdata and new\_ydata are not

provided.

tau proportion of observations used in the training set. Only used if new\_xdata and

new\_ydata are not provided.

seed value of the seed to ensure reproducibility of the results. Only used if new\_xdata

and new\_ydata are not provided.

n\_thr number of thresholds to use to construct the ROC curve. If n\_thr=NULL, all

predicted probability values are iteratively used as thresholds. For faster computations on large data, less thresholds can be used. Only applicable to logistic

regression.

time numeric indicating the time for which the survival probabilities are computed.

Only applicable to Cox regression.

verbose logical indicating if a loading bar and messages should be printed.

... additional parameters passed to the function provided in resampling.

#### Value

An object of class incremental.

For logistic regression, a list with:

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FPR	A list with, for each of the models (sequentially added predictors), the False Positive Rates for different thresholds (columns) and different data splits (rows).
TPR	A list with, for each of the models (sequentially added predictors), the True Positive Rates for different thresholds (columns) and different data splits (rows).
AUC	A list with, for each of the models (sequentially added predictors), a vector of Area Under the Curve (AUC) values obtained with different data splits.
Beta	Estimated regression coefficients from visited models.
names	Names of the predictors by order of inclusion.
stable	Binary vector indicating which predictors are stably selected. Only returned if stability is provided.

### For Cox regression, a list with:

concordance A list with, for each of the models (sequentially added predictors), a vector of

concordance indices obtained with different data splits.

Beta Estimated regression coefficients from visited models.

names Names of the predictors by order of inclusion.

stable Binary vector indicating which predictors are stably selected. Only returned if

stability is provided.

For linear regression, a list with:

Q\_squared A list with, for each of the models (sequentially added predictors), a vector of

Q-squared obtained with different data splits.

Beta Estimated regression coefficients from visited models.

names Names of the predictors by order of inclusion.

stable Binary vector indicating which predictors are stably selected. Only returned if

stability is provided.

#### See Also

#### VariableSelection, Refit

Other prediction performance functions: ExplanatoryPerformance()

```
# Data simulation
set.seed(1)
simul <- SimulateRegression(
    n = 1000, pk = 20,
    family = "binomial", ev_xy = 0.8
)

# Data split: selection, training and test set
ids <- Split(
    data = simul$ydata,
    family = "binomial",
    tau = c(0.4, 0.3, 0.3)</pre>
```

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```
xselect <- simul$xdata[ids[[1]], ]</pre>
yselect <- simul$ydata[ids[[1]], ]</pre>
xtrain <- simul$xdata[ids[[2]], ]</pre>
ytrain <- simul$ydata[ids[[2]], ]</pre>
xtest <- simul$xdata[ids[[3]], ]</pre>
ytest <- simul$ydata[ids[[3]], ]</pre>
# Stability selection
stab <- VariableSelection(</pre>
  xdata = xselect,
  ydata = yselect,
  family = "binomial"
# Performances in test set of model refitted in training set
incr <- Incremental(</pre>
  xdata = xtrain, ydata = ytrain,
  new_xdata = xtest, new_ydata = ytest,
  stability = stab, n_predictors = 10
)
plot(incr)
# Alternative with multiple training/test splits
incr <- Incremental(</pre>
  xdata = rbind(xtrain, xtest),
  ydata = c(ytrain, ytest),
  stability = stab, K = 10, n_predictors = 10
plot(incr)
```

**KMeansClustering** 

(Sparse) K-means clustering

## Description

Runs k-means clustering using implementation from kmeans. This function is not using stability.

# Usage

```
KMeansClustering(xdata, nc = NULL, Lambda = NULL, ...)
```

### **Arguments**

xdata

data matrix with observations as rows and variables as columns.

nc

matrix of parameters controlling the number of clusters in the underlying algorithm specified in implementation. If nc is not provided, it is set to seq(1, tau\*nrow(xdata)).

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```
Lambda vector of penalty parameters (see argument wbounds in KMeansSparseCluster).
... additional parameters passed to kmeans (if Lambda is NULL) or KMeansSparseCluster.
```

### Value

A list with:

comembership an array of binary and symmetric co-membership matrices.

weights a matrix of median weights by feature.

#### References

Witten DM, Tibshirani R (2010). "A Framework for Feature Selection in Clustering." *Journal of the American Statistical Association*, **105**(490), 713-726. doi:10.1198/jasa.2010.tm09415, PMID: 20811510.

#### See Also

Other clustering algorithms: DBSCANClustering(), GMMClustering(), HierarchicalClustering(), PAMClustering()

# Examples

```
# Data simulation
set.seed(1)
simul <- SimulateClustering(n = c(10, 10), pk = 50)

# K means clustering
mykmeans <- KMeansClustering(xdata = simul$data, nc = seq_len(20))

# Sparse K means clustering
if (requireNamespace("sparcl", quietly = TRUE)) {
   mykmeans <- KMeansClustering(
      xdata = simul$data, nc = seq_len(20),
      Lambda = c(2, 5)
   )
}</pre>
```

LambdaGridGraphical

Grid of penalty parameters (graphical model)

### Description

Generates a relevant grid of penalty parameter values for penalised graphical models.

### Usage

```
LambdaGridGraphical(
  xdata,
  pk = NULL
  lambda_other_blocks = 0.1,
 K = 100,
  tau = 0.5,
  n_cat = 3,
  implementation = PenalisedGraphical,
  start = "cold",
  scale = TRUE,
  resampling = "subsampling",
 PFER_method = "MB",
 PFER_thr = Inf,
  FDP_thr = Inf,
 Lambda_cardinal = 50,
  lambda_max = NULL,
  lambda_path_factor = 0.001,
 max_density = 0.5,
)
```

## **Arguments**

xdata

data matrix with observations as rows and variables as columns. For multi-block stability selection, the variables in data have to be ordered by group.

pk

optional vector encoding the grouping structure. Only used for multi-block stability selection where pk indicates the number of variables in each group. If pk=NULL, single-block stability selection is performed.

lambda\_other\_blocks

optional vector of parameters controlling the level of sparsity in neighbour blocks for the multi-block procedure. To use jointly a specific set of parameters for each block, lambda\_other\_blocks must be set to NULL (not recommended). Only used for multi-block stability selection, i.e. if length(pk)>1.

Κ number of resampling iterations.

subsample size. Only used if resampling="subsampling" and cpss=FALSE. tau

computation options for the stability score. Default is NULL to use the score n\_cat

based on a z test. Other possible values are 2 or 3 to use the score based on the

negative log-likelihood.

implementation function to use for graphical modelling. If implementation=PenalisedGraphical,

the algorithm implemented in glassoFast is used for regularised estimation of a conditional independence graph. Alternatively, a user-defined function can be

provided.

character string indicating if the algorithm should be initialised at the estimated start

(inverse) covariance with previous penalty parameters (start="warm") or not (start="cold"). Using start="warm" can speed-up the computations, but

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could lead to convergence issues (in particular with small Lambda\_cardinal). Only used for implementation=PenalisedGraphical (see argument "start" in glassoFast).

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scale logical indicating if the correlation (scale=TRUE) or covariance (scale=FALSE)

matrix should be used as input of glassoFast if implementation=PenalisedGraphical.

Otherwise, this argument must be used in the function provided in implementation.

resampling resampling approach. Possible values are: "subsampling" for sampling with-

out replacement of a proportion tau of the observations, or "bootstrap" for sampling with replacement generating a resampled dataset with as many observations as in the full sample. Alternatively, this argument can be a function to use for resampling. This function must use arguments named data and tau and

return the IDs of observations to be included in the resampled dataset.

PFER\_method method used to compute the upper-bound of the expected number of False Posi-

tives (or Per Family Error Rate, PFER). If PFER\_method="MB", the method proposed by Meinshausen and Bühlmann (2010) is used. If PFER\_method="SS", the method proposed by Shah and Samworth (2013) under the assumption of

unimodality is used.

PFER\_thr threshold in PFER for constrained calibration by error control. If PFER\_thr=Inf

and FDP\_thr=Inf, unconstrained calibration is used (the default).

FDP\_thr threshold in the expected proportion of falsely selected features (or False Dis-

covery Proportion) for constrained calibration by error control. If PFER\_thr=Inf

and FDP\_thr=Inf, unconstrained calibration is used (the default).

Lambda\_cardinal

number of values in the grid of parameters controlling the level of sparsity in the

underlying algorithm.

lambda\_max optional maximum value for the grid in penalty parameters. If lambda\_max=NULL,

the maximum value is set to the maximum covariance in absolute value. Only

used if implementation=PenalisedGraphical.

lambda\_path\_factor

multiplicative factor used to define the minimum value in the grid.

max\_density threshold on the density. The grid is defined such that the density of the esti-

mated graph does not exceed max\_density.

.. additional parameters passed to the functions provided in implementation or

resampling.

### Value

A matrix of lambda values with length(pk) columns and Lambda\_cardinal rows.

#### See Also

Other lambda grid functions: LambdaGridRegression(), LambdaSequence()

### **Examples**

# Single-block simulation

```
set.seed(1)
simul <- SimulateGraphical()</pre>
# Generating grid of 10 values
Lambda <- LambdaGridGraphical(xdata = simul$data, Lambda_cardinal = 10)</pre>
# Ensuring PFER < 5
Lambda <- LambdaGridGraphical(xdata = simul$data, Lambda_cardinal = 10, PFER_thr = 5)</pre>
# Multi-block simulation
set.seed(1)
simul <- SimulateGraphical(pk = c(10, 10))
# Multi-block grid
Lambda <- LambdaGridGraphical(xdata = simul$data, pk = c(10, 10), Lambda_cardinal = 10)
# Denser neighbouring blocks
Lambda <- LambdaGridGraphical(</pre>
  xdata = simul data, pk = c(10, 10),
  Lambda_cardinal = 10, lambda_other_blocks = 0
)
# Using different neighbour penalties
Lambda <- LambdaGridGraphical(</pre>
  xdata = simul data, pk = c(10, 10),
  Lambda_cardinal = 10, lambda_other_blocks = c(0.1, 0, 0.1)
stab <- GraphicalModel(</pre>
  xdata = simul data, pk = c(10, 10),
  Lambda = Lambda, lambda_other_blocks = c(0.1, 0, 0.1)
)
stab$Lambda
# Visiting from empty to full graphs with max_density=1
Lambda <- LambdaGridGraphical(</pre>
  xdata = simul data, pk = c(10, 10),
  Lambda_cardinal = 10, max_density = 1
bigblocks <- BlockMatrix(pk = c(10, 10))</pre>
bigblocks_vect <- bigblocks[upper.tri(bigblocks)]</pre>
N_blocks <- unname(table(bigblocks_vect))</pre>
N_blocks # max number of edges per block
tab \leftarrow GraphicalModel(xdata = simul\$data, pk = c(10, 10), Lambda = Lambda)
apply(stab$Q, 2, max, na.rm = TRUE) # max average number of edges from underlying algo
```

## **Description**

Generates a relevant grid of penalty parameter values for penalised regression using the implementation in glmnet.

### Usage

```
LambdaGridRegression(
  xdata,
 ydata,
  tau = 0.5,
  seed = 1,
  family = "gaussian",
  resampling = "subsampling",
 Lambda_cardinal = 100,
  check_input = TRUE,
)
```

## **Arguments**

xdata	matrix of predictors with observations as rows and variables as columns.	
ydata	optional vector or matrix of outcome(s). If family is set to "binomial" or "multinomial", ydata can be a vector with character/numeric values or a factor.	
tau	subsample size. Only used if resampling="subsampling" and cpss=FALSE.	
seed	value of the seed to initialise the random number generator and ensure reproducibility of the results (see set.seed).	
family	type of regression model. This argument is defined as in glmnet. Possible values include "gaussian" (linear regression), "binomial" (logistic regression), "multinomial" (multinomial regression), and "cox" (survival analysis).	
resampling	resampling approach. Possible values are: "subsampling" for sampling without replacement of a proportion tau of the observations, or "bootstrap" for sampling with replacement generating a resampled dataset with as many observations as in the full sample. Alternatively, this argument can be a function to use for resampling. This function must use arguments named data and tau and return the IDs of observations to be included in the resampled dataset.	
Lambda_cardinal		
	number of values in the grid of parameters controlling the level of sparsity in the	

underlying algorithm.

logical indicating if input values should be checked (recommended). check\_input

additional parameters passed to the functions provided in implementation or . . .

resampling.

## Value

A matrix of lambda values with one column and as many rows as indicated in Lambda\_cardinal.

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### See Also

Other lambda grid functions: LambdaGridGraphical(), LambdaSequence()

### **Examples**

```
# Data simulation
set.seed(1)
simul <- SimulateRegression(n = 100, pk = 50, family = "gaussian") # simulated data

# Lambda grid for linear regression
Lambda <- LambdaGridRegression(
    xdata = simul$xdata, ydata = simul$ydata,
    family = "gaussian", Lambda_cardinal = 20
)

# Grid can be used in VariableSelection()
stab <- VariableSelection(
    xdata = simul$xdata, ydata = simul$ydata,
    family = "gaussian", Lambda = Lambda
)
print(SelectedVariables(stab))</pre>
```

LambdaSequence

Sequence of penalty parameters

### **Description**

Generates a sequence of penalty parameters from extreme values and the required number of elements. The sequence is defined on the log-scale.

### Usage

```
LambdaSequence(lmax, lmin, cardinal = 100)
```

### **Arguments**

lmax maximum value in the grid.lmin minimum value in the grid.cardinal number of values in the grid.

## Value

A vector with values between "lmin" and "lmax" and as many values as indicated by "cardinal".

### See Also

Other lambda grid functions: LambdaGridGraphical(), LambdaGridRegression()

LinearSystemMatrix 67

## **Examples**

```
# Grid from extreme values
mygrid <- LambdaSequence(lmax = 0.7, lmin = 0.001, cardinal = 10)</pre>
```

LinearSystemMatrix

Matrix from linear system outputs

## Description

Returns a matrix from output of PenalisedLinearSystem.

## Usage

LinearSystemMatrix(vect, adjacency)

# **Arguments**

vect vector of coefficients to assign to entries of the matrix.

adjacency binary adjacency matrix of the Directed Acyclic Graph (transpose of the asym-

metric matrix A in Reticular Action Model notation). The row and column

names of this matrix must be defined.

### Value

An asymmetric matrix.

### See Also

PenalisedLinearSystem

OpenMxMatrix

Matrix from OpenMx outputs

## **Description**

Returns a matrix from output of mxPenaltySearch.

### Usage

```
OpenMxMatrix(vect, adjacency, residual_covariance = NULL)
```

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### **Arguments**

vect vector of coefficients to assign to entries of the matrix.

adjacency binary adjacency matrix of the Directed Acyclic Graph (transpose of the asym-

metric matrix A in Reticular Action Model notation). The row and column

names of this matrix must be defined.

residual\_covariance

binary and symmetric matrix encoding the nonzero entries in the residual covariance matrix (symmetric matrix S in Reticular Action Model notation). By default, this is the identity matrix (no residual covariance).

#### Value

An asymmetric matrix.

### See Also

PenalisedOpenMx, OpenMxModel

OpenMxModel

Writing OpenMx model (matrix specification)

## Description

Returns matrix specification for use in mxModel from (i) the adjacency matrix of a Directed Acyclic Graph (asymmetric matrix A in Reticular Action Model notation), and (ii) a binary matrix encoding nonzero entries in the residual covariance matrix (symmetric matrix S in Reticular Action Model notation).

#### Usage

OpenMxModel(adjacency, residual\_covariance = NULL, manifest = NULL)

### **Arguments**

adjacency binary adjacency matrix of the Directed Acyclic Graph (transpose of the asym-

metric matrix A in Reticular Action Model notation). The row and column

names of this matrix must be defined.

residual\_covariance

binary and symmetric matrix encoding the nonzero entries in the residual covariance matrix (symmetric matrix S in Reticular Action Model notation). By

default, this is the identity matrix (no residual covariance).

manifest optional vector of manifest variable names.

### Value

A list of RAM matrices that can be used in mxRun.

OpenMxModel 69

### See Also

PenalisedOpenMx, OpenMxMatrix

```
if (requireNamespace("OpenMx", quietly = TRUE)) {
 # Definition of simulated effects
 pk < -c(3, 2, 3)
 dag <- LayeredDAG(layers = pk)</pre>
 theta <- dag
 theta[2, 4] <- 0
 theta[3, 7] <- 0
 theta[4, 7] <- 0
 # Data simulation
 set.seed(1)
 simul <- SimulateStructural(n = 500, v_between = 1, theta = theta, pk = pk)</pre>
 # Writing RAM matrices for mxModel
 ram_matrices <- OpenMxModel(adjacency = dag)</pre>
 # Running unpenalised model
 unpenalised <- OpenMx::mxRun(OpenMx::mxModel(</pre>
    "Model",
    OpenMx::mxData(simul$data, type = "raw"),
    ram_matrices$Amat,
    ram_matrices$Smat,
    ram_matrices$Fmat,
    ram_matrices$Mmat,
    OpenMx::mxExpectationRAM("A", "S", "F", "M", dimnames = colnames(dag)),
    OpenMx::mxFitFunctionML()
 ), silent = TRUE, suppressWarnings = TRUE)
 unpenalised$A$values
 # Incorporating latent variables
 ram_matrices <- OpenMxModel(</pre>
    adjacency = dag,
    manifest = paste0("x", seq_len(7))
 )
 ram_matrices$Fmat$values
 # Running unpenalised model
 unpenalised <- OpenMx::mxRun(OpenMx::mxModel(</pre>
    "Model",
    OpenMx::mxData(simul$data[, seq_len(7)], type = "raw"),
    ram_matrices$Amat,
    ram_matrices$Smat,
    ram_matrices$Fmat,
    ram_matrices$Mmat,
    OpenMx::mxExpectationRAM("A", "S", "F", "M", dimnames = colnames(dag)),
    OpenMx::mxFitFunctionML()
 ), silent = TRUE, suppressWarnings = TRUE)
```

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```
unpenalised$A$values
}
```

**PAMClustering** 

(Weighted) Partitioning Around Medoids

#### Description

Runs Partitioning Around Medoids (PAM) clustering using implementation from pam. This is also known as the k-medoids algorithm. If Lambda is provided, clustering is applied on the weighted distance matrix calculated using the COSA algorithm as implemented in cosa2. Otherwise, distances are calculated using dist. This function is not using stability.

### Usage

```
PAMClustering(xdata, nc = NULL, Lambda = NULL, distance = "euclidean", ...)
```

### Arguments

data matrix with observations as rows and variables as columns. xdata nc matrix of parameters controlling the number of clusters in the underlying algorithm specified in implementation. If nc is not provided, it is set to seq(1, tau\*nrow(xdata)). vector of penalty parameters (see argument lambda in cosa2). Unweighted dis-Lambda tance matrices are used if Lambda=NULL. distance character string indicating the type of distance to use. If Lambda=NULL, possible values include "euclidean", "maximum", "canberra", "binary", and "minkowski" (see argument method in dist). Otherwise, possible values include "euclidean" (pwr=2) or "absolute" (pwr=1) (see argument pwr in cosa2). additional parameters passed to pam, dist, or cosa2. If weighted=TRUE, parameters niter (default to 1) and noit (default to 100) correspond to the number of

iterations in cosa2 to calculate weights and may need to be modified.

#### Value

#### A list with:

comembership an array of binary and symmetric co-membership matrices. weights a matrix of median weights by feature.

### References

Kampert MM, Meulman JJ, Friedman JH (2017). "rCOSA: A Software Package for Clustering Objects on Subsets of Attributes." *Journal of Classification*, **34**(3), 514–547. doi:10.1007/s00357-0179240z.

Friedman JH, Meulman JJ (2004). "Clustering objects on subsets of attributes (with discussion)." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **66**(4), 815-849. doi:10.1111/j.14679868.2004.02059.x, https://rss.onlinelibrary.wiley.com/doi/pdf/10.1111/j.1467-9868.2004.02059.x, https://rss.onlinelibrary.wiley.com/doi/abs/10.1111/j.1467-9868.2004.02059.x.

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### See Also

Other clustering algorithms: DBSCANClustering(), GMMClustering(), HierarchicalClustering(), KMeansClustering()

# **Examples**

```
if (requireNamespace("cluster", quietly = TRUE)) {
 # Data simulation
 set.seed(1)
 simul \leftarrow SimulateClustering(n = c(10, 10), pk = 50)
 # PAM clustering
 myclust <- PAMClustering(</pre>
   xdata = simul$data,
   nc = seq_len(20)
 )
 # Weighted PAM clustering (using COSA)
 if (requireNamespace("rCOSA", quietly = TRUE)) {
   myclust <- PAMClustering(</pre>
      xdata = simul$data,
      nc = seq_len(20),
      Lambda = c(0.2, 0.5)
   )
 }
}
```

PenalisedGraphical

Graphical LASSO

# Description

Runs the graphical LASSO algorithm for estimation of a Gaussian Graphical Model (GGM). This function is not using stability.

## Usage

```
PenalisedGraphical(
  xdata,
  pk = NULL,
  Lambda,
  Sequential_template = NULL,
  scale = TRUE,
  start = "cold",
  output_omega = FALSE,
  ...
)
```

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#### **Arguments**

xdata matrix with observations as rows and variables as columns.

pk optional vector encoding the grouping structure. Only used for multi-block sta-

bility selection where pk indicates the number of variables in each group. If

pk=NULL, single-block stability selection is performed.

Lambda matrix of parameters controlling the level of sparsity.

Sequential\_template

logical matrix encoding the type of procedure to use for data with multiple blocks in stability selection graphical modelling. For multi-block estimation, the stability selection model is constructed as the union of block-specific stable edges estimated while the others are weakly penalised (TRUE only for the block currently being calibrated and FALSE for other blocks). Other approaches with

joint calibration of the blocks are allowed (all entries are set to TRUE).

scale logical indicating if the correlation (scale=TRUE) or covariance (scale=FALSE)

matrix should be used as input of glassoFast if implementation=PenalisedGraphical. Otherwise, this argument must be used in the function provided in implementation.

start character string indicating if the algorithm should be initialised at the estimated

(inverse) covariance with previous penalty parameters (start="warm") or not (start="cold"). Using start="warm" can speed-up the computations, but could lead to convergence issues (in particular with small Lambda\_cardinal). Only used for implementation=PenalisedGraphical (see argument "start"

in glassoFast).

output\_omega logical indicating if the estimated precision matrices should be stored and re-

turned.

... additional parameters passed to the function provided in implementation.

#### **Details**

The use of the procedure from Equation (4) or (5) is controlled by the argument "Sequential\_template".

### Value

An array with binary and symmetric adjacency matrices along the third dimension.

#### References

Friedman J, Hastie T, Tibshirani R (2008). "Sparse inverse covariance estimation with the graphical lasso." *Biostatistics*, **9**(3), 432–441.

#### See Also

### GraphicalModel

Other underlying algorithm functions: CART(), ClusteringAlgo(), PenalisedOpenMx(), PenalisedRegression()

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### **Examples**

```
# Data simulation
set.seed(1)
simul <- SimulateGraphical()

# Running graphical LASSO
myglasso <- PenalisedGraphical(
    xdata = simul$data,
    Lambda = matrix(c(0.1, 0.2), ncol = 1)
)

# Returning estimated precision matrix
myglasso <- PenalisedGraphical(
    xdata = simul$data,
    Lambda = matrix(c(0.1, 0.2), ncol = 1),
    output_omega = TRUE
)</pre>
```

PenalisedOpenMx

Penalised Structural Equation Model

## **Description**

Runs penalised Structural Equation Modelling using implementations from OpenMx functions (for PenalisedOpenMx), or using series of penalised regressions with glmnet (for PenalisedLinearSystem). The function PenalisedLinearSystem does not accommodate latent variables. These functions are not using stability.

## Usage

```
PenalisedOpenMx(
    xdata,
    adjacency,
    penalised = NULL,
    residual_covariance = NULL,
    Lambda,
    ...
)

PenalisedLinearSystem(xdata, adjacency, penalised = NULL, Lambda = NULL, ...)
```

#### **Arguments**

xdata matrix with observations as rows and variables as columns. Column names must

be defined and in line with the row and column names of adjacency.

adjacency binary adjacency matrix of the Directed Acyclic Graph (transpose of the asym-

metric matrix A in Reticular Action Model notation). The row and column

names of this matrix must be defined.

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optional binary matrix indicating which coefficients are regularised. penalised residual\_covariance binary and symmetric matrix encoding the nonzero entries in the residual covariance matrix (symmetric matrix S in Reticular Action Model notation). By default, this is the identity matrix (no residual covariance). Lambda matrix of parameters controlling the level of sparsity. Only the minimum, max-

imum and length are used in PenalisedOpenMx.

additional parameters passed to OpenMx functions (for PenalisedOpenMx), or . . .

glmnet (for PenalisedLinearSystem).

### Value

A list with:

selected matrix of binary selection status. Rows correspond to different regularisation

parameters. Columns correspond to different parameters to estimated.

matrix of model coefficients. Rows correspond to different regularisation pabeta\_full

rameters. Columns correspond to different parameters to estimated.

#### References

Jacobucci R, Grimm KJ, McArdle JJ (2016). "Regularized structural equation modeling." Structural equation modeling: a multidisciplinary journal, 23(4), 555-566. doi:10.1080/10705511.2016.1154793.

#### See Also

SelectionAlgo, VariableSelection, OpenMxMatrix, LinearSystemMatrix

Other underlying algorithm functions: CART(), ClusteringAlgo(), PenalisedGraphical(), PenalisedRegression()

```
# Data simulation
pk <- c(3, 2, 3)
dag <- LayeredDAG(layers = pk)</pre>
theta <- dag
theta[2, 4] <- 0
set.seed(1)
simul <- SimulateStructural(theta = theta, pk = pk, output_matrices = TRUE)</pre>
# Running regularised SEM (OpenMx)
if (requireNamespace("OpenMx", quietly = TRUE)) {
 mysem <- PenalisedOpenMx(</pre>
    xdata = simul$data, adjacency = dag,
    Lambda = seq(1, 10, 1)
 OpenMxMatrix(vect = mysem$selected[3, ], adjacency = dag)
}
# Running regularised SEM (glmnet)
mysem <- PenalisedLinearSystem(</pre>
```

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```
xdata = simul$data, adjacency = dag
)
LinearSystemMatrix(vect = mysem$selected[20, ], adjacency = dag)
```

PenalisedRegression

Penalised regression

# Description

Runs penalised regression using implementation from glmnet. This function is not using stability.

# Usage

```
PenalisedRegression(
   xdata,
   ydata,
   Lambda = NULL,
   family,
   penalisation = c("classic", "randomised", "adaptive"),
   gamma = NULL,
   ...
)
```

# Arguments

xdata	matrix of predictors with observations as rows and variables as columns.
ydata	optional vector or matrix of outcome(s). If family is set to "binomial" or "multinomial", ydata can be a vector with character/numeric values or a factor.
Lambda	matrix of parameters controlling the level of sparsity.
family	type of regression model. This argument is defined as in glmnet. Possible values include "gaussian" (linear regression), "binomial" (logistic regression), "multinomial" (multinomial regression), and "cox" (survival analysis).
penalisation	type of penalisation to use. If penalisation="classic" (the default), penalised regression is done with the same regularisation parameter, or using penalty.factor, if specified. If penalisation="randomised", the regularisation for each of the variables is uniformly chosen between lambda and lambda/gamma. If penalisation="adaptive", the regularisation for each of the variables is weighted by 1/abs(beta)^gamma where beta is the regression coefficient obtained from unpenalised regression.
gamma	parameter for randomised or adaptive regularisation. Default is gamma=0.5 for randomised regularisation and gamma=2 for adaptive regularisation. The parameter gamma should be between 0 and 1 for randomised regularisation.
	additional parameters passed to glmnet.

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### Value

A list with:

selected matrix of binary selection status. Rows correspond to different model parame-

ters. Columns correspond to predictors.

beta\_full array of model coefficients. Rows correspond to different model parameters.

Columns correspond to predictors. Indices along the third dimension correspond

to outcome variable(s).

## References

Zou H (2006). "The adaptive lasso and its oracle properties." *Journal of the American statistical association*, **101**(476), 1418–1429.

Tibshirani R (1996). "Regression Shrinkage and Selection via the Lasso." *Journal of the Royal Statistical Society. Series B (Methodological)*, **58**(1), 267–288. ISSN 00359246, http://www.jstor.org/stable/2346178.

#### See Also

SelectionAlgo, VariableSelection

 $Other \ underlying \ algorithm \ functions: \ CART(), Clustering Algo(), Penalised Graphical(), Penalised Open Mx()$ 

```
# Data simulation
set.seed(1)
simul <- SimulateRegression(pk = 50)

# Running the LASSO
mylasso <- PenalisedRegression(
    xdata = simul$xdata, ydata = simul$ydata,
    Lambda = c(0.1, 0.2), family = "gaussian"
)

# Using glmnet arguments
mylasso <- PenalisedRegression(
    xdata = simul$xdata, ydata = simul$ydata,
    Lambda = c(0.1), family = "gaussian",
    penalty.factor = c(rep(0, 10), rep(1, 40))
)
mylasso$beta_full</pre>
```

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PFER Per Family Error Rate

### **Description**

Computes the Per Family Error Rate upper-bound of a stability selection model using the methods proposed by Meinshausen and Bühlmann (2010) or Shah and Samworth (2013). In stability selection, the PFER corresponds to the expected number of stably selected features that are not relevant to the outcome (i.e. False Positives).

### Usage

```
PFER(q, pi, N, K, PFER_method = "MB")
```

### Arguments

q average number of features selected by the underlying algorithm.

pi threshold in selection proportions.

N total number of features.

K number of resampling iterations.

PFER\_method method used to compute the upper-bound of the expected number of False Posi-

tives (or Per Family Error Rate, PFER). If PFER\_method="MB", the method proposed by Meinshausen and Bühlmann (2010) is used. If PFER\_method="SS", the method proposed by Shah and Samworth (2013) under the assumption of

unimodality is used.

#### Value

The estimated upper-bound in PFER.

### References

Meinshausen N, Bühlmann P (2010). "Stability selection." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **72**(4), 417-473. doi:10.1111/j.14679868.2010.00740.x.

Shah RD, Samworth RJ (2013). "Variable selection with error control: another look at stability selection." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **75**(1), 55-80. doi:10.1111/j.14679868.2011.01034.x.

## See Also

Other stability metric functions: ConsensusScore(), FDP(), StabilityMetrics(), StabilityScore()

```
# Computing PFER for 10/50 selected features and threshold of 0.8 pfer_mb <- PFER(q = 10, pi = 0.8, N = 50, K = 100, PFER_method = "MB") pfer_ss <- PFER(q = 10, pi = 0.8, N = 50, K = 100, PFER_method = "SS")
```

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plot.clustering

Consensus matrix heatmap

## **Description**

Creates a heatmap of the (calibrated) consensus matrix. See examples in Clustering.

# Usage

```
## S3 method for class 'clustering'
plot(
  х,
  linkage = "complete",
  argmax_id = NULL,
  theta = NULL,
  theta_star = NULL,
  col = c("ivory", "navajowhite", "tomato", "darkred"),
  lines = TRUE,
  col.lines = c("blue"),
  lwd.lines = 2,
  tick = TRUE,
  axes = TRUE,
 col.axis = NULL,
  cex.axis = 1,
 xlas = 2,
 ylas = 2,
 bty = "n",
)
```

# Arguments

x	output of Clustering.
linkage	character string indicating the type of linkage used in hierarchical clustering to define the stable clusters. Possible values include "complete", "single" and "average" (see argument "method" in hclust for a full list).
argmax_id	optional indices of hyper-parameters. If ${\tt argmax\_id=NULL},$ the calibrated hyper-parameters are used.
theta	optional vector of cluster membership. If provided, the ordering of the items should be the same as in Clusters. This argument is used to re-order the consensus matrix.
theta_star	optional vector of true cluster membership. If provided, the ordering of the items should be the same as in Clusters. This argument is used to define item colours.
col	vector of colours.

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lines	logical indicating if lines separating the clusters provided in theta should be displayed.
col.lines	colour of the lines separating the clusters.
lwd.lines	width of the lines separating the clusters.
tick	logical indicating if axis tickmarks should be displayed.
axes	logical indicating if item labels should be displayed.
col.axis	optional vector of cluster colours.
cex.axis	font size for axes.
xlas	orientation of labels on the x-axis, as las in par.
ylas	orientation of labels on the y-axis, as las in par.
bty	character string indicating if the box around the plot should be drawn. Possible values include: "o" (default, the box is drawn), or "n" (no box).
	additional arguments passed to Heatmap.

### Value

A heatmap.

plot.incremental Plot of increm

Plot of incremental performance

# Description

Represents prediction performances upon sequential inclusion of the predictors in a logistic or Cox regression model as produced by Incremental. The median and quantiles of the performance metric are reported. See examples in Incremental.

## Usage

```
## S3 method for class 'incremental'
plot(
    x,
    quantiles = c(0.05, 0.95),
    col = c("red", "grey"),
    col.axis = NULL,
    xgrid = FALSE,
    ygrid = FALSE,
    output_data = FALSE,
    ...
)

IncrementalPlot(
    x,
    quantiles = c(0.05, 0.95),
```

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```
col = c("red", "grey"),
col.axis = NULL,
xgrid = FALSE,
ygrid = FALSE,
output_data = FALSE,
...
)

PlotIncremental(
    x,
    quantiles = c(0.05, 0.95),
    col = c("red", "grey"),
    col.axis = NULL,
    xgrid = FALSE,
    ygrid = FALSE,
    output_data = FALSE,
...
)
```

### **Arguments**

Χ	output of Incremental.
quantiles	quantiles defining the lower and upper bounds.
col	vector of colours by stable selection status.
col.axis	optional vector of label colours by stable selection status.
xgrid	logical indicating if a vertical grid should be drawn.
ygrid	logical indicating if a horizontal grid should be drawn.
output_data	logical indicating if the median and quantiles should be returned in a matrix.
	additional plotting arguments (see par).

## Value

A plot.

### See Also

Incremental

plot.roc\_band Receiver Operating Characteristic (ROC) band

### **Description**

Plots the True Positive Rate (TPR) as a function of the False Positive Rate (FPR) for different thresholds in predicted probabilities. If the results from multiple ROC analyses are provided (e.g. output of ExplanatoryPerformance with large K), the point-wise median is represented and flanked by a transparent band defined by point-wise quantiles. See examples in ROC and ExplanatoryPerformance.

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## Usage

```
## $3 method for class 'roc_band'
plot(
    x,
    col_band = NULL,
    alpha = 0.5,
    quantiles = c(0.05, 0.95),
    add = FALSE,
    ...
)
```

### **Arguments**

```
x output of ROC or ExplanatoryPerformance.
col_band colour of the band defined by point-wise quantiles.
alpha level of opacity for the band.
quantiles point-wise quantiles of the performances defining the band.
add logical indicating if the curve should be added to the current plot.
... additional plotting arguments (see par).
```

### Value

A base plot.

#### See Also

ROC, ExplanatoryPerformance

```
plot.variable_selection

Plot of selection proportions
```

## **Description**

Makes a barplot of selection proportions in decreasing order. See examples in VariableSelection.

## Usage

```
## S3 method for class 'variable_selection'
plot(
    x,
    col = c("red", "grey"),
    col.axis = NULL,
    col.thr = "darkred",
    lty.thr = 2,
    n_predictors = NULL,
    ...
)
```

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## **Arguments**

```
output of VariableSelection.
vector of colours by stable selection status.
optional vector of label colours by stable selection status.
thr threshold colour.
thry.thr threshold line type as lty in par.
n_predictors number of predictors to display.
additional plotting arguments (see par).
```

### Value

A plot.

#### See Also

VariableSelection

PLS

Partial Least Squares 'a la carte'

## **Description**

Runs a Partial Least Squares (PLS) model in regression mode using algorithm implemented in pls. This function allows for the construction of components based on different sets of predictor and/or outcome variables. This function is not using stability.

## Usage

```
PLS(
   xdata,
   ydata,
   selectedX = NULL,
   selectedY = NULL,
   family = "gaussian",
   ncomp = NULL,
   scale = TRUE
)
```

tor.

## **Arguments**

xdata matrix of predictors with observations as rows and variables as columns.

ydata optional vector or matrix of outcome(s). If family is set to "binomial" or "multinomial", ydata can be a vector with character/numeric values or a fac-

selectedX binary matrix of size (ncol(xdata) \* ncomp). The binary entries indicate which

predictors (in rows) contribute to the definition of each component (in columns).

If selectedX=NULL, all predictors are selected for all components.

selectedY binary matrix of size (ncol(ydata) \* ncomp). The binary entries indicate which

outcomes (in rows) contribute to the definition of each component (in columns).

If selectedY=NULL, all outcomes are selected for all components.

family type of PLS model. Only family="gaussian" is supported. This corresponds

to a PLS model as defined in pls (for continuous outcomes).

ncomp number of components.

scale logical indicating if the data should be scaled (i.e. transformed so that all vari-

ables have a standard deviation of one).

#### **Details**

All matrices are defined as in (Wold et al. 2001). The weight matrix Wmat is the equivalent of loadings\$X in pls. The loadings matrix Pmat is the equivalent of mat.c in pls. The score matrices Tmat and Qmat are the equivalent of variates\$X and variates\$Y in pls.

#### Value

A list with:

Wmat matrix of X-weights.

Wstar matrix of transformed X-weights.

Pmat matrix of X-loadings.

Cmat matrix of Y-weights.

Tmat matrix of X-scores.

Umat matrix of Y-scores.

Qmat matrix needed for predictions.

Rmat matrix needed for predictions.

meansX vector used for centering of predictors, needed for predictions.

sigmaX vector used for scaling of predictors, needed for predictions.

wector used for centering of outcomes, needed for predictions.

sigmaY vector used for scaling of outcomes, needed for predictions.

methods a list with family and scale values used for the run.

params a list with selectedX and selectedY values used for the run.

### References

Wold S, Sjöström M, Eriksson L (2001). "PLS-regression: a basic tool of chemometrics." *Chemometrics and Intelligent Laboratory Systems*, **58**(2), 109-130. ISSN 0169-7439, doi:10.1016/S0169-7439(01)001551, PLS Methods.

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### See Also

VariableSelection, BiSelection

```
if (requireNamespace("mixOmics", quietly = TRUE)) {
 oldpar <- par(no.readonly = TRUE)</pre>
 # Data simulation
 set.seed(1)
 simul <- SimulateRegression(n = 200, pk = 15, q = 3, family = "gaussian")</pre>
 x <- simul$xdata
 y <- simul$ydata
 # PLS
 mypls \leftarrow PLS(xdata = x, ydata = y, ncomp = 3)
 if (requireNamespace("sgPLS", quietly = TRUE)) {
    # Sparse PLS to identify relevant variables
    stab <- BiSelection(</pre>
      xdata = x, ydata = y,
      family = "gaussian", ncomp = 3,
      LambdaX = seq_len(ncol(x) - 1),
      LambdaY = seq_len(ncol(y) - 1),
      implementation = SparsePLS,
      n_cat = 2
    plot(stab)
    # Refitting of PLS model
   mypls <- PLS(</pre>
      xdata = x, ydata = y,
      selectedX = stab$selectedX,
      selectedY = stab$selectedY
    # Nonzero entries in weights are the same as in selectedX
    par(mfrow = c(2, 2))
   Heatmap(stab$selectedX,
      legend = FALSE
    title("Selected in X")
    Heatmap(ifelse(mypls$Wmat != 0, yes = 1, no = 0),
      legend = FALSE
    title("Nonzero entries in Wmat")
   Heatmap(stab$selectedY,
      legend = FALSE
    title("Selected in Y")
   Heatmap(ifelse(myplsCmat != 0, yes = 1, no = 0),
      legend = FALSE
```

```
    title("Nonzero entries in Cmat")
}

# Multilevel PLS
# Generating random design
z <- rep(seq_len(50), each = 4)

# Extracting the within-variability
x_within <- mixOmics::withinVariation(X = x, design = cbind(z))

# Running PLS on within-variability
mypls <- PLS(xdata = x_within, ydata = y, ncomp = 3)

par(oldpar)
}
</pre>
```

predict.variable\_selection

Predict method for stability selection

# Description

Computes predicted values from the output of VariableSelection.

### Usage

```
## $3 method for class 'variable_selection'
predict(
   object,
   xdata,
   ydata,
   newdata = NULL,
   method = c("ensemble", "refit"),
   ...
)
```

# **Arguments**

```
object output of VariableSelection.

xdata predictor data (training set).

ydata outcome data (training set).

newdata optional predictor data (test set).

method character string indicating if predictions should be obtained from an Ensemble model (if method="ensemble") or a Refitted model (if method="refit").

... additional arguments passed to predict.
```

#### Value

Predicted values.

#### See Also

```
Refit, Ensemble, EnsemblePredictions
```

```
## Linear regression
# Data simulation
set.seed(1)
simul <- SimulateRegression(n = 500, pk = 50, family = "gaussian")</pre>
# Training/test split
ids <- Split(data = simul$ydata, tau = c(0.8, 0.2))
# Stability selection
stab <- VariableSelection(</pre>
  xdata = simul$xdata[ids[[1]], ],
  ydata = simul$ydata[ids[[1]], ]
)
\# Predictions from post stability selection estimation
yhat <- predict(stab,</pre>
  xdata = simul$xdata[ids[[1]], ],
  ydata = simul$ydata[ids[[1]], ],
 newdata = simul$xdata[ids[[2]], ],
  method = "refit"
)
cor(simul$ydata[ids[[2]], ], yhat)^2 # Q-squared
# Predictions from ensemble model
yhat <- predict(stab,</pre>
  xdata = simul$xdata[ids[[1]], ],
  ydata = simul$ydata[ids[[1]], ],
  newdata = simul$xdata[ids[[2]], ],
  method = "ensemble"
cor(simul$ydata[ids[[2]], ], yhat)^2 # Q-squared
## Logistic regression
# Data simulation
set.seed(1)
simul <- SimulateRegression(n = 500, pk = 20, family = "binomial", ev_xy = 0.9)</pre>
# Training/test split
ids <- Split(data = simulydata, family = "binomial", tau = c(0.8, 0.2))
```

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```
# Stability selection
stab <- VariableSelection(</pre>
 xdata = simul$xdata[ids[[1]], ],
 ydata = simul$ydata[ids[[1]], ],
 family = "binomial"
)
# Predictions from post stability selection estimation
yhat <- predict(stab,</pre>
 xdata = simul$xdata[ids[[1]], ],
 ydata = simul$ydata[ids[[1]], ],
 newdata = simul$xdata[ids[[2]], ],
 method = "refit", type = "response"
plot(ROC(predicted = yhat, observed = simul$ydata[ids[[2]], ]))
# Predictions from ensemble model
yhat <- predict(stab,</pre>
 xdata = simul$xdata[ids[[1]], ],
 ydata = simul$ydata[ids[[1]], ],
 newdata = simul$xdata[ids[[2]], ],
 method = "ensemble", type = "response"
)
plot(ROC(predicted = yhat, observed = simul$ydata[ids[[2]], ]),
 add = TRUE,
 col = "blue"
```

PredictPLS

Partial Least Squares predictions

## **Description**

Computes predicted values from a Partial Least Squares (PLS) model in regression mode applied on xdata. This function is using the algorithm implemented in predict.pls.

## Usage

```
PredictPLS(xdata, model)
```

## **Arguments**

xdata matrix of predictors with observations as rows and variables as columns.
model output of PLS.

### Value

An array of predicted values.

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### See Also

**PLS** 

### **Examples**

```
if (requireNamespace("mixOmics", quietly = TRUE)) {
    # Data simulation
    set.seed(1)
    simul <- SimulateRegression(n = 100, pk = c(5, 5, 5), family = "gaussian")
    x <- simul$xdata
    y <- simul$ydata

# PLS
    mypls <- PLS(xdata = x, ydata = y, ncomp = 3)

# Predicted values
    predicted <- PredictPLS(xdata = x, model = mypls)
}</pre>
```

Refit

Regression model refitting

## **Description**

Refits the regression model with stably selected variables as predictors (without penalisation). Variables in xdata not evaluated in the stability selection model will automatically be included as predictors.

### Usage

```
Refit(
  xdata,
  ydata,
  stability = NULL,
  family = NULL,
  implementation = NULL,
  Lambda = NULL,
  seed = 1,
  verbose = TRUE,
)
Recalibrate(
  xdata,
  ydata,
  stability = NULL,
  family = NULL,
  implementation = NULL,
```

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```
Lambda = NULL,
seed = 1,
verbose = TRUE,
...
```

#### **Arguments**

xdata matrix of predictors with observations as rows and variables as columns.

ydata optional vector or matrix of outcome(s). If family is set to "binomial" or

"multinomial", ydata can be a vector with character/numeric values or a fac-

tor.

stability output of VariableSelection or BiSelection. If stability=NULL (the de-

fault), a model including all variables in xdata as predictors is fitted. Argument

family must be provided in this case.

family type of regression model. Possible values include "gaussian" (linear regres-

sion), "binomial" (logistic regression), "multinomial" (multinomial regression), and "cox" (survival analysis). If provided, this argument must be consis-

tent with input stability.

implementation optional function to refit the model. If stability is the output of VariableSelection,

a regression model is refitted. If implementation=NULL and Lambda=0, this is done using lm (for linear regression), coxph (Cox regression), glm (logistic regression), or multinom (multinomial regression). If Lambda=NULL, a Ridge regression is fitted and calibrated by cross validation using cv.glmnet. The

function PLS is used if stability is the output of BiSelection.

Lambda optional vector of penalty parameters.

seed value of the seed to initialise the random number generator and ensure repro-

ducibility of the results (see set.seed).

verbose logical indicating if a loading bar and messages should be printed.

... additional arguments to be passed to the function provided in implementation.

## Value

The output as obtained from:

\link[stats]{lm}

for logistic regression ("binomial" family).

\link[nnet]{multinom}

for multinomial regression ("multinomial" family).

#### See Also

VariableSelection

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```
## Linear regression
# Data simulation
set.seed(1)
simul <- SimulateRegression(n = 100, pk = 50, family = "gaussian")</pre>
# Data split
ids_train <- Resample(</pre>
  data = simul$ydata,
  tau = 0.5, family = "gaussian"
)
xtrain <- simul$xdata[ids_train, , drop = FALSE]</pre>
ytrain <- simul$ydata[ids_train, , drop = FALSE]</pre>
xrefit <- simul$xdata[-ids_train, , drop = FALSE]</pre>
yrefit <- simul$ydata[-ids_train, , drop = FALSE]</pre>
# Stability selection
stab <- VariableSelection(xdata = xtrain, ydata = ytrain, family = "gaussian")</pre>
print(SelectedVariables(stab))
# Refitting the model
refitted <- Refit(</pre>
 xdata = xrefit, ydata = yrefit,
  stability = stab
)
refitted$coefficients # refitted coefficients
head(refitted$fitted.values) # refitted predicted values
# Fitting the full model (including all possible predictors)
refitted <- Refit(</pre>
  xdata = simul$xdata, ydata = simul$ydata,
  family = "gaussian"
refitted$coefficients # refitted coefficients
## Logistic regression
# Data simulation
set.seed(1)
simul <- SimulateRegression(n = 200, pk = 20, family = "binomial")</pre>
# Data split
ids_train <- Resample(</pre>
  data = simul$ydata,
  tau = 0.5, family = "binomial"
xtrain <- simul$xdata[ids_train, , drop = FALSE]</pre>
ytrain <- simul$ydata[ids_train, , drop = FALSE]</pre>
xrefit <- simul$xdata[-ids_train, , drop = FALSE]</pre>
yrefit <- simul$ydata[-ids_train, , drop = FALSE]</pre>
```

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```
# Stability selection
stab <- VariableSelection(xdata = xtrain, ydata = ytrain, family = "binomial")</pre>
# Refitting the model
refitted <- Refit(</pre>
 xdata = xrefit, ydata = yrefit,
 stability = stab
)
refitted$coefficients # refitted coefficients
head(refitted$fitted.values) # refitted predicted probabilities
## Partial Least Squares (multiple components)
if (requireNamespace("sgPLS", quietly = TRUE)) {
 # Data simulation
 set.seed(1)
 simul \leftarrow SimulateRegression(n = 500, pk = 15, q = 3, family = "gaussian")
 # Data split
 ids_train <- Resample(</pre>
    data = simul$ydata,
    tau = 0.5, family = "gaussian"
 )
 xtrain <- simul$xdata[ids_train, , drop = FALSE]</pre>
 ytrain <- simul$ydata[ids_train, , drop = FALSE]</pre>
 xrefit <- simul$xdata[-ids_train, , drop = FALSE]</pre>
 yrefit <- simul$ydata[-ids_train, , drop = FALSE]</pre>
 # Stability selection
 stab <- BiSelection(</pre>
   xdata = xtrain, ydata = ytrain,
    family = "gaussian", ncomp = 3,
   LambdaX = seq_len(ncol(xtrain) - 1),
   LambdaY = seq_len(ncol(ytrain) - 1),
    implementation = SparsePLS
 )
 plot(stab)
 # Refitting the model
 refitted <- Refit(</pre>
    xdata = xrefit, ydata = yrefit,
    stability = stab
 refitted$Wmat # refitted X-weights
 refitted$Cmat # refitted Y-weights
}
```

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### **Description**

Generates a vector of resampled observation IDs.

### Usage

```
Resample(data, family = NULL, tau = 0.5, resampling = "subsampling", ...)
```

### **Arguments**

data vector or matrix of data. In regression, this should be the outcome data.

family type of regression model. This argument is defined as in glmnet. Possible val-

ues include "gaussian" (linear regression), "binomial" (logistic regression), "multinomial" (multinomial regression), and "cox" (survival analysis).

tau subsample size. Only used if resampling "subsampling" and cpss=FALSE.

resampling resampling approach. Possible values are: "subsampling" for sampling with-

out replacement of a proportion tau of the observations, or "bootstrap" for sampling with replacement generating a resampled dataset with as many observations as in the full sample. Alternatively, this argument can be a function to use for resampling. This function must use arguments named data and tau and

return the IDs of observations to be included in the resampled dataset.

... additional parameters passed to the function provided in resampling.

#### **Details**

With categorical outcomes (i.e. "family" argument is set to "binomial", "multinomial" or "cox"), the resampling is done such that the proportion of observations from each of the categories is representative of that of the full sample.

### Value

A vector of resampled IDs.

```
## Linear regression framework
# Data simulation
simul <- SimulateRegression()

# Subsampling
ids <- Resample(data = simul$ydata, family = "gaussian")
sum(duplicated(ids))

# Bootstrapping
ids <- Resample(data = simul$ydata, family = "gaussian", resampling = "bootstrap")
sum(duplicated(ids))

## Logistic regression framework
# Data simulation
simul <- SimulateRegression(family = "binomial")</pre>
```

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```
# Subsampling
ids <- Resample(data = simul$ydata, family = "binomial")</pre>
sum(duplicated(ids))
prop.table(table(simul$ydata))
prop.table(table(simul$ydata[ids]))
# Data simulation for a binary confounder
conf \leftarrow ifelse(runif(n = 100) > 0.5, yes = 1, no = 0)
# User-defined resampling function
BalancedResampling <- function(data, tau, Z, ...) {</pre>
  s <- NULL
  for (z in unique(Z)) {
  s \leftarrow c(s, sample(which((data == "0") & (Z == z)), size = tau * sum((data == "0") & (Z == z))))
  s \leftarrow c(s, sample(which((data == "1") & (Z == z)), size = tau * sum((data == "1") & (Z == z))))
  }
  return(s)
}
\# Resampling keeping proportions by Y and Z
ids <- Resample(data = simul$ydata, family = "binomial", resampling = BalancedResampling, Z = conf)</pre>
prop.table(table(simul$ydata, conf))
prop.table(table(simul$ydata[ids], conf[ids]))
# User-defined resampling for stability selection
stab <- VariableSelection(</pre>
  xdata = simul$xdata, ydata = simul$ydata, family = "binomial",
  resampling = BalancedResampling, Z = conf
)
```

SelectionAlgo

Variable selection algorithm

# Description

Runs the variable selection algorithm specified in the argument implementation. This function is not using stability.

### Usage

```
SelectionAlgo(
  xdata,
  ydata = NULL,
  Lambda,
  group_x = NULL,
  scale = TRUE,
  family = NULL,
  implementation = PenalisedRegression,
  ...
)
```

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#### **Arguments**

xdata matrix of predictors with observations as rows and variables as columns. ydata optional vector or matrix of outcome(s). If family is set to "binomial" or "multinomial", ydata can be a vector with character/numeric values or a fac-Lambda matrix of parameters controlling the level of sparsity in the underlying feature selection algorithm specified in implementation. If Lambda=NULL and implementation=PenalisedRegression, LambdaGridRegression is used to define a relevant grid. vector encoding the grouping structure among predictors. This argument indigroup\_x cates the number of variables in each group. Only used for models with group penalisation (e.g. implementation=GroupPLS or implementation=SparseGroupPLS). logical indicating if the predictor data should be scaled. scale family type of regression model. This argument is defined as in glmnet. Possible values include "gaussian" (linear regression), "binomial" (logistic regression), "multinomial" (multinomial regression), and "cox" (survival analysis). implementation function to use for variable selection. Possible functions are: PenalisedRegression, SparsePLS, GroupPLS and SparseGroupPLS. Alternatively, a user-defined function can be provided.

### Value

A list with:

selected matrix of binary selection status. Rows correspond to different model parame-

ters. Columns correspond to predictors.

beta\_full array of model coefficients. Rows correspond to different model parameters.

Columns correspond to predictors. Indices along the third dimension correspond

additional parameters passed to the function provided in implementation.

to outcome variable(s).

### See Also

VariableSelection, PenalisedRegression, SparsePCA, SparsePLS, GroupPLS, SparseGroupPLS Other wrapping functions: GraphicalAlgo()

```
# Data simulation (univariate outcome)
set.seed(1)
simul <- SimulateRegression(pk = 50)

# Running the LASSO
mylasso <- SelectionAlgo(
   xdata = simul$xdata, ydata = simul$ydata,
   Lambda = c(0.1, 0.2), family = "gaussian",
)</pre>
```

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```
# Data simulation (multivariate outcome)
set.seed(1)
simul <- SimulateRegression(pk = 50, q = 3)
# Running multivariate Gaussian LASSO
mylasso <- SelectionAlgo(
   xdata = simul$xdata, ydata = simul$ydata,
   Lambda = c(0.1, 0.2), family = "mgaussian"
)
str(mylasso)</pre>
```

 ${\tt SelectionPerformance} \quad \textit{Selection performance} \quad$ 

## **Description**

Computes different metrics of selection performance by comparing the set of selected features to the set of true predictors/edges. This function can only be used in simulation studies (i.e. when the true model is known).

## Usage

```
SelectionPerformance(theta, theta_star, pk = NULL, cor = NULL, thr = 0.5)
```

## **Arguments**

theta	output from VariableSelection, BiSelection, or GraphicalModel. Alternatively, it can be a binary matrix of selected variables (in variable selection) or a binary adjacency matrix (in graphical modelling)
theta_star	output from SimulateRegression, SimulateComponents, or SimulateGraphical. Alternatively, it can be a binary matrix of true predictors (in variable selection) or the true binary adjacency matrix (in graphical modelling).
pk	optional vector encoding the grouping structure. Only used for multi-block stability selection where pk indicates the number of variables in each group. If pk=NULL, single-block stability selection is performed.
cor	optional correlation matrix. Only used in graphical modelling.
thr	optional threshold in correlation. Only used in graphical modelling and when argument "cor" is not NULL.

## Value

A matrix of selection metrics including:

TP	number of True Positives (TP)
FN	number of False Negatives (TN)
FP	number of False Positives (FP)

```
number of True Negatives (TN)
sensitivity sensitivity, i.e. TP/(TP+FN)
specificity specificity, i.e. TN/(TN+FP)
accuracy accuracy, i.e. (TP+TN)/(TP+TN+FP+FN)
precision precision (p), i.e. TP/(TP+FP)
recall recall (r), i.e. TP/(TP+FN)
F1_score F1-score, i.e. 2*p*r/(p+r)
```

If argument "cor" is provided, the number of False Positives among correlated (FP\_c) and uncorrelated (FP\_i) pairs, defined as having correlations (provided in "cor") above or below the threshold "thr", are also reported.

Block-specific performances are reported if "pk" is not NULL. In this case, the first row of the matrix corresponds to the overall performances, and subsequent rows correspond to each of the blocks. The order of the blocks is defined as in BlockStructure.

#### See Also

Other functions for model performance: ClusteringPerformance(), SelectionPerformanceGraph()

## **Examples**

```
# Variable selection model
set.seed(1)
simul <- SimulateRegression(pk = 30, nu_xy = 0.5)
stab <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata)
# Selection performance
SelectionPerformance(theta = stab, theta_star = simul)
# Alternative formulation
SelectionPerformance(
    theta = SelectedVariables(stab),
    theta_star = simul$theta
)</pre>
```

SelectionPerformanceGraph

Graph representation of selection performance

## **Description**

Generates an igraph object representing the True Positive, False Positive and False Negative edges by comparing the set of selected edges to the set of true edges. This function can only be used in simulation studies (i.e. when the true model is known).

## Usage

```
SelectionPerformanceGraph(
   theta,
   theta_star,
   col = c("tomato", "forestgreen", "navy"),
   lty = c(2, 3, 1),
   node_colour = NULL,
   show_labels = TRUE,
   ...
)
```

# Arguments

theta	binary adjacency matrix or output of GraphicalModel, VariableSelection, or BiSelection.
theta_star	$true\ binary\ adjacency\ matrix\ or\ output\ of\ {\tt SimulateGraphical}\ or\ {\tt SimulateRegression}.$
col	vector of edge colours. The first entry of the vector defines the colour of False Positive edges, second entry is for True Negatives and third entry is for True Positives.
lty	vector of line types for edges. The order is defined as for argument col.
node_colour	optional vector of node colours. This vector must contain as many entries as there are rows/columns in the adjacency matrix and must be in the same order (the order is used to assign colours to nodes). Integers, named colours or RGB values can be used.
show_labels	logical indicating if the node labels should be displayed.
	additional arguments to be passed to Graph.

### Value

An igraph object.

### See Also

```
SimulateGraphical, SimulateRegression, GraphicalModel, VariableSelection, BiSelection Other functions for model performance: ClusteringPerformance(), SelectionPerformance()
```

```
# Data simulation
set.seed(1)
simul <- SimulateGraphical(pk = 30)

# Stability selection
stab <- GraphicalModel(xdata = simul$data, K = 10)

# Performance graph
perfgraph <- SelectionPerformanceGraph(</pre>
```

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```
theta = stab,
  theta_star = simul
)
plot(perfgraph)
```

SelectionProportions Selection/co-membership proportions

## **Description**

Extracts selection proportions (for stability selection) or co-membership proportions (for consensus clustering).

### Usage

```
SelectionProportions(stability, argmax_id = NULL)
ConsensusMatrix(stability, argmax_id = NULL)
```

# Arguments

```
stability output of VariableSelection, GraphicalModel, BiSelection, or Clustering.

argmax_id optional indices of hyper-parameters. If argmax_id=NULL, the calibrated hyper-parameters are used.
```

## Value

A vector or matrix of proportions.

### See Also

VariableSelection, GraphicalModel, BiSelection, Clustering

```
# Stability selection
set.seed(1)
simul <- SimulateRegression(pk = 50)
stab <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata)
SelectionProportions(stab)

# Consensus clustering
set.seed(1)
simul <- SimulateClustering(
   n = c(30, 30, 30), nu_xc = 1, ev_xc = 0.5
)
stab <- Clustering(xdata = simul$data)</pre>
```

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ConsensusMatrix(stab)

SparseGroupPLS

Sparse group Partial Least Squares

# Description

Runs a sparse group Partial Least Squares model using implementation from sgPLS-package. This function is not using stability.

# Usage

```
SparseGroupPLS(
  xdata,
  ydata,
  family = "gaussian",
  group_x,
  group_y = NULL,
  Lambda,
  alpha.x,
  alpha.y = NULL,
  keepX_previous = NULL,
  keepY = NULL,
  ncomp = 1,
  scale = TRUE,
  ...
)
```

# Arguments

xdata	matrix of predictors with observations as rows and variables as columns.
ydata	optional vector or matrix of outcome(s). If family is set to "binomial" or "multinomial", ydata can be a vector with character/numeric values or a factor.
family	type of PLS model. If family="gaussian", a sparse group PLS model as defined in sgPLS is run (for continuous outcomes). If family="binomial", a PLS-DA model as defined in sgPLSda is run (for categorical outcomes).
group_x	vector encoding the grouping structure among predictors. This argument indicates the number of variables in each group.
group_y	optional vector encoding the grouping structure among outcomes. This argument indicates the number of variables in each group.
Lambda	matrix of parameters controlling the number of selected groups at current component, as defined by ncomp.
alpha.x	vector of parameters controlling the level of sparsity within groups of predictors.

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alpha.y	optional vector of parameters controlling the level of sparsity within groups of outcomes. Only used if family="gaussian".
keepX_previous	number of selected groups in previous components. Only used if $ncomp > 1$ . The argument keepX in sgPLS is obtained by concatenating keepX_previous and Lambda.
keepY	number of selected groups of outcome variables. This argument is defined as in $sgPLS$ . Only used if family="gaussian".
ncomp	number of components.
scale	logical indicating if the data should be scaled (i.e. transformed so that all variables have a standard deviation of one). Only used if family="gaussian".
	additional arguments to be passed to sgPLS or sgPLSda.

### Value

A list with:

selected matrix of binary selection status. Rows correspond to different model parame-

ters. Columns correspond to predictors.

beta\_full array of model coefficients. Rows correspond to different model parameters.

Columns correspond to predictors (starting with "X") or outcomes (starting with

"Y") variables for different components (denoted by "PC").

### References

Liquet B, de Micheaux PL, Hejblum BP, Thiébaut R (2016). "Group and sparse group partial least square approaches applied in genomics context." *Bioinformatics*, **32**(1), 35-42. ISSN 1367-4803, doi:10.1093/bioinformatics/btv535.

#### See Also

```
VariableSelection, BiSelection
```

Other penalised dimensionality reduction functions: GroupPLS(), SparsePCA(), SparsePLS()

```
if (requireNamespace("sgPLS", quietly = TRUE)) {
    ## Sparse group PLS
    # Data simulation
    set.seed(1)
    simul <- SimulateRegression(n = 100, pk = 30, q = 3, family = "gaussian")
    x <- simul$xdata
    y <- simul$ydata

# Running sgPLS with 1 group and sparsity of 0.5
mypls <- SparseGroupPLS(
    xdata = x, ydata = y, Lambda = 1, family = "gaussian",
    group_x = c(10, 15, 5), alpha.x = 0.5
)</pre>
```

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```
# Running sgPLS with groups on outcomes
mypls <- SparseGroupPLS(
    xdata = x, ydata = y, Lambda = 1, family = "gaussian",
    group_x = c(10, 15, 5), alpha.x = 0.5,
    group_y = c(2, 1), keepY = 1, alpha.y = 0.9
)

## Sparse group PLS-DA
# Data simulation
set.seed(1)
simul <- SimulateRegression(n = 100, pk = 50, family = "binomial")

# Running sgPLS-DA with 1 group and sparsity of 0.9
mypls <- SparseGroupPLS(
    xdata = simul$xdata, ydata = simul$ydata, Lambda = 1, family = "binomial",
    group_x = c(10, 15, 25), alpha.x = 0.9
)
}</pre>
```

SparsePCA

Sparse Principal Component Analysis

## Description

Runs a sparse Principal Component Analysis model using implementation from spca (if algo="sPCA") or spca (if algo="rSVD"). This function is not using stability.

### Usage

```
SparsePCA(
  xdata,
  Lambda,
  ncomp = 1,
  scale = TRUE,
  keepX_previous = NULL,
  algorithm = "sPCA",
  ...
)
```

#### **Arguments**

xdata data matrix with observations as rows and variables as columns.

Lambda matrix of parameters controlling the number of selected variables at current

component, as defined by ncomp.

ncomp number of components.

scale logical indicating if the data should be scaled (i.e. transformed so that all vari-

ables have a standard deviation of one).

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keepX\_previous number of selected predictors in previous components. Only used if ncomp > 1.

algorithm character string indicating the name of the algorithm to use for sparse PCA. Possible values are: "sPCA" (for the algorithm proposed by Zou, Hastie and Tibshirani and implemented in spca) or "rSVD" (for the regularised SVD approach proposed by Shen and Huang and implemented in spca).

... additional arguments to be passed to spca (if algorithm="sPCA") or spca (if algorithm="rSVD").

### Value

A list with:

selected matrix of binary selection status. Rows correspond to different model parame-

ters. Columns correspond to predictors.

beta\_full array of model coefficients. Rows correspond to different model parameters.

Columns correspond to predictors (starting with "X") or outcomes (starting with

"Y") variables for different components (denoted by "PC").

#### References

Zou H, Hastie T, Tibshirani R (2006). "Sparse Principal Component Analysis." *Journal of Computational and Graphical Statistics*, **15**(2), 265-286. doi:10.1198/106186006X113430.

Shen H, Huang JZ (2008). "Sparse principal component analysis via regularized low rank matrix approximation." *Journal of Multivariate Analysis*, **99**(6), 1015-1034. ISSN 0047-259X, doi:10.1016/j.jmva.2007.06.007.

# See Also

#### VariableSelection, BiSelection

Other penalised dimensionality reduction functions: GroupPLS(), SparseGroupPLS(), SparsePLS()

```
# Data simulation
set.seed(1)
simul <- SimulateRegression(n = 100, pk = 50, family = "gaussian")
x <- simul$xdata

# Sparse PCA (by Zou, Hastie, Tibshirani)
if (requireNamespace("elasticnet", quietly = TRUE)) {
   mypca <- SparsePCA(
      xdata = x, ncomp = 2,
      Lambda = c(1, 2), keepX_previous = 10, algorithm = "sPCA"
   )
}

# Sparse PCA (by Shen and Huang)
if (requireNamespace("mixOmics", quietly = TRUE)) {
   mypca <- SparsePCA(
      xdata = x, ncomp = 2,
   }
</pre>
```

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```
Lambda = c(1, 2), keepX_previous = 10, algorithm = "rSVD"
)
}
```

SparsePLS

Sparse Partial Least Squares

# Description

Runs a sparse Partial Least Squares model using implementation from sgPLS-package. This function is not using stability.

# Usage

```
SparsePLS(
  xdata,
  ydata,
  Lambda,
  family = "gaussian",
  ncomp = 1,
  scale = TRUE,
  keepX_previous = NULL,
  keepY = NULL,
  ...
)
```

# **Arguments**

xdata	matrix of predictors with observations as rows and variables as columns.
ydata	optional vector or matrix of outcome(s). If family is set to "binomial" or "multinomial", ydata can be a vector with character/numeric values or a factor.
Lambda	matrix of parameters controlling the number of selected predictors at current component, as defined by ncomp.
family	type of PLS model. If family="gaussian", a sparse PLS model as defined in sPLS is run (for continuous outcomes). If family="binomial", a PLS-DA model as defined in sPLSda is run (for categorical outcomes).
ncomp	number of components.
scale	logical indicating if the data should be scaled (i.e. transformed so that all variables have a standard deviation of one). Only used if family="gaussian".
keepX_previous	number of selected predictors in previous components. Only used if ncomp > 1. The argument keepX in sPLS is obtained by concatenating keepX_previous and Lambda.
keepY	number of selected outcome variables. This argument is defined as in sPLS. Only used if family="gaussian".
	additional arguments to be passed to sPLS or sPLSda.

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### Value

A list with:

selected matrix of binary selection status. Rows correspond to different model parame-

ters. Columns correspond to predictors.

beta\_full array of model coefficients. Rows correspond to different model parameters.

Columns correspond to predictors (starting with "X") or outcomes (starting with

"Y") variables for different components (denoted by "PC").

#### References

KA LC, Rossouw D, Robert-Granié C, Besse P (2008). "A sparse PLS for variable selection when integrating omics data." *Stat Appl Genet Mol Biol*, **7**(1), Article 35. ISSN 1544-6115, doi:10.2202/15446115.1390.

### See Also

```
VariableSelection, BiSelection
```

Other penalised dimensionality reduction functions: GroupPLS(), SparseGroupPLS(), SparsePCA()

```
if (requireNamespace("sgPLS", quietly = TRUE)) {
    ## Sparse PLS

# Data simulation
    set.seed(1)
    simul <- SimulateRegression(n = 100, pk = 20, q = 3, family = "gaussian")
    x <- simul$xdata
    y <- simul$ydata

# Running sPLS with 2 X-variables and 1 Y-variable
    mypls <- SparsePLS(xdata = x, ydata = y, Lambda = 2, family = "gaussian", keepY = 1)

## Sparse PLS-DA

# Data simulation
    set.seed(1)
    simul <- SimulateRegression(n = 100, pk = 20, family = "binomial")

# Running sPLS-DA with 2 X-variables and 1 Y-variable
    mypls <- SparsePLS(xdata = simul$xdata, ydata = simul$ydata, Lambda = 2, family = "binomial")
}</pre>
```

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Split

Splitting observations into non-overlapping sets

# Description

Generates a list of length(tau) non-overlapping sets of observation IDs.

### Usage

```
Split(data, family = NULL, tau = c(0.5, 0.25, 0.25))
```

### **Arguments**

data vector or matrix of data. In regression, this should be the outcome data.

family type of regression model. This argument is defined as in glmnet. Possible values include "gaussian" (linear regression), "binomial" (logistic regression), "multinomial" (multinomial regression), and "cox" (survival analysis).

tau vector of the proportion of observations in each of the sets.

#### **Details**

With categorical outcomes (i.e. family argument is set to "binomial", "multinomial" or "cox"), the split is done such that the proportion of observations from each of the categories in each of the sets is representative of that of the full sample.

### Value

A list of length length(tau) with sets of non-overlapping observation IDs.

```
# Splitting into 3 sets
simul <- SimulateRegression()
ids <- Split(data = simul$ydata)
lapply(ids, length)

# Balanced splits with respect to a binary variable
simul <- SimulateRegression(family = "binomial")
ids <- Split(data = simul$ydata, family = "binomial")
lapply(ids, FUN = function(x) {
  table(simul$ydata[x, ])
})</pre>
```

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Square

Adjacency from bipartite

# **Description**

Generates a symmetric adjacency matrix encoding a bipartite graph.

## Usage

```
Square(x)
```

# Arguments

Χ

matrix encoding the edges between two types of nodes (rows and columns).

### Value

A symmetric adjacency matrix encoding a bipartite graph.

# **Examples**

```
# Simulated links between two sets
set.seed(1)
mat <- matrix(sample(c(0, 1), size = 15, replace = TRUE),
    nrow = 5, ncol = 3
)
# Adjacency matrix of a bipartite graph
Square(mat)</pre>
```

 ${\it Stability Metrics}$ 

Stability selection metrics

# Description

Computes the stability score (see StabilityScore) and upper-bounds of the PFER and FDP from selection proportions of models with a given parameter controlling the sparsity of the underlying algorithm and for different thresholds in selection proportions.

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### Usage

```
StabilityMetrics(
   selprop,
   pk = NULL,
   pi_list = seq(0.6, 0.9, by = 0.01),
   K = 100,
   n_cat = NULL,
   PFER_method = "MB",
   PFER_thr_blocks = Inf,
   FDP_thr_blocks = Inf,
   Sequential_template = NULL,
   graph = TRUE,
   group = NULL
)
```

#### **Arguments**

selprop array of selection proportions.

pk optional vector encoding the grouping structure. Only used for multi-block sta-

bility selection where pk indicates the number of variables in each group. If

pk=NULL, single-block stability selection is performed.

pi\_list vector of thresholds in selection proportions. If n\_cat=NULL or n\_cat=2, these

values must be >0 and <1. If  $n_{cat}=3$ , these values must be >0.5 and <1.

K number of resampling iterations.

n\_cat computation options for the stability score. Default is NULL to use the score

based on a z test. Other possible values are 2 or 3 to use the score based on the

negative log-likelihood.

PFER\_method method used to compute the upper-bound of the expected number of False Posi-

tives (or Per Family Error Rate, PFER). If PFER\_method="MB", the method proposed by Meinshausen and Bühlmann (2010) is used. If PFER\_method="SS", the method proposed by Shah and Samworth (2013) under the assumption of

unimodality is used.

PFER\_thr\_blocks

vector of block-specific thresholds in PFER for constrained calibration by error control. If PFER\_thr=Inf and FDP\_thr=Inf, unconstrained calibration is used.

FDP\_thr\_blocks vector of block-specific thresholds in the expected proportion of falsely selected

features (or False Discovery Proportion, FDP) for constrained calibration by error control. If PFER\_thr=Inf and FDP\_thr=Inf, unconstrained calibration is

used.

Sequential\_template

logical matrix encoding the type of procedure to use for data with multiple blocks in stability selection graphical modelling. For multi-block estimation, the stability selection model is constructed as the union of block-specific stable edges estimated while the others are weakly penalised (TRUE only for the block currently being calibrated and FALSE for other blocks). Other approaches with joint calibration of the blocks are allowed (all entries are set to TRUE).

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graph logical indicating if stability selection is performed in a regression (if FALSE) or

graphical (if TRUE) framework.

group vector encoding the grouping structure among predictors. This argument indi-

cates the number of variables in each group and only needs to be provided for

group (but not sparse group) penalisation.

#### Value

A list with:

S a matrix of the best (block-specific) stability scores for different (sets of) penalty

parameters. In multi-block stability selection, rows correspond to different sets of penalty parameters, (values are stored in the output "Lambda") and columns

correspond to different blocks.

Lambda a matrix of (block-specific) penalty parameters. In multi-block stability selec-

tion, rows correspond to sets of penalty parameters and columns correspond to

different blocks.

Q a matrix of average numbers of (block-specific) edges selected by the underlying algorithm for different (sets of) penalty parameters. In multi-block stability selection, rows correspond to different sets of penalty parameters, (values are

stored in the output "Lambda") and columns correspond to different blocks.

Q\_s a matrix of calibrated numbers of (block-specific) stable edges for different (sets

of) penalty parameters. In multi-block stability selection, rows correspond to different sets of penalty parameters, (values are stored in the output "Lambda")

and columns correspond to different blocks.

P a matrix of calibrated (block-specific) thresholds in selection proportions for

different (sets of) penalty parameters. In multi-block stability selection, rows correspond to different sets of penalty parameters, (values are stored in the out-

put "Lambda") and columns correspond to different blocks.

PFER a matrix of computed (block-specific) upper-bounds in PFER of calibrated graphs

for different (sets of) penalty parameters. In multi-block stability selection, rows correspond to different sets of penalty parameters, (values are stored in the out-

put "Lambda") and columns correspond to different blocks.

FDP a matrix of computed (block-specific) upper-bounds in FDP of calibrated sta-

bility selection models for different (sets of) penalty parameters. In multi-block stability selection, rows correspond to different sets of penalty parameters, (values are stored in the output "Lambda") and columns correspond to different

blocks.

S\_2d an array of (block-specific) stability scores obtained with different combinations

of parameters. Rows correspond to different (sets of) penalty parameters and columns correspond to different thresholds in selection proportions. In multiblock stability selection, indices along the third dimension correspond to differ-

ent blocks.

PFER\_2d an array of computed upper-bounds of PFER obtained with different combi-

nations of parameters. Rows correspond to different penalty parameters and columns correspond to different thresholds in selection proportions. Not avail-

able in multi-block stability selection graphical modelling.

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FDP\_2d

an array of computed upper-bounds of FDP obtained with different combinations of parameters. Rows correspond to different penalty parameters and columns correspond to different thresholds in selection proportions. Not available in multi-block stability selection graphical modelling.

#### References

Bodinier B, Filippi S, Nøst TH, Chiquet J, Chadeau-Hyam M (2023). "Automated calibration for stability selection in penalised regression and graphical models." *Journal of the Royal Statistical Society Series C: Applied Statistics*, qlad058. ISSN 0035-9254, doi:10.1093/jrsssc/qlad058, https://academic.oup.com/jrsssc/advance-article-pdf/doi/10.1093/jrsssc/qlad058/50878777/qlad058.pdf.

Meinshausen N, Bühlmann P (2010). "Stability selection." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **72**(4), 417-473. doi:10.1111/j.14679868.2010.00740.x.

Shah RD, Samworth RJ (2013). "Variable selection with error control: another look at stability selection." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **75**(1), 55-80. doi:10.1111/j.14679868.2011.01034.x.

#### See Also

Other stability metric functions: ConsensusScore(), FDP(), PFER(), StabilityScore()

## **Examples**

```
## Sparse or sparse group penalisation
# Simulating set of selection proportions
selprop <- matrix(round(runif(n = 20), digits = 2), nrow = 2)</pre>
# Computing stability scores for different thresholds
metrics <- StabilityMetrics(</pre>
  selprop = selprop, pi = c(0.6, 0.7, 0.8),
  K = 100, graph = FALSE
## Group penalisation
# Simulating set of selection proportions
selprop <- matrix(round(runif(n = 6), digits = 2), nrow = 2)</pre>
selprop <- cbind(</pre>
  selprop[, 1], selprop[, 1],
  selprop[, 2], selprop[, 2],
  matrix(rep(selprop[, 3], each = 6), nrow = 2, byrow = TRUE)
# Computing stability scores for different thresholds
metrics <- StabilityMetrics(</pre>
  selprop = selprop, pi = c(0.6, 0.7, 0.8),
  K = 100, graph = FALSE, group = c(2, 2, 6)
```

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)

StabilityScore

Stability score

# **Description**

Computes the stability score from selection proportions of models with a given parameter controlling the sparsity and for different thresholds in selection proportions. The score measures how unlikely it is that the selection procedure is uniform (i.e. uninformative) for a given combination of parameters.

## Usage

```
StabilityScore(
  selprop,
  pi_list = seq(0.6, 0.9, by = 0.01),
  K,
  n_cat = 3,
  group = NULL
)
```

# Arguments

selprop	array of selection proportions.
pi_list	vector of thresholds in selection proportions. If n_cat=NULL or n_cat=2, these values must be >0 and <1. If n_cat=3, these values must be >0.5 and <1.
K	number of resampling iterations.
n_cat	computation options for the stability score. Default is NULL to use the score based on a z test. Other possible values are 2 or 3 to use the score based on the negative log-likelihood.
group	vector encoding the grouping structure among predictors. This argument indicates the number of variables in each group and only needs to be provided for group (but not sparse group) penalisation.

# **Details**

The stability score is derived from the likelihood under the assumption of uniform (uninformative) selection.

We classify the features into three categories: the stably selected ones (that have selection proportions  $\geq \pi$ ), the stably excluded ones (selection proportion  $\leq 1-\pi$ ), and the unstable ones (selection proportions between  $1-\pi$  and  $\pi$ ).

Under the hypothesis of equiprobability of selection (instability), the likelihood of observing stably selected, stably excluded and unstable features can be expressed as:

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$$L_{\lambda,\pi} = \prod_{j=1}^{N} [(1 - F(K\pi - 1))^{1_{H_{\lambda}(j) \ge K\pi}} \times (F(K\pi - 1) - F(K(1 - \pi))^{1_{(1-\pi)K} < H_{\lambda}(j) < K\pi} \times F(K(1 - \pi))^{1_{H_{\lambda}(j) \le K(1-\pi)}}]$$

where  $H_{\lambda}(j)$  is the selection count of feature j and F(x) is the cumulative probability function of the binomial distribution with parameters K and the average proportion of selected features over resampling iterations.

The stability score is computed as the minus log-transformed likelihood under the assumption of equiprobability of selection:

$$S_{\lambda,\pi} = -log(L_{\lambda,\pi})$$

The stability score increases with stability.

Alternatively, the stability score can be computed by considering only two sets of features: stably selected (selection proportions  $\geq \pi$ ) or not (selection proportions  $< \pi$ ). This can be done using n\_cat=2.

#### Value

A vector of stability scores obtained with the different thresholds in selection proportions.

### References

Bodinier B, Filippi S, Nøst TH, Chiquet J, Chadeau-Hyam M (2023). "Automated calibration for stability selection in penalised regression and graphical models." *Journal of the Royal Statistical Society Series C: Applied Statistics*, qlad058. ISSN 0035-9254, doi:10.1093/jrsssc/qlad058, https://academic.oup.com/jrsssc/advance-article-pdf/doi/10.1093/jrsssc/qlad058/50878777/qlad058.pdf.

#### See Also

Other stability metric functions: ConsensusScore(), FDP(), PFER(), StabilityMetrics()

### **Examples**

```
# Simulating set of selection proportions
set.seed(1)
selprop <- round(runif(n = 20), digits = 2)
# Computing stability scores for different thresholds
score <- StabilityScore(selprop, pi_list = c(0.6, 0.7, 0.8), K = 100)</pre>
```

Stable

Stable results

## Description

Extracts stable results for stability selection or consensus clustering.

Stable Stable

# Usage

```
Stable(stability, argmax_id = NULL, linkage = "complete")
SelectedVariables(stability, argmax_id = NULL)
Adjacency(stability, argmax_id = NULL)
Clusters(stability, linkage = "complete", argmax_id = NULL)
```

## **Arguments**

output of VariableSelection, BiSelection, GraphicalModel or Clustering.

argmax\_id optional indices of hyper-parameters. If argmax\_id=NULL, the calibrated hyper-parameters are used.

linkage character string indicating the type of linkage used in hierarchical clustering to define the stable clusters. Possible values include "complete", "single" and "average" (see argument "method" in hclust for a full list).

#### Value

A binary vector or matrix encoding the selection status (1 if selected, 0 otherwise) in stability selection or stable cluster membership in consensus clustering.

#### See Also

VariableSelection, BiSelection, GraphicalModel, Clustering

## **Examples**

```
# Variable selection
set.seed(1)
simul <- SimulateRegression(pk = 20)</pre>
stab <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata)</pre>
SelectedVariables(stab)
Stable(stab)
# Graphical model
set.seed(1)
simul <- SimulateGraphical(pk = 10)</pre>
stab <- GraphicalModel(xdata = simul$data)</pre>
Adjacency(stab)
Stable(stab)
# Clustering
set.seed(1)
simul <- SimulateClustering(</pre>
  n = c(30, 30, 30),
  nu_xc = 1
stab <- Clustering(xdata = simul$data)</pre>
```

```
Clusters(stab)
Stable(stab)
```

StructuralModel

Stability selection in Structural Equation Modelling

## **Description**

Performs stability selection for Structural Equation Models. The underlying arrow selection algorithm (e.g. regularised Structural Equation Modelling) is run with different combinations of parameters controlling the sparsity (e.g. penalty parameter) and thresholds in selection proportions. These two hyper-parameters are jointly calibrated by maximisation of the stability score.

# Usage

```
StructuralModel(
  xdata,
  adjacency,
  residual_covariance = NULL,
  Lambda = NULL,
  pi_list = seq(0.01, 0.99, by = 0.01),
 K = 100,
  tau = 0.5,
  seed = 1,
  n_cat = NULL,
  implementation = PenalisedLinearSystem,
  resampling = "subsampling",
  cpss = FALSE,
  PFER_method = "MB",
  PFER_thr = Inf,
  FDP_thr = Inf,
  Lambda_cardinal = 100,
  optimisation = c("grid_search", "nloptr"),
  n_{cores} = 1,
  output_data = FALSE,
  verbose = TRUE,
)
```

#### **Arguments**

xdata

matrix with observations as rows and variables as columns. Column names must be defined and in line with the row and column names of adjacency.

adjacency

binary adjacency matrix of the Directed Acyclic Graph (transpose of the asymmetric matrix A in Reticular Action Model notation). The row and column names of this matrix must be defined.

residual\_covariance

binary and symmetric matrix encoding the nonzero entries in the residual covariance matrix (symmetric matrix S in Reticular Action Model notation). By

default, this is the identity matrix (no residual covariance).

Lambda matrix of parameters controlling the level of sparsity in the underlying feature

selection algorithm specified in implementation.

pi\_list vector of thresholds in selection proportions. If n\_cat=NULL or n\_cat=2, these

values must be >0 and <1. If  $n_{cat}=3$ , these values must be >0.5 and <1.

Κ number of resampling iterations.

tau subsample size. Only used if resampling="subsampling" and cpss=FALSE.

seed value of the seed to initialise the random number generator and ensure repro-

ducibility of the results (see set.seed).

n\_cat computation options for the stability score. Default is NULL to use the score

based on a z test. Other possible values are 2 or 3 to use the score based on the

negative log-likelihood.

implementation function to use for variable selection.

resampling resampling approach. Possible values are: "subsampling" for sampling with-

out replacement of a proportion tau of the observations, or "bootstrap" for sampling with replacement generating a resampled dataset with as many observations as in the full sample. Alternatively, this argument can be a function to use for resampling. This function must use arguments named data and tau and

return the IDs of observations to be included in the resampled dataset.

logical indicating if complementary pair stability selection should be done. For cpss

> this, the algorithm is applied on two non-overlapping subsets of half of the observations. A feature is considered as selected if it is selected for both subsamples. With this method, the data is split K/2 times (K models are fitted). Only used if

PFER\_method="MB".

PFER\_method method used to compute the upper-bound of the expected number of False Posi-

> tives (or Per Family Error Rate, PFER). If PFER\_method="MB", the method proposed by Meinshausen and Bühlmann (2010) is used. If PFER\_method="SS", the method proposed by Shah and Samworth (2013) under the assumption of

unimodality is used.

threshold in PFER for constrained calibration by error control. If PFER\_thr=Inf PFER\_thr

and FDP\_thr=Inf, unconstrained calibration is used (the default).

FDP\_thr threshold in the expected proportion of falsely selected features (or False Dis-

covery Proportion) for constrained calibration by error control. If PFER\_thr=Inf

and FDP\_thr=Inf, unconstrained calibration is used (the default).

Lambda\_cardinal

number of values in the grid of parameters controlling the level of sparsity in the

underlying algorithm. Only used if Lambda=NULL.

optimisation character string indicating the type of optimisation method. With optimisation="grid\_search"

> (the default), all values in Lambda are visited. Alternatively, optimisation algorithms implemented in nloptr can be used with optimisation="nloptr". By default, we use "algorithm"="NLOPT\_GN\_DIRECT\_L", "xtol\_abs"=0.1, "ftol\_abs"=0.1 and "maxeval"=Lambda\_cardinal. These values can be changed

by providing the argument opts (see nloptr). For stability selection using penalised regression, optimisation="grid\_search" may be faster as it allows

for warm start.

n\_cores number of cores to use for parallel computing (see argument workers in multisession).

Using n\_cores>1 is only supported with optimisation="grid\_search".

output\_data logical indicating if the input datasets xdata and ydata should be included in

the output.

verbose logical indicating if a loading bar and messages should be printed.

... additional parameters passed to the functions provided in implementation or

resampling.

#### **Details**

In stability selection, a feature selection algorithm is fitted on K subsamples (or bootstrap samples) of the data with different parameters controlling the sparsity (Lambda). For a given (set of) sparsity parameter(s), the proportion out of the K models in which each feature is selected is calculated. Features with selection proportions above a threshold pi are considered stably selected. The stability selection model is controlled by the sparsity parameter(s) for the underlying algorithm, and the threshold in selection proportion:

$$V_{\lambda,\pi} = \{j : p_{\lambda}(j) \ge \pi\}$$

In Structural Equation Modelling, "feature" refers to an arrow in the corresponding Directed Acyclic Graph.

These parameters can be calibrated by maximisation of a stability score (see ConsensusScore if n\_cat=NULL or StabilityScore otherwise) calculated under the null hypothesis of equiprobability of selection.

It is strongly recommended to examine the calibration plot carefully to check that the grids of parameters Lambda and pi\_list do not restrict the calibration to a region that would not include the global maximum (see CalibrationPlot). In particular, the grid Lambda may need to be extended when the maximum stability is observed on the left or right edges of the calibration heatmap. In some instances, multiple peaks of stability score can be observed. Simulation studies suggest that the peak corresponding to the largest number of selected features tend to give better selection performances. This is not necessarily the highest peak (which is automatically retained by the functions in this package). The user can decide to manually choose another peak.

To control the expected number of False Positives (Per Family Error Rate) in the results, a threshold PFER\_thr can be specified. The optimisation problem is then constrained to sets of parameters that generate models with an upper-bound in PFER below PFER\_thr (see Meinshausen and Bühlmann (2010) and Shah and Samworth (2013)).

Possible resampling procedures include defining (i) K subsamples of a proportion tau of the observations, (ii) K bootstrap samples with the full sample size (obtained with replacement), and (iii) K/2 splits of the data in half for complementary pair stability selection (see arguments resampling and cpss). In complementary pair stability selection, a feature is considered selected at a given resampling iteration if it is selected in the two complementary subsamples.

To ensure reproducibility of the results, the starting number of the random number generator is set to seed.

For parallelisation, stability selection with different sets of parameters can be run on  $n_{cores}$  cores. Using  $n_{cores} > 1$  creates a multisession. Alternatively, the function can be run manually with different seeds and all other parameters equal. The results can then be combined using Combine.

# Value

An object of class variable\_selection. A list with:

S	a matrix of the best stability scores for different parameters controlling the level of sparsity in the underlying algorithm.
Lambda	a matrix of parameters controlling the level of sparsity in the underlying algorithm.
Q	a matrix of the average number of selected features by the underlying algorithm with different parameters controlling the level of sparsity.
Q_s	a matrix of the calibrated number of stably selected features with different parameters controlling the level of sparsity.
P	a matrix of calibrated thresholds in selection proportions for different parameters controlling the level of sparsity in the underlying algorithm.
PFER	a matrix of upper-bounds in PFER of calibrated stability selection models with different parameters controlling the level of sparsity.
FDP	a matrix of upper-bounds in FDP of calibrated stability selection models with different parameters controlling the level of sparsity.
S_2d	a matrix of stability scores obtained with different combinations of parameters. Columns correspond to different thresholds in selection proportions.
PFER_2d	a matrix of upper-bounds in FDP obtained with different combinations of parameters. Columns correspond to different thresholds in selection proportions.
FDP_2d	a matrix of upper-bounds in PFER obtained with different combinations of parameters. Columns correspond to different thresholds in selection proportions.
selprop	a matrix of selection proportions. Columns correspond to predictors from xdata.
Beta	an array of model coefficients. Columns correspond to predictors from xdata. Indices along the third dimension correspond to different resampling iterations. With multivariate outcomes, indices along the fourth dimension correspond to outcome-specific coefficients.
method	a list with type="variable_selection" and values used for arguments implementation, family, resampling, cpss and PFER_method.
params	a list with values used for arguments K, pi_list, tau, n_cat, pk, n (number of observations), PFER_thr, FDP_thr and seed. The datasets xdata and ydata are also included if output_data=TRUE.

For all matrices and arrays returned, the rows are ordered in the same way and correspond to parameter values stored in Lambda.

#### References

Bodinier B, Rodrigues S, Karimi M, Filippi S, Chiquet J, Chadeau-Hyam M (2025). "Stability Selection and Consensus Clustering in R: The R Package sharp." *Journal of Statistical Software*, **112**(5), btad635. doi:10.18637/jss.v112.i05.

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#### See Also

SelectionAlgo, Resample, StabilityScore

Other stability functions: BiSelection(), Clustering(), GraphicalModel(), VariableSelection()

## **Examples**

```
oldpar <- par(no.readonly = TRUE)
par(mar = rep(7, 4))
# Data simulation
set.seed(1)
pk < -c(3, 2, 3)
simul <- SimulateStructural(</pre>
  n = 500,
  pk = pk,
 nu_between = 0.5,
  v_between = 1,
  v_sign = 1
# Stability selection (using glmnet)
dag <- LayeredDAG(layers = pk)</pre>
stab <- StructuralModel(</pre>
  xdata = simul$data,
  adjacency = dag
CalibrationPlot(stab)
LinearSystemMatrix(vect = Stable(stab), adjacency = dag)
# Stability selection (using OpenMx)
if (requireNamespace("OpenMx", quietly = TRUE)) {
```

```
stab <- StructuralModel(</pre>
    xdata = simul$data,
    implementation = PenalisedOpenMx,
   Lambda = seq(50, 500, by = 50),
   adjacency = dag
 CalibrationPlot(stab)
 OpenMxMatrix(SelectedVariables(stab), adjacency = dag)
}
## Not run:
# Data simulation with latent variables
set.seed(1)
pk < -c(3, 2, 3)
simul <- SimulateStructural(</pre>
 n = 500,
 pk = pk,
 nu\_between = 0.5,
 v_sign = 1,
 v_between = 1,
 n_{manifest} = 3,
 ev_manifest = 0.95
)
# Stability selection (using OpenMx)
if (requireNamespace("OpenMx", quietly = TRUE)) {
 dag <- LayeredDAG(layers = pk, n_manifest = 3)</pre>
 penalised <- dag
 penalised[, seq_len(ncol(simul$data))] <- 0</pre>
 stab <- StructuralModel(</pre>
   xdata = simul$data,
    implementation = PenalisedOpenMx,
    adjacency = dag,
   penalised = penalised,
   Lambda = seq(10, 100, by = 20),
   K = 10 \# to increase for real use
 CalibrationPlot(stab)
 ids_latent <- grep("f", colnames(dag))</pre>
 OpenMxMatrix(SelectedVariables(stab),
    adjacency = dag
 )[ids_latent, ids_latent]
## End(Not run)
par(oldpar)
```

VariableSelection

Stability selection in regression

## **Description**

Performs stability selection for regression models. The underlying variable selection algorithm (e.g. LASSO regression) is run with different combinations of parameters controlling the sparsity (e.g. penalty parameter) and thresholds in selection proportions. These two hyper-parameters are jointly calibrated by maximisation of the stability score.

# Usage

```
VariableSelection(
  xdata,
  ydata = NULL,
 Lambda = NULL,
 pi_list = seq(0.01, 0.99, by = 0.01),
 K = 100,
  tau = 0.5,
  seed = 1,
  n_cat = NULL,
  family = "gaussian",
  implementation = PenalisedRegression,
  resampling = "subsampling",
  cpss = FALSE,
  PFER_method = "MB",
  PFER_thr = Inf,
  FDP_thr = Inf,
  Lambda_cardinal = 100,
  group_x = NULL,
  group_penalisation = FALSE,
  optimisation = c("grid_search", "nloptr"),
  n_{cores} = 1,
  output_data = FALSE,
  verbose = TRUE,
  beep = NULL,
)
```

## **Arguments**

xdata	matrix of predictors with observations as rows and variables as columns.
ydata	optional vector or matrix of outcome(s). If family is set to "binomial" or "multinomial", ydata can be a vector with character/numeric values or a factor.
Lambda	matrix of parameters controlling the level of sparsity in the underlying feature selection algorithm specified in implementation. If Lambda=NULL and implementation=PenalisedRegression, LambdaGridRegression is used to define a relevant grid.
pi_list	vector of thresholds in selection proportions. If $n_{cat}=NULL$ or $n_{cat}=2$ , these values must be >0 and <1. If $n_{cat}=3$ , these values must be >0.5 and <1.

K number of resampling iterations.

tau subsample size. Only used if resampling "subsampling" and cpss=FALSE.

seed value of the seed to initialise the random number generator and ensure repro-

ducibility of the results (see set.seed).

n\_cat computation options for the stability score. Default is NULL to use the score

based on a z test. Other possible values are 2 or 3 to use the score based on the

negative log-likelihood.

family type of regression model. This argument is defined as in glmnet. Possible val-

ues include "gaussian" (linear regression), "binomial" (logistic regression),

"multinomial" (multinomial regression), and "cox" (survival analysis).

implementation function to use for variable selection. Possible functions are: PenalisedRegression,

SparsePLS, GroupPLS and SparseGroupPLS. Alternatively, a user-defined func-

tion can be provided.

resampling resampling approach. Possible values are: "subsampling" for sampling with-

out replacement of a proportion tau of the observations, or "bootstrap" for sampling with replacement generating a resampled dataset with as many observations as in the full sample. Alternatively, this argument can be a function to use for resampling. This function must use arguments named data and tau and

return the IDs of observations to be included in the resampled dataset.

cpss logical indicating if complementary pair stability selection should be done. For

this, the algorithm is applied on two non-overlapping subsets of half of the observations. A feature is considered as selected if it is selected for both subsamples. With this method, the data is split K/2 times (K models are fitted). Only used if

PFER\_method="MB".

PFER\_method method used to compute the upper-bound of the expected number of False Posi-

tives (or Per Family Error Rate, PFER). If PFER\_method="MB", the method proposed by Meinshausen and Bühlmann (2010) is used. If PFER\_method="SS", the method proposed by Shah and Samworth (2013) under the assumption of

unimodality is used.

PFER\_thr threshold in PFER for constrained calibration by error control. If PFER\_thr=Inf

and FDP\_thr=Inf, unconstrained calibration is used (the default).

FDP\_thr threshold in the expected proportion of falsely selected features (or False Dis-

covery Proportion) for constrained calibration by error control. If PFER\_thr=Inf

and FDP\_thr=Inf, unconstrained calibration is used (the default).

Lambda\_cardinal

number of values in the grid of parameters controlling the level of sparsity in the

underlying algorithm. Only used if Lambda=NULL.

group\_x vector encoding the grouping structure among predictors. This argument indi-

cates the number of variables in each group. Only used for models with group

 $penalisation \ (e.g.\ implementation = Group PLS\ or\ implementation = Sparse Group PLS).$ 

group\_penalisation

logical indicating if a group penalisation should be considered in the stability score. The use of group\_penalisation=TRUE strictly applies to group (not

sparse-group) penalisation.

optimisation character string indicating the type of optimisation method. With optimisation="grid\_search"

(the default), all values in Lambda are visited. Alternatively, optimisation algorithms implemented in nloptr can be used with optimisation="nloptr". By default, we use "algorithm"="NLOPT\_GN\_DIRECT\_L", "xtol\_abs"=0.1, "ftol\_abs"=0.1 and "maxeval"=Lambda\_cardinal. These values can be changed by providing the argument opts (see nloptr). For stability selection using penalised regression, optimisation="grid\_search" may be faster as it allows

for warm start.

n\_cores number of cores to use for parallel computing (see argument workers in multisession).

Using n\_cores>1 is only supported with optimisation="grid\_search".

output\_data logical indicating if the input datasets xdata and ydata should be included in

the output.

verbose logical indicating if a loading bar and messages should be printed.

beep sound indicating the end of the run. Possible values are: NULL (no sound) or an

integer between 1 and 11 (see argument sound in beep).

... additional parameters passed to the functions provided in implementation or

resampling.

## **Details**

In stability selection, a feature selection algorithm is fitted on K subsamples (or bootstrap samples) of the data with different parameters controlling the sparsity (Lambda). For a given (set of) sparsity parameter(s), the proportion out of the K models in which each feature is selected is calculated. Features with selection proportions above a threshold pi are considered stably selected. The stability selection model is controlled by the sparsity parameter(s) for the underlying algorithm, and the threshold in selection proportion:

$$V_{\lambda,\pi} = \{j : p_{\lambda}(j) \ge \pi\}$$

If argument group\_penalisation=FALSE, "feature" refers to variable (variable selection model). If argument group\_penalisation=TRUE, "feature" refers to group (group selection model). In this case, groups need to be defined *a priori* and specified in argument group\_x.

These parameters can be calibrated by maximisation of a stability score (see ConsensusScore if n\_cat=NULL or StabilityScore otherwise) calculated under the null hypothesis of equiprobability of selection.

It is strongly recommended to examine the calibration plot carefully to check that the grids of parameters Lambda and pi\_list do not restrict the calibration to a region that would not include the global maximum (see CalibrationPlot). In particular, the grid Lambda may need to be extended when the maximum stability is observed on the left or right edges of the calibration heatmap. In some instances, multiple peaks of stability score can be observed. Simulation studies suggest that the peak corresponding to the largest number of selected features tend to give better selection performances. This is not necessarily the highest peak (which is automatically retained by the functions in this package). The user can decide to manually choose another peak.

To control the expected number of False Positives (Per Family Error Rate) in the results, a threshold PFER\_thr can be specified. The optimisation problem is then constrained to sets of parameters that generate models with an upper-bound in PFER below PFER\_thr (see Meinshausen and Bühlmann (2010) and Shah and Samworth (2013)).

Possible resampling procedures include defining (i) K subsamples of a proportion tau of the observations, (ii) K bootstrap samples with the full sample size (obtained with replacement), and (iii) K/2 splits of the data in half for complementary pair stability selection (see arguments resampling and cpss). In complementary pair stability selection, a feature is considered selected at a given resampling iteration if it is selected in the two complementary subsamples.

For categorical or time to event outcomes (argument family is "binomial", "multinomial" or "cox"), the proportions of observations from each category in all subsamples or bootstrap samples are the same as in the full sample.

To ensure reproducibility of the results, the starting number of the random number generator is set to seed.

For parallelisation, stability selection with different sets of parameters can be run on n\_cores cores. Using n\_cores > 1 creates a multisession. Alternatively, the function can be run manually with different seeds and all other parameters equal. The results can then be combined using Combine.

# Value

An object of class variable\_selection. A list with:

S	a matrix of the best stability scores for different parameters controlling the level of sparsity in the underlying algorithm.
Lambda	a matrix of parameters controlling the level of sparsity in the underlying algorithm.
Q	a matrix of the average number of selected features by the underlying algorithm with different parameters controlling the level of sparsity.
Q_s	a matrix of the calibrated number of stably selected features with different parameters controlling the level of sparsity.
P	a matrix of calibrated thresholds in selection proportions for different parameters controlling the level of sparsity in the underlying algorithm.
PFER	a matrix of upper-bounds in PFER of calibrated stability selection models with different parameters controlling the level of sparsity.
FDP	a matrix of upper-bounds in FDP of calibrated stability selection models with different parameters controlling the level of sparsity.
S_2d	a matrix of stability scores obtained with different combinations of parameters. Columns correspond to different thresholds in selection proportions.
PFER_2d	a matrix of upper-bounds in FDP obtained with different combinations of parameters. Columns correspond to different thresholds in selection proportions.
FDP_2d	a matrix of upper-bounds in PFER obtained with different combinations of parameters. Columns correspond to different thresholds in selection proportions.
selprop	a matrix of selection proportions. Columns correspond to predictors from xdata.
Beta	an array of model coefficients. Columns correspond to predictors from xdata. Indices along the third dimension correspond to different resampling iterations. With multivariate outcomes, indices along the fourth dimension correspond to outcome-specific coefficients.
method	a list with type="variable_selection" and values used for arguments implementation, family, resampling, cpss and PFER_method.

params

a list with values used for arguments K, pi\_list, tau, n\_cat, pk, n (number of observations), PFER\_thr, FDP\_thr and seed. The datasets xdata and ydata are also included if output\_data=TRUE.

For all matrices and arrays returned, the rows are ordered in the same way and correspond to parameter values stored in Lambda.

#### References

Bodinier B, Rodrigues S, Karimi M, Filippi S, Chiquet J, Chadeau-Hyam M (2025). "Stability Selection and Consensus Clustering in R: The R Package sharp." *Journal of Statistical Software*, **112**(5), btad635. doi:10.18637/jss.v112.i05.

Bodinier B, Filippi S, Nøst TH, Chiquet J, Chadeau-Hyam M (2023). "Automated calibration for stability selection in penalised regression and graphical models." *Journal of the Royal Statistical Society Series C: Applied Statistics*, qlad058. ISSN 0035-9254, doi:10.1093/jrsssc/qlad058, https://academic.oup.com/jrsssc/advance-article-pdf/doi/10.1093/jrsssc/qlad058/50878777/qlad058.pdf.

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Tibshirani R (1996). "Regression Shrinkage and Selection via the Lasso." *Journal of the Royal Statistical Society. Series B (Methodological)*, **58**(1), 267–288. ISSN 00359246, http://www.jstor.org/stable/2346178.

# See Also

PenalisedRegression, SelectionAlgo, LambdaGridRegression, Resample, StabilityScore Refit, ExplanatoryPerformance, Incremental,

Other stability functions: BiSelection(), Clustering(), GraphicalModel(), StructuralModel()

## **Examples**

```
oldpar <- par(no.readonly = TRUE)
par(mar = rep(7, 4))

# Linear regression
set.seed(1)
simul <- SimulateRegression(n = 100, pk = 50, family = "gaussian")
stab <- VariableSelection(
   xdata = simul$xdata, ydata = simul$ydata,
   family = "gaussian"
)

# Calibration plot
CalibrationPlot(stab)

# Extracting the results
summary(stab)</pre>
```

```
Stable(stab)
SelectionProportions(stab)
plot(stab)
# Using randomised LASSO
stab <- VariableSelection(</pre>
  xdata = simul$xdata, ydata = simul$ydata,
  family = "gaussian", penalisation = "randomised"
)
plot(stab)
# Using adaptive LASSO
stab <- VariableSelection(</pre>
  xdata = simul$xdata, ydata = simul$ydata,
  family = "gaussian", penalisation = "adaptive"
plot(stab)
# Using additional arguments from glmnet (e.g. penalty.factor)
stab <- VariableSelection(</pre>
  xdata = simul$xdata, ydata = simul$ydata, family = "gaussian",
  penalty.factor = c(rep(1, 45), rep(0, 5))
head(coef(stab))
# Using CART
if (requireNamespace("rpart", quietly = TRUE)) {
  stab <- VariableSelection(</pre>
    xdata = simul$xdata, ydata = simul$ydata,
    implementation = CART,
    family = "gaussian",
  plot(stab)
}
# Regression with multivariate outcomes
simul <- SimulateRegression(n = 100, pk = 20, q = 3, family = "gaussian")</pre>
stab <- VariableSelection(</pre>
  xdata = simul$xdata, ydata = simul$ydata,
  family = "mgaussian"
summary(stab)
# Logistic regression
set.seed(1)
simul <- SimulateRegression(n = 200, pk = 10, family = "binomial", ev_xy = 0.8)</pre>
stab <- VariableSelection(</pre>
  xdata = simul$xdata, ydata = simul$ydata,
  family = "binomial"
)
summary(stab)
```

```
# Sparse PCA (1 component, see BiSelection for more components)
if (requireNamespace("elasticnet", quietly = TRUE)) {
 set.seed(1)
 simul <- SimulateComponents(pk = c(5, 3, 4))
 stab <- VariableSelection(</pre>
    xdata = simul$data,
   Lambda = seq_len(ncol(simul$data) - 1),
    implementation = SparsePCA
 CalibrationPlot(stab, xlab = "")
 summary(stab)
}
# Sparse PLS (1 outcome, 1 component, see BiSelection for more options)
if (requireNamespace("sgPLS", quietly = TRUE)) {
 set.seed(1)
 simul <- SimulateRegression(n = 100, pk = 50, family = "gaussian")</pre>
 stab <- VariableSelection(</pre>
    xdata = simul$xdata, ydata = simul$ydata,
   Lambda = seq_len(ncol(simul$xdata) - 1),
    implementation = SparsePLS, family = "gaussian"
 CalibrationPlot(stab, xlab = "")
 SelectedVariables(stab)
}
# Group PLS (1 outcome, 1 component, see BiSelection for more options)
if (requireNamespace("sgPLS", quietly = TRUE)) {
 stab <- VariableSelection(</pre>
   xdata = simul$xdata, ydata = simul$ydata,
   Lambda = seq_len(5),
    group_x = c(5, 5, 10, 20, 10),
   group_penalisation = TRUE,
    implementation = GroupPLS, family = "gaussian"
 CalibrationPlot(stab, xlab = "")
 SelectedVariables(stab)
}
# Example with more hyper-parameters: elastic net
simul <- SimulateRegression(n = 100, pk = 50, family = "gaussian")</pre>
TuneElasticNet <- function(xdata, ydata, family, alpha) {</pre>
 stab <- VariableSelection(</pre>
    xdata = xdata, ydata = ydata,
    family = family, alpha = alpha, verbose = FALSE
 )
 return(max(stab$S, na.rm = TRUE))
}
myopt <- optimise(TuneElasticNet,</pre>
 lower = 0.1, upper = 1, maximum = TRUE,
 xdata = simul$xdata, ydata = simul$ydata,
 family = "gaussian"
```

```
stab <- VariableSelection(</pre>
  xdata = simul$xdata, ydata = simul$ydata,
  family = "gaussian", alpha = myopt$maximum
)
summary(stab)
enet <- SelectedVariables(stab)</pre>
# Comparison with LASSO
stab <- VariableSelection(xdata = simul$xdata, ydata = simul$ydata, family = "gaussian")</pre>
summary(stab)
lasso <- SelectedVariables(stab)</pre>
table(lasso, enet)
# Example using an external function: group-LASSO with gglasso
if (requireNamespace("gglasso", quietly = TRUE)) {
  set.seed(1)
  simul <- SimulateRegression(n = 200, pk = 20, family = "binomial")</pre>
  ManualGridGroupLasso <- function(xdata, ydata, family, group_x, ...) {</pre>
    # Defining the grouping
    group <- do.call(c, lapply(seq_len(length(group_x)), FUN = function(i) {</pre>
      rep(i, group_x[i])
    }))
    if (family == "binomial") {
      ytmp <- ydata
      ytmp[ytmp == min(ytmp)] <- -1
      ytmp[ytmp == max(ytmp)] <- 1
      return(gglasso::gglasso(xdata, ytmp, loss = "logit", group = group, ...))
    return(gglasso::gglasso(xdata, ydata, lambda = lambda, loss = "ls", group = group, ...))
    }
  }
  Lambda <- LambdaGridRegression(</pre>
    xdata = simul$xdata, ydata = simul$ydata,
    family = "binomial", Lambda_cardinal = 20,
    implementation = ManualGridGroupLasso,
    group_x = rep(5, 4)
  GroupLasso <- function(xdata, ydata, Lambda, family, group_x, ...) {</pre>
    # Defining the grouping
    group <- do.call(c, lapply(seq_len(length(group_x)), FUN = function(i) {</pre>
      rep(i, group_x[i])
    }))
    # Running the regression
    if (family == "binomial") {
      ytmp <- ydata
      ytmp[ytmp == min(ytmp)] <- -1
      ytmp[ytmp == max(ytmp)] <- 1</pre>
    mymodel <- gglasso::gglasso(xdata, ytmp, lambda = Lambda, loss = "logit", group = group, ...)</pre>
    if (family == "gaussian") {
```

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```
mymodel <- gglasso::gglasso(xdata, ydata, lambda = Lambda, loss = "ls", group = group, ...)
}
# Extracting and formatting the beta coefficients
beta_full <- t(as.matrix(mymodel$beta))
beta_full <- beta_full[, colnames(xdata)]

selected <- ifelse(beta_full != 0, yes = 1, no = 0)

return(list(selected = selected, beta_full = beta_full))
}
stab <- VariableSelection(
    xdata = simul$xdata, ydata = simul$ydata,
    implementation = GroupLasso, family = "binomial", Lambda = Lambda,
    group_x = rep(5, 4),
    group_penalisation = TRUE
)
summary(stab)
}
par(oldpar)</pre>
```

WeightBoxplot

Stable attribute weights

# **Description**

Creates a boxplots of the distribution of (calibrated) median attribute weights obtained from the COSA algorithm across the subsampling iterations. See examples in Clustering.

## Usage

```
WeightBoxplot(
   stability,
   at = NULL,
   argmax_id = NULL,
   col = NULL,
   boxwex = 0.3,
   xlab = "",
   ylab = "Weight",
   cex.lab = 1.5,
   las = 3,
   frame = "F",
   add = FALSE,
   ...
)
```

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## **Arguments**

stability output of Clustering.

at coordinates along the x-axis (more details in boxplot).

argmax\_id optional indices of hyper-parameters. If argmax\_id=NULL, the calibrated hyper-

parameters are used.

col optional vector of colours.

boxwex box width (more details in boxplot).

xlab label of the x-axis.
ylab label of the y-axis.
cex.lab font size for labels.

las orientation of labels on the x-axis (see par).

frame logical indicating if the box around the plot should be drawn (more details in

boxplot).

add logical indicating if the boxplot should be added to the current plot.

. . . additional parameters passed to boxplot).

# Value

A boxplot.

# See Also

Clustering

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