# Package 'SDModels'

June 5, 2025

```
Title Spectrally Deconfounded Models
Version 1.0.13
Description Screen for and analyze non-linear sparse direct effects in the presence of unobserved con-
     founding using the spectral deconfounding techniques (Čevid, Bühlmann, and Mein-
     shausen (2020)<jmlr.org/papers/v21/19-545.html>, Guo, Će-
     vid, and Bühlmann (2022) <doi:10.1214/21-AOS2152>). These meth-
     ods have been shown to be a good estimate for the true direct effect if we observe many covari-
     ates, e.g., high-dimensional settings, and we have fairly dense confounding. Even if the assump-
     tions are violated, it seems like there is not much to lose, and the deconfounded mod-
     els will, in general, estimate a function closer to the true one than classical least squares opti-
     mization. 'SDModels' provides functions SDAM() for Spectrally Deconfounded Additive Mod-
     els (Scheidegger, Guo, and Bühlmann (2025) <doi:10.1145/3711116>) and SDForest() for Spec-
     trally Deconfounded Random Forests (Ulmer, Scheideg-
     ger, and Bühlmann (2025) <doi:10.48550/arXiv.2502.03969>).
License GPL-3
Imports data.tree, DiagrammeR, doParallel, future.apply, future,
     ggplot2, GPUmatrix, gridExtra, locatexec, parallel, pbapply,
     Rdpack, tidyr, fda, grplasso, rlang
Suggests plotly, datasets, rpart, knitr, rmarkdown, ranger, HDclassif,
     qpdf, igraph, testthat (>= 3.0.0)
RdMacros Rdpack
Encoding UTF-8
RoxygenNote 7.3.2
VignetteBuilder knitr
URL https://www.markus-ulmer.ch/SDModels/
BugReports https://github.com/markusul/SDModels/issues
Config/testthat/edition 3
NeedsCompilation no
Author Markus Ulmer [aut, cre, cph] (ORCID:
       <https://orcid.org/0000-0001-7783-8475>),
     Cyrill Scheidegger [aut] (ORCID:
       <https://orcid.org/0009-0005-2851-1384>)
```

2 Contents

Maintainer Markus Ulmer <markus.ulmer@stat.math.ethz.ch>
Repository CRAN

**Date/Publication** 2025-06-05 16:10:05 UTC

# **Contents**

1 7	3
	4
cvSDTree	5
in i	7
	8
	9
6 - 1 - · 1 · · · · · · · · · · · · · · ·	0
get_cp_seq.SDTree	_
get_Q	
get_W	
mergeForest	
partDependence	
	6
	7
plot.SDForest	
plot.SDTree	
plotOOB	9
predict.SDAM	0
predict.SDForest	
predict.SDTree	2
predictOOB	
predict_individual_fj	3
print.partDependence	4
print.SDAM	5
print.SDForest	6
print.SDTree 2	7
prune.SDForest	8
prune.SDTree	9
regPath.SDForest	0
regPath.SDTree	_
SDAM	2
SDForest	5
SDTree	0
simulate_data_nonlinear	4
simulate_data_step	5
stabilitySelection.SDForest	7
toList.SDForest	8
toList.SDTree	9
varImp.SDAM	0
varImp.SDForest	1
varImp.SDTree	2

copy.SDForest 3

Index 53

copy.SDForest

Copy a forest

# Description

Returns a copy of the forest object. Might be useful if you want to keep the original forest in comparison to the pruned forest.

# Usage

```
## S3 method for class 'SDForest'
copy(object, ...)
```

# Arguments

object an SDForest object

Further arguments passed to or from other methods.

#### Value

A copy of the SDForest object

# Author(s)

Markus Ulmer

### See Also

prune

```
set.seed(1)
X <- matrix(rnorm(10 * 20), nrow = 10)
Y <- rnorm(10)
fit <- SDForest(x = X, y = Y, nTree = 2, cp = 0.5)
fit2 <- copy(fit)</pre>
```

4 copy.SDTree

copy.SDTree

Copy a tree

# Description

Returns a copy of the tree object. Might be useful if you want to keep the original tree in comparison to the pruned tree.

# Usage

```
## S3 method for class 'SDTree'
copy(object, ...)
```

# Arguments

object an SDTree object

... Further arguments passed to or from other methods.

#### Value

A copy of the SDTree object

# Author(s)

Markus Ulmer

### See Also

prune

```
set.seed(1)
X <- matrix(rnorm(10 * 20), nrow = 10)
Y <- rnorm(10)
fit <- SDTree(x = X, y = Y, cp = 0.5)
fit2 <- copy(fit)</pre>
```

cvSDTree 5

 ${\tt cvSDTree}$ 

Cross-validation for the SDTree

### **Description**

Estimates the optimal complexity parameter for the SDTree using cross-validation. The transformations are estimated for each training set and validation set separately to ensure independence of the validation set.

### Usage

```
cvSDTree(
  formula = NULL,
  data = NULL,
  x = NULL,
 y = NULL,
 max_leaves = NULL,
  cp = 0,
 min_sample = 5,
 mtry = NULL,
  fast = TRUE,
  Q_type = "trim",
  trim_quantile = 0.5,
  q_hat = 0,
  Qf = NULL,
  A = NULL
  gamma = 0.5,
  gpu = FALSE,
 mem_size = 1e+07,
 max_candidates = 100,
  nfolds = 3,
  cp\_seq = NULL,
  mc.cores = 1,
  Q_scale = TRUE
)
```

# **Arguments**

formula	Object of class formula or describing the model to fit of the form $y \sim x1 + x2 + \dots$ where y is a numeric response and x1, x2, \dots are vectors of covariates. Interactions are not supported.
data	Training data of class data. frame containing the variables in the model.
X	Predictor data, alternative to formula and data.
у	Response vector, alternative to formula and data.
max_leaves	Maximum number of leaves for the grown tree.

6 cvSDTree

cp Complexity parameter, minimum loss decrease to split a node. A split is only

performed if the loss decrease is larger than cp \* initial\_loss, where initial\_loss

is the loss of the initial estimate using only a stump.

min\_sample Minimum number of observations per leaf. A split is only performed if both

resulting leaves have at least min\_sample observations.

mtry Number of randomly selected covariates to consider for a split, if NULL all co-

variates are available for each split.

fast If TRUE, only the optimal splits in the new leaves are evaluated and the previously

optimal splits and their potential loss-decrease are reused. If FALSE all possible

splits in all the leaves are reevaluated after every split.

Q\_type Type of deconfounding, one of 'trim', 'pca', 'no\_deconfounding'. 'trim' corre-

sponds to the Trim transform (Ćevid et al. 2020) as implemented in the Doubly debiased lasso (Guo et al. 2022), 'pca' to the PCA transformation(Paul et al.

2008). See get\_Q.

trim\_quantile Quantile for Trim transform, only needed for trim and DDL\_trim, see get\_Q.

q\_hat Assumed confounding dimension, only needed for pca, see get\_Q.

Qf Spectral transformation, if NULL it is internally estimated using get\_Q.

A Numerical Anchor of class matrix. See get\_W.

gamma Strength of distributional robustness,  $\gamma \in [0, \infty]$ . See get\_W.

gpu If TRUE, the calculations are performed on the GPU. If it is properly set up.

mem\_size Amount of split candidates that can be evaluated at once. This is a trade-off be-

tween memory and speed can be decreased if either the memory is not sufficient

or the gpu is to small.

max\_candidates Maximum number of split points that are proposed at each node for each covari-

ate.

nfolds Number of folds for cross-validation. It is recommended to not use more than

5 folds if the number of covariates is larger than the number of observations. In this case the spectral transformation could differ to much if the validation data

is substantially smaller than the training data.

cp\_seq Sequence of complexity parameters cp to compare using cross-validation, if

NULL a sequence from 0 to 0.6 with stepsize 0.002 is used.

mc.cores Number of cores to use for parallel computation.

Q\_scale Should data be scaled to estimate the spectral transformation? Default is TRUE

to not reduce the signal of high variance covariates, and we do not know of a

scenario where this hurts.

#### Value

A list containing

cp\_min The optimal complexity parameter.

cp\_table A table containing the complexity parameter, the mean and the standard devia-

tion of the loss on the validation sets for the complexity parameters. If multiple complexity parameters result in the same loss, only the one with the largest

complexity parameter is shown.

fromList.SDForest 7

#### Author(s)

Markus Ulmer

#### References

Guo Z, Ćevid D, Bühlmann P (2022). "Doubly debiased lasso: High-dimensional inference under hidden confounding." *The Annals of Statistics*, **50**(3). ISSN 0090-5364, doi:10.1214/21AOS2152.

Paul D, Bair E, Hastie T, Tibshirani R (2008). ""Preconditioning" for feature selection and regression in high-dimensional problems." *The Annals of Statistics*, **36**(4). ISSN 0090-5364, doi:10.1214/009053607000000578.

Ćevid D, Bühlmann P, Meinshausen N (2020). "Spectral Deconfounding via Perturbed Sparse Linear Models." *J. Mach. Learn. Res.*, **21**(1). ISSN 1532-4435, http://jmlr.org/papers/v21/19-545.html.

#### See Also

```
SDTree prune.SDTree regPath.SDTree
```

### **Examples**

```
set.seed(1)
n <- 50
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n, 0, 5)
cp <- cvSDTree(x = X, y = y, Q_type = 'no_deconfounding')
cp</pre>
```

fromList.SDForest

SDForest fromList method

### **Description**

Converts the trees in an SDForest object from class list to class Node (Glur 2023).

### Usage

```
## S3 method for class 'SDForest'
fromList(object, ...)
```

#### **Arguments**

object an SDForest object with the trees in list format
... Further arguments passed to or from other methods.

8 fromList.SDTree

#### Value

an SDForest object with the trees in Node format

#### Author(s)

Markus Ulmer

#### References

```
Glur C (2023). "data.tree: General Purpose Hierarchical Data Structure." https://CRAN.R-project.org/package=data.tree.
```

#### See Also

```
fromList fromList.SDTree
```

# **Examples**

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n)
model <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5, nTree = 2)
fromList(toList(model))</pre>
```

fromList.SDTree

SDTree fromList method

### **Description**

Converts the tree in an SDTree object from class list to class Node (Glur 2023).

# Usage

```
## S3 method for class 'SDTree'
fromList(object, ...)
```

#### **Arguments**

object an SDTree object with the tree in list format
... Further arguments passed to or from other methods.

#### Value

an SDTree object with the tree in Node format

### Author(s)

Markus Ulmer

f\_four 9

#### References

Glur C (2023). "data.tree: General Purpose Hierarchical Data Structure." https://CRAN.R-project.org/package=data.tree.

### See Also

toList

### **Examples**

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n)
model <- SDTree(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5)
fromList(toList(model))</pre>
```

f\_four

Function of x on a fourier basis

# Description

Function of x on a fourier basis with a subset of covariates having a causal effect on Y using the parameters beta. The function is given by:

$$f(x_i) = \sum_{j=1}^{p} 1_{j \in js} \sum_{k=1}^{K} (\beta_{j,k}^{(1)} \cos(0.2kx_j) + \beta_{j,k}^{(2)} \sin(0.2kx_j))$$

#### **Usage**

```
f_four(x, beta, js)
```

# **Arguments**

x a vector of covariates beta the parameter vector for the function f(X)

js the indices of the causal covariates in X

#### Value

the value of the function f(x)

### Author(s)

Markus Ulmer

#### See Also

```
simulate_data_nonlinear
```

### **Examples**

```
set.seed(42)
# simulation of confounded data
sim_data <- simulate_data_nonlinear(q = 2, p = 150, n = 100, m = 2)
X <- sim_data$X
j <- sim_data$j[1]
apply(X, 1, function(x) f_four(x, sim_data$beta, j))</pre>
```

get\_cp\_seq.SDForest

Get the sequence of complexity parameters of an SDForest

### **Description**

This function extracts the sequence of complexity parameters of an SDForest that result in changes of the SDForest if pruned. Only cp values that differ in the first three digits after the decimal point are returned.

# Usage

```
## S3 method for class 'SDForest'
get_cp_seq(object, ...)
```

### Arguments

object an SDForest object

... Further arguments passed to or from other methods.

#### Value

A sequence of complexity parameters

#### Author(s)

Markus Ulmer

#### See Also

```
regPath stabilitySelection get_cp_seq.SDTree
```

get\_cp\_seq.SDTree 11

#### **Examples**

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n)
model <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', cp = 0, nTree = 2)
get_cp_seq(model)</pre>
```

get\_cp\_seq.SDTree

Get the sequence of complexity parameters of an SDTree

#### **Description**

This function extracts the sequence of complexity parameters of an SDTree that result in changes of the tree structure if pruned. Only cp values that differ in the first three digits after the decimal point are returned.

#### Usage

```
## S3 method for class 'SDTree'
get_cp_seq(object, ...)
```

### **Arguments**

object an SDTree object

... Further arguments passed to or from other methods.

#### Value

A sequence of complexity parameters

#### Author(s)

Markus Ulmer

### See Also

```
regPath stabilitySelection
```

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n)
model <- SDTree(x = X, y = y, Q_type = 'no_deconfounding', cp = 0)
get_cp_seq(model)</pre>
```

 $get_Q$ 

		_
ge	τ	L.

Estimation of spectral transformation

#### **Description**

Estimates the spectral transformation Q for spectral deconfounding by shrinking the leading singular values of the covariates.

### Usage

```
get_Q(X, type, trim_quantile = 0.5, q_hat = 0, gpu = FALSE, scaling = TRUE)
```

### **Arguments**

X Numerical covariates of class matrix.

type Type of deconfounding, one of 'trim', 'pca', 'no\_deconfounding'. 'trim' corre-

sponds to the Trim transform (Ćevid et al. 2020) as implemented in the Doubly debiased lasso (Guo et al. 2022), 'pca' to the PCA transformation(Paul et al.

2008) and 'no\_deconfounding' to the Identity.

trim\_quantile Quantile for Trim transform, only needed for trim.

q\_hat Assumed confounding dimension, only needed for pca.

gpu If TRUE, the calculations are performed on the GPU. If it is properly set up. scaling Whether X should be scaled before calculating the spectral transformation.

#### Value

Q of class matrix, the spectral transformation matrix.

#### Author(s)

Markus Ulmer

# References

Guo Z, Ćevid D, Bühlmann P (2022). "Doubly debiased lasso: High-dimensional inference under hidden confounding." *The Annals of Statistics*, **50**(3). ISSN 0090-5364, doi:10.1214/21AOS2152.

Paul D, Bair E, Hastie T, Tibshirani R (2008). ""Preconditioning" for feature selection and regression in high-dimensional problems." *The Annals of Statistics*, **36**(4). ISSN 0090-5364, doi:10.1214/009053607000000578.

Ćevid D, Bühlmann P, Meinshausen N (2020). "Spectral Deconfounding via Perturbed Sparse Linear Models." *J. Mach. Learn. Res.*, **21**(1). ISSN 1532-4435, http://jmlr.org/papers/v21/19-545.html.

get\_W 13

#### **Examples**

```
set.seed(1)
X <- matrix(rnorm(50 * 20), nrow = 50)
Q_trim <- get_Q(X, 'trim')
Q_pca <- get_Q(X, 'pca', q_hat = 5)
Q_plain <- get_Q(X, 'no_deconfounding')</pre>
```

get\_W

Estimation of anchor transformation

# **Description**

Estimates the anchor transformation for the Anchor-Objective. The anchor transformation is  $W=I-(1-\sqrt{\gamma}))\Pi_A$ , where  $\Pi_A=A(A^TA)^{-1}A^T$ . For  $\gamma=1$  this is just the identity. For  $\gamma=0$  this corresponds to residuals after orthogonal projecting onto A. For large  $\gamma$  this is close to the orthogonal projection onto A, scaled by  $\gamma$ . The estimator  $\underset{f}{\operatorname{argmin}}|W(Y-f(X))||^2$  corresponds to the Anchor-Regression Estimator (Rothenhäusler et al. 2021), (Bühlmann 2020).

### Usage

```
get_W(A, gamma, intercept = FALSE, gpu = FALSE)
```

#### **Arguments**

A Numerical Anchor of class matrix.

gamma Strength of distributional robustness,  $\gamma \in [0, \infty]$ .

intercept Logical, whether to include an intercept in the anchor.

gpu If TRUE, the calculations are performed on the GPU. If it is properly set up.

#### Value

W of class matrix, the anchor transformation matrix.

#### Author(s)

Markus Ulmer

#### References

Bühlmann P (2020). "Invariance, Causality and Robustness." *Statistical Science*, **35**(3). ISSN 0883-4237, doi:10.1214/19STS721.

Rothenhäusler D, Meinshausen N, Bühlmann P, Peters J (2021). "Anchor Regression: Heterogeneous Data Meet Causality." *Journal of the Royal Statistical Society Series B: Statistical Methodology*, **83**(2), 215–246. ISSN 1369-7412, doi:10.1111/rssb.12398.

14 mergeForest

#### **Examples**

```
set.seed(1)
n <- 50
X <- matrix(rnorm(n * 1), nrow = n)
Y <- 3 * X + rnorm(n)
W <- get_W(X, gamma = 0)
resid <- W %*% Y</pre>
```

mergeForest

Merge two forests

### **Description**

This function merges two forests. The trees are combined and the variable importance is calculated as a weighted average of the two forests. If the forests are trained on the same data, the predictions and oob\_predictions are combined as well.

# Usage

```
mergeForest(fit1, fit2)
```

# Arguments

```
fit1 first SDForest object
fit2 second SDForest object
```

### Value

```
merged SDForest object set.seed(1) n <- 50 X <- matrix(rnorm(n * 5), nrow = n) y <- sign(X[, 1]) * 3 + rnorm(n) fit1 <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', nTree = 5, cp = 0.5) fit2 <- SDForest(x = X, y = y, nTree = 5, cp = 0.5) mergeForest(fit1, fit2)
```

#### Author(s)

Markus Ulmer

partDependence 15

|--|--|

### **Description**

This function calculates the partial dependence of a model on a single variable. For that predictions are made for all observations in the dataset while varying the value of the variable of interest. The overall partial effect is the average of all predictions. (Friedman 2001)

# Usage

```
partDependence(object, j, X = NULL, subSample = NULL, mc.cores = 1)
```

### **Arguments**

object	A model object that has a predict method that takes newdata as argument and returns predictions.
j	The variable for which the partial dependence should be calculated. Either the column index of the variable in the dataset or the name of the variable.
X	The dataset on which the partial dependence should be calculated. Should contain the same variables as the dataset used to train the model. If NULL, tries to extract the dataset from the model object.
subSample	Number of samples to draw from the original data for the empirical partial dependence. If NULL, all the observations are used.
mc.cores	Number of cores to use for parallel computation. Parallel computing is only supported for unix.

### Value

An object of class partDependence containing

preds_mean	The average prediction for each value of the variable of interest.
x_seq	The sequence of values for the variable of interest.
preds	The predictions for each value of the variable of interest for each observation.
j	The name of the variable of interest.
хj	The values of the variable of interest in the dataset.

#### Author(s)

Markus Ulmer

# References

Friedman JH (2001). "Greedy Function Approximation: A Gradient Boosting Machine." *The Annals of Statistics*, **29**(5), 1189–1232. ISSN 00905364, http://www.jstor.org/stable/2699986.

plot.partDependence

#### See Also

```
SDForest, SDTree
```

### **Examples**

```
set.seed(1)
x <- rnorm(100)
y <- sign(x) * 3 + rnorm(100)
model <- SDTree(x = x, y = y, Q_type = 'no_deconfounding')
pd <- partDependence(model, 1, X = x, subSample = 10)
plot(pd)</pre>
```

plot.partDependence

Plot partial dependence

# Description

This function plots the partial dependence of a model on a single variable.

### Usage

```
## S3 method for class 'partDependence'
plot(x, n_examples = 19, ...)
```

#### **Arguments**

x An object of class partDependence returned by partDependence.
 n\_examples Number of examples to plot in addition to the average prediction.
 ... Further arguments passed to or from other methods.

#### Value

A ggplot object.

#### Author(s)

Markus Ulmer

### See Also

```
partDependence set.seed(1) x < rnorm(10) y < sign(x) * 3 + rnorm(10) model < SDTree(x = x, y = y, Q_type = 'no_deconfounding', cp = 0.5) pd <math>< rnorm(10) partDependence(model, 1, X = x) plot(pd)
```

plot.paths 17

plot.paths Visualize the paths of an S	DTree or SDForest
--	-------------------

### **Description**

This function visualizes the variable importance of an SDTree or SDForest for different complexity parameters. Both the regularization path and the stability selection path can be visualized.

# Usage

```
## S3 method for class 'paths'
plot(x, plotly = FALSE, selection = NULL, sqrt_scale = FALSE, ...)
```

#### **Arguments**

X	A paths object
plotly	If TRUE the plot is returned interactive using plotly. Might be slow for large data.
selection	A vector of indices of the covariates to be plotted. Can be used to plot only a subset of the covariates in case of many covariates.
sqrt_scale	If TRUE the y-axis is on a square root scale.
	Further arguments passed to or from other methods.

#### Value

A ggplot object with the variable importance for different regularization. If the path object includes a cp\_min value, a black dashed line is added to indicate the out-of-bag optimal variable selection.

#### Author(s)

Markus Ulmer

#### See Also

```
regPath stabilitySelection
```

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + sign(X[, 2]) + rnorm(n)
model <- SDTree(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5)
paths <- regPath(model)
plot(paths)</pre>
```

plot.SDTree

```
plot(paths, plotly = TRUE)
```

plot.SDForest

Plot performance of SDForest against number of trees

# Description

This plot helps to analyze whether enough trees were used. If the loss does not stabilize one can fit another SDForest and merge the two.

# Usage

```
## S3 method for class 'SDForest' plot(x, ...)
```

# **Arguments**

x Fitted object of class SDForest.

. . . Further arguments passed to or from other methods.

#### Value

A ggplot object

### Author(s)

Markus Ulmer

#### See Also

```
 \begin{aligned} & \text{SDForest set.seed}(1) \text{ n <- } 10 \text{ X <- } matrix(rnorm(n * 5), nrow = n) \text{ y <- } sign(X[, 1]) * 3 + rnorm(n) \\ & \text{model <- SDForest}(x = X, y = y, Q\_type = \text{'no\_deconfounding'}, cp = 0.5, nTree = 500) \text{ plot(model)} \end{aligned}
```

plot.SDTree

Plot SDTree

### **Description**

Plot the SDTree.

#### Usage

```
## S3 method for class 'SDTree' plot(x, ...)
```

plotOOB 19

# Arguments

x Fitted object of class SDTree.

... Further arguments for DiagrammeR::render\_graph()

#### Value

```
graph object from DiagrammeR::render_graph()
```

### Author(s)

Markus Ulmer

#### See Also

```
SDTree set.seed(1) n <- 10 \text{ X} <- matrix(rnorm(n * 5), nrow = n) y <- \operatorname{sign}(X[, 1]) * 3 + rnorm(n) model <- SDTree(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5) plot(model)
```

plot00B

Visualize the out-of-bag performance of an SDForest

### **Description**

This function visualizes the out-of-bag performance of an SDForest for different complexity parameters. Can be used to choose the optimal complexity parameter.

# Usage

```
plot00B(object, sqrt_scale = FALSE)
```

# **Arguments**

object A paths object with loss\_path matrix with the out-of-bag performance for each

complexity parameter.

sqrt\_scale If TRUE the x-axis is on a square root scale.

#### Value

A ggplot object

## Author(s)

Markus Ulmer

#### See Also

```
regPath.SDForest
```

20 predict.SDAM

#### **Examples**

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + sign(X[, 2]) + rnorm(n)
model <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5)
paths <- regPath(model)
plot00B(paths)</pre>
```

predict.SDAM

Predictions for SDAM

### **Description**

Predicts the response for new data using a fitted SDAM.

### Usage

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

### **Arguments**

object Fitted object of class SDAM.

newdata New test data of class data. frame containing the covariates for which to predict

the response.

Further arguments passed to or from other methods.

#### Value

A vector of predictions for the new data.

### Author(s)

Cyrill Scheidegger

### See Also

SDAM

```
set.seed(1)
X <- matrix(rnorm(10 * 5), ncol = 5)
Y <- sin(X[, 1]) - X[, 2] + rnorm(10)
model <- SDAM(x = X, y = Y, Q_type = "trim", trim_quantile = 0.5, nfold = 2, n_K = 1)
predict(model, newdata = data.frame(X))</pre>
```

predict.SDForest 21

predic	+ CD	For	20+
preare	. L	יוטחי	25 L

Predictions for the SDForest

# Description

Predicts the response for new data using a fitted SDForest.

#### Usage

```
## S3 method for class 'SDForest'
predict(object, newdata, mc.cores = 1, ...)
```

### **Arguments**

object Fitted object of class SDForest.

newdata New test data of class data. frame containing the covariates for which to predict

the response.

mc.cores Number of cores to use for parallel processing, if mc.cores > 1 the trees predict

in parallel.

. . . Further arguments passed to or from other methods.

### Value

A vector of predictions for the new data.

#### Author(s)

Markus Ulmer

#### See Also

**SDForest** 

```
set.seed(1)
n <- 50
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n)
model <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', nTree = 5, cp = 0.5)
predict(model, newdata = data.frame(X))</pre>
```

22 predict.SDTree

predict.SDTree

Predictions for the SDTree

# Description

Predicts the response for new data using a fitted SDTree.

### Usage

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

# Arguments

object Fitted object of class SDTree.

newdata New test data of class data. frame containing the covariates for which to predict

the response.

... Further arguments passed to or from other methods.

### Value

A vector of predictions for the new data.

# Author(s)

Markus Ulmer

#### See Also

SDTree

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n)
model <- SDTree(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5)
predict(model, newdata = data.frame(X))</pre>
```

predictOOB 23

		٠			$\overline{}$	$\overline{}$	_
pr	മപ	7	ς.	t	( )	( )	к
D.	u	_	_	L	v	v	$\mathbf{\mathcal{L}}$

Out-of-bag predictions for the SDForest

#### **Description**

Predicts the response for the training data using only the trees in the SDForest that were not trained on the observation.

#### Usage

```
predictOOB(object, X = NULL)
```

### Arguments

object Fitted object of class SDForest.

X Covariates of the training data. If NULL, the data saved in the object is used.

#### Value

```
A vector of out-of-bag predictions for the training data. #' set.seed(1) n <- 50 X <- matrix(rnorm(n * 5), nrow = n) y <- sign(X[, 1]) * 3 + rnorm(n) model <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', nTree = 5, cp = 0.5) predictOOB(model)
```

#### Author(s)

Markus Ulmer

#### See Also

```
SDForest prune.SDForest plot00B
```

predict\_individual\_fj Predictions of individual component functions for SDAM

# Description

Predicts the contribution of an individual component j using a fitted SDAM.

### Usage

```
predict_individual_fj(object, j, x = NULL)
```

#### **Arguments**

object	Fitted object of class SDAM.
j	Which component to evaluate.
X	New numeric data to predict for.

### Value

A vector of predictions for fj evaluated at Xjnew.

### Author(s)

Cyrill Scheidegger

#### See Also

**SDAM** 

# **Examples**

```
set.seed(1)
X <- matrix(rnorm(10 * 5), ncol = 5)
Y <- sin(X[, 1]) - X[, 2] + rnorm(10)
model <- SDAM(x = X, y = Y, Q_type = "trim", trim_quantile = 0.5, nfold = 2, n_K = 1)
predict_individual_fj(model, j = 1, seq(-2, 2, length.out = 100))</pre>
```

print.partDependence Print partDependence

### **Description**

Print contents of the partDependence.

# Usage

```
## S3 method for class 'partDependence'
print(x, ...)
```

## **Arguments**

- x Fitted object of class partDependence.
- . . . Further arguments passed to or from other methods.

#### Value

No return value, called for side effects

## Author(s)

Markus Ulmer

#### See Also

```
partDependence, plot.partDependence
```

print.SDAM 25

#### **Examples**

```
set.seed(1)
x <- rnorm(10)
y <- sign(x) * 3 + rnorm(10)
model <- SDTree(x = x, y = y, Q_type = 'no_deconfounding', cp = 0.5)
pd <- partDependence(model, 1, X = x)
print(pd)</pre>
```

print.SDAM

Print SDAM

### **Description**

Print number of covariates and number of active covariates for SDAM object.

# Usage

```
## S3 method for class 'SDAM'
print(x, ...)
```

### **Arguments**

x Fitted object of class SDAM.

. . . Further arguments passed to or from other methods.

#### Value

No return value, called for side effects

### Author(s)

Cyrill Scheidegger

#### See Also

**SDAM** 

```
set.seed(1)
X <- matrix(rnorm(10 * 5), ncol = 5)
Y <- sin(X[, 1]) - X[, 2] + rnorm(10)
model <- SDAM(x = X, y = Y, Q_type = "trim", trim_quantile = 0.5, nfold = 2, n_K = 1)
print(model)</pre>
```

26 print.SDForest

print.SDForest

Print SDForest

# Description

Print contents of the SDForest.

# Usage

```
## S3 method for class 'SDForest' print(x, ...)
```

### **Arguments**

x Fitted object of class SDForest.

... Further arguments passed to or from other methods.

#### Value

No return value, called for side effects

# Author(s)

Markus Ulmer

### See Also

**SDForest** 

```
set.seed(1)
n <- 50
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n)
model <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', nTree = 5, cp = 0.5)
print(model)</pre>
```

print.SDTree 27

print.SDTree

Print a SDTree

# Description

Print contents of the SDTree.

# Usage

```
## S3 method for class 'SDTree' print(x, ...)
```

### **Arguments**

x Fitted object of class SDTree.

... Further arguments passed to or from other methods.

#### Value

No return value, called for side effects

# Author(s)

Markus Ulmer

### See Also

SDTree

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n)
model <- SDTree(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5)
print(model)</pre>
```

28 prune.SDForest

nruno	SDForest	
or une.	JULULEST	

Prune an SDForest

### **Description**

Prunes all trees in the forest and re-calculates the out-of-bag predictions and performance measures. The training data is needed to calculate the out-of-bag statistics. Note that the forest is pruned in place. If you intend to keep the original forest, make a copy of it before pruning.

### Usage

```
## S3 method for class 'SDForest'
prune(object, cp, X = NULL, Y = NULL, Q = NULL, pred = TRUE, ...)
```

### **Arguments**

object	an SDForest object
ср	Complexity parameter, the higher the value the more nodes are pruned.
Χ	The training data, if NULL the data from the forest object is used.
Υ	The training response variable, if NULL the data from the forest object is used.
Q	The transformation function, if NULL the data from the forest object is used.
pred	If TRUE the predictions are calculated, if FALSE only the out-of-bag statistics are calculated. This can set to FALSE to save computation time if only the out-of-bag statistics are needed.
	Further arguments passed to or from other methods.

### Value

A pruned SDForest object

#### Author(s)

Markus Ulmer

#### See Also

```
copy prune. SDTree regPath
```

```
set.seed(1)
X <- matrix(rnorm(10 * 20), nrow = 10)
Y <- rnorm(10)
fit <- SDForest(x = X, y = Y, nTree = 2)
pruned_fit <- prune(copy(fit), 0.2)</pre>
```

prune.SDTree 29

prune.SDTree

Prune an SDTree

### **Description**

Removes all nodes that did not improve the loss by more than cp times the initial loss. Either by themselves or by one of their successors. Note that the tree is pruned in place. If you intend to keep the original tree, make a copy of it before pruning.

# Usage

```
## S3 method for class 'SDTree'
prune(object, cp, ...)
```

#### **Arguments**

object an SDTree object

cp Complexity parameter, the higher the value the more nodes are pruned.

... Further arguments passed to or from other methods.

#### Value

A pruned SDTree object

### Author(s)

Markus Ulmer

# See Also

сору

```
set.seed(1)
X <- matrix(rnorm(10 * 20), nrow = 10)
Y <- rnorm(10)
tree <- SDTree(x = X, y = Y)
pruned_tree <- prune(copy(tree), 0.2)
tree
pruned_tree</pre>
```

30 regPath.SDForest

regPath.SDForest	Calculate the regularization path of an SDForest	

# Description

This function calculates the variable importance of an SDForest and the out-of-bag performance for different complexity parameters.

# Usage

```
## S3 method for class 'SDForest'
regPath(object, cp_seq = NULL, X = NULL, Y = NULL, Q = NULL, copy = TRUE, ...)
```

# **Arguments**

object	an SDForest object
cp_seq	A sequence of complexity parameters. If NULL, the sequence is calculated automatically using only relevant values.
Χ	The training data, if NULL the data from the forest object is used.
Υ	The training response variable, if NULL the data from the forest object is used.
Q	The transformation matrix, if NULL the data from the forest object is used.
сору	Whether the tree should be copied for the regularization path. If FALSE, the pruning is done in place and will change the SDForest. This might be reasonable, if the SDForest is to large to copy.
	Further arguments passed to or from other methods.

# Value

An object of class paths containing

ср	The sequence of complexity parameters.
varImp_path	A matrix with the variable importance for each complexity parameter.
loss_path	A matrix with the out-of-bag performance for each complexity parameter.
cp_min	The complexity parameter with the lowest out-of-bag performance.
type	Path type

# Author(s)

Markus Ulmer

### See Also

plot.paths plot00B regPath.SDTree prune get\_cp\_seq SDForest

regPath.SDTree 31

#### **Examples**

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + sign(X[, 2]) + rnorm(n)
model <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5)
paths <- regPath(model)
plot00B(paths)
plot(paths)
plot(paths, plotly = TRUE)</pre>
```

regPath.SDTree

Calculate the regularization path of an SDTree

#### **Description**

This function calculates the variable importance of an SDTree for different complexity parameters.

#### Usage

```
## S3 method for class 'SDTree'
regPath(object, cp_seq = NULL, ...)
```

#### **Arguments**

object an SDTree object

cp\_seq A sequence of complexity parameters. If NULL, the sequence is calculated

automatically using only relevant values.

... Further arguments passed to or from other methods.

#### Value

An object of class paths containing

cp The sequence of complexity parameters.

varImp\_path A matrix with the variable importance for each complexity parameter.

type Path type

#### Author(s)

Markus Ulmer

#### See Also

```
plot.paths prune get_cp_seq SDTree
```

32 SDAM

#### **Examples**

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + sign(X[, 2]) + rnorm(n)
model <- SDTree(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5)
paths <- regPath(model)
plot(paths)
plot(paths, plotly = TRUE)</pre>
```

**SDAM** 

Spectrally Deconfounded Additive Models

### **Description**

Estimate high-dimensional additive models using spectral deconfounding (Scheidegger et al. 2025). The covariates are expanded into B-spline basis functions. A spectral transformation is used to remove bias arising from hidden confounding and a group lasso objective is minimized to enforce component-wise sparsity. Optimal number of basis functions per component and sparsity penalty are chosen by cross validation.

### Usage

```
SDAM(
  formula = NULL,
 data = NULL,
 x = NULL
  y = NULL,
  Q_type = "trim",
  trim_quantile = 0.5,
  q_hat = 0,
  nfolds = 5,
  cv_method = "1se",
  n_K = 4,
  n_{\text{lambda1}} = 10,
  n_{\text{lambda2}} = 20,
  Q_scale = TRUE,
  ind_lin = NULL,
 mc.cores = 1,
  verbose = TRUE,
  notRegularized = NULL
)
```

SDAM 33

#### **Arguments**

formula Object of class formula or describing the model to fit of the form  $y \sim x1 + x2$ + ... where y is a numeric response and x1, x2, ... are vectors of covariates. Interactions are not supported. data Training data of class data. frame containing the variables in the model. Matrix of covariates, alternative to formula and data. Vector of responses, alternative to formula and data. У Type of deconfounding, one of 'trim', 'pca', 'no\_deconfounding'. 'trim' corre-Q\_type sponds to the Trim transform (Ćevid et al. 2020) as implemented in the Doubly debiased lasso (Guo et al. 2022), 'pca' to the PCA transformation(Paul et al. 2008). See get\_Q. trim\_quantile Quantile for Trim transform, only needed for trim, see get\_Q. q\_hat Assumed confounding dimension, only needed for pca, see get\_0. nfolds The number of folds for cross-validation. Default is 5. cv\_method The method for selecting the regularization parameter during cross-validation. One of "min" (minimum cv-loss) and "1se" (one-standard-error rule) Default is "1se". n\_K The number of candidate values for the number of basis functions for B-splines. Default is 4. n\_lambda1 The number of candidate values for the regularization parameter in the initial cross-validation step. Default is 10. n\_lambda2 The number of candidate values for the regularization parameter in the second stage of cross-validation (once the optimal number of basis function K is decided, a second stage of cross-validation for the regularization parameter is performed on a finer grid). Default is 20. Q\_scale Should data be scaled to estimate the spectral transformation? Default is TRUE to not reduce the signal of high variance covariates. ind\_lin A vector of indices specifying which covariates to model linearly (i.e. not expanded into basis function). Default is 'NULL'. Number of cores to use for parallel processing, if mc.cores > 1 the cross valimc.cores dation is parallelized. Default is '1'. (only supported for unix) If TRUE fitting information is shown. verbose notRegularized A vector of indices specifying which covariates not to regularize. Default is 'NULL'.

#### Value

An object of class 'SDAM' containing the following elements:

X The original design matrix.

p The number of covariates in 'X'.

var\_names Names of the covariates in the training data.

intercept The intercept term of the fitted model.

34 SDAM

К	A vector of the number of basis functions for each covariate, where 1 corresponds to a linear term. The entries of the vector will mostly by the same, but some entries might be lower if the corresponding component of X contains only few unique values.
breaks	A list of breakpoints used for the B-splines. Used to reconstruct the B-spline basis functions.
coefs	A list of coefficients for the B-spline basis functions for each component.
active	A vector of active covariates that contribute to the model.

#### Author(s)

Cyrill Scheidegger

#### References

Guo Z, Ćevid D, Bühlmann P (2022). "Doubly debiased lasso: High-dimensional inference under hidden confounding." *The Annals of Statistics*, **50**(3). ISSN 0090-5364, doi:10.1214/21AOS2152.

Paul D, Bair E, Hastie T, Tibshirani R (2008). ""Preconditioning" for feature selection and regression in high-dimensional problems." *The Annals of Statistics*, **36**(4). ISSN 0090-5364, doi:10.1214/009053607000000578.

Scheidegger C, Guo Z, Bühlmann P (2025). "Spectral Deconfounding for High-Dimensional Sparse Additive Models." *ACM / IMS J. Data Sci.*. doi:10.1145/3711116.

Ćevid D, Bühlmann P, Meinshausen N (2020). "Spectral Deconfounding via Perturbed Sparse Linear Models." *J. Mach. Learn. Res.*, **21**(1). ISSN 1532-4435, http://jmlr.org/papers/v21/19-545.html.

### See Also

```
get_Q, predict.SDAM, varImp.SDAM, predict_individual_fj, partDependence
```

SDForest 35

```
"colIntens", "hue", "OD", "proline")
wine <- log(wine)
# estimate model
# do not use class in the model and restrict proline to be linear
model <- SDAM(alcohol ~ . - class, wine, ind_lin = "proline")</pre>
# extract variable importance
varImp(model)
# most important variable
mostImp <- names(which.max(varImp(model)))</pre>
mostImp
# predict for individual Xj
x <- seq(min(wine[, mostImp]), max(wine[, mostImp]), length.out = 100)</pre>
predJ <- predict_individual_fj(object = model, j = mostImp, x = x)</pre>
plot(x, predJ,
     xlab = paste0("log ", mostImp), ylab = "log alcohol")
# partial dependece
plot(partDependence(model, mostImp))
# predict
predict(model, newdata = wine[42, ])
## alternative function call
mod\_none \leftarrow SDAM(x = as.matrix(wine[1:10, -c(1, 2)]), y = wine alcohol[1:10],
                  Q_type = "no_deconfounding", nfolds = 2, n_K = 4,
                  n_{\text{lambda1}} = 4, n_{\text{lambda2}} = 8)
```

**SDForest** 

Spectrally Deconfounded Random Forests

## Description

Estimate regression Random Forest using spectral deconfounding. The spectrally deconfounded Random Forest (SDForest) combines SDTrees in the same way, as in the original Random Forest (Breiman 2001). The idea is to combine multiple regression trees into an ensemble in order to decrease variance and get a smooth function. Ensembles work best if the different models are independent of each other. To decorrelate the regression trees as much as possible from each other, we have two mechanisms. The first one is bagging (Breiman 1996), where we train each regression tree on an independent bootstrap sample of the observations, e.g., we draw a random sample of size n with replacement from the observations. The second mechanic to decrease the correlation is that only a random subset of the covariates is available for each split. Before each split, we sample

36 SDForest

 $mtry \le p$  from all the covariates and choose the one that reduces the loss the most only from those.

$$\widehat{f(X)} = \frac{1}{N_{tree}} \sum_{t=1}^{N_{tree}} SDTree_t(X)$$

### Usage

```
SDForest(
  formula = NULL,
  data = NULL,
  x = NULL,
 y = NULL,
  nTree = 100,
  cp = 0,
 min_sample = 5,
 mtry = NULL,
 mc.cores = 1,
  Q_{type} = "trim",
  trim_quantile = 0.5,
  q_hat = 0,
 Qf = NULL,
 A = NULL
  gamma = 7,
 max_size = NULL,
  gpu = FALSE,
  return_data = TRUE,
 mem_size = 1e+07,
  leave_out_ind = NULL,
  envs = NULL,
  nTree_leave_out = NULL,
  nTree_env = NULL,
 max_candidates = 100,
  Q_scale = TRUE,
 verbose = TRUE,
  predictors = NULL
)
```

### **Arguments**

formula	Object of class formula or describing the model to fit of the form $y \sim x1 + x + \dots$ where y is a numeric response and x1, x2, \ldots are vectors of covariates. Interactions are not supported.
data	Training data of class data. frame containing the variables in the model.
х	Matrix of covariates, alternative to formula and data.
у	Vector of responses, alternative to formula and data.
nTree	Number of trees to grow.

SDForest 37

Complexity parameter, minimum loss decrease to split a node. A split is only ср performed if the loss decrease is larger than cp \* initial\_loss, where initial\_loss is the loss of the initial estimate using only a stump. Minimum number of observations per leaf. A split is only performed if both min\_sample resulting leaves have at least min\_sample observations. mtry Number of randomly selected covariates to consider for a split, if NULL half of the covariates are available for each split. mtry =  $\left| \frac{p}{2} \right|$ Number of cores to use for parallel processing, if mc.cores > 1 the trees are mc.cores estimated in parallel. Type of deconfounding, one of 'trim', 'pca', 'no\_deconfounding'. 'trim' corre-Q\_type sponds to the Trim transform (Ćevid et al. 2020) as implemented in the Doubly debiased lasso (Guo et al. 2022), 'pca' to the PCA transformation(Paul et al. 2008). See get\_Q. trim\_quantile Quantile for Trim transform, only needed for trim, see get\_0. q\_hat Assumed confounding dimension, only needed for pca, see get\_Q. Qf Spectral transformation, if NULL it is internally estimated using get\_Q. Numerical Anchor of class matrix. See get\_W. Strength of distributional robustness,  $\gamma \in [0, \infty]$ . See get\_W. gamma Maximum number of observations used for a bootstrap sample. If NULL n sammax\_size ples with replacement are drawn. If TRUE, the calculations are performed on the GPU. If it is properly set up. gpu return\_data If TRUE, the training data is returned in the output. This is needed for prune. SDForest, regPath. SDForest, and for mergeForest. Amount of split candidates that can be evaluated at once. This is a trade-off bemem\_size tween memory and speed can be decreased if either the memory is not sufficient or the gpu is to small. Indices of observations that should not be used for training. leave\_out\_ind Vector of environments of class factor which can be used for stratified tree envs fitting. nTree\_leave\_out Number of trees that should be estimated while leaving one of the environments out. Results in number of environments times number of trees. Number of trees that should be estimated for each environment. Results in numnTree\_env ber of environments times number of trees. max\_candidates Maximum number of split points that are proposed at each node for each covari-Should data be scaled to estimate the spectral transformation? Default is TRUE Q\_scale to not reduce the signal of high variance covariates, and we do not know of a scenario where this hurts. verbose If TRUE fitting information is shown. predictors Subset of colnames(X) or numerical indices of the covariates for which an effect on y should be estimated. All the other covariates are only used for deconfound-

ing.

38 SDForest

#### Value

Object of class SDForest containing:

predictions Vector of predictions for each observation.

forest List of SDTree objects.

var\_names Names of the covariates.

oob\_loss Out-of-bag loss. MSE

oob\_SDloss Out-of-bag loss using the spectral transformation.

var\_importance Variable importance. The variable importance is calculated as the sum of the

decrease in the loss function resulting from all splits that use a covariate for each tree. The mean of the variable importance of all trees results in the variable

importance for the forest.

oob\_ind List of indices of trees that did not contain the observation in the training set.

oob\_predictions

Out-of-bag predictions.

If return\_data is TRUE the following are also returned:

X Matrix of covariates.

Y Vector of responses.

Q Spectral transformation.

If envs is provided the following are also returned:

envs Vector of environments.

nTree\_env Number of trees for each environment.

ooEnv\_ind List of indices of trees that did not contain the observation or the same environ-

ment in the training set for each observation.

ooEnv\_loss Out-of-bag loss using only trees that did not contain the observation or the same

environment.

ooEnv\_SDloss Out-of-bag loss using the spectral transformation and only trees that did not

contain the observation or the same environment.

ooEnv\_predictions

Out-of-bag predictions using only trees that did not contain the observation or

the same environment.

nTree\_leave\_out

If environments are left out, the environment for each tree, that was left out.

#### Author(s)

Markus Ulmer

SDForest 39

#### References

Breiman L (1996). "Bagging predictors." *Machine Learning*, **24**(2), 123–140. ISSN 0885-6125, doi:10.1007/BF00058655.

Breiman L (2001). "Random Forests." *Machine Learning*, **45**(1), 5–32. ISSN 08856125, doi:10.1023/A:1010933404324.

Guo Z, Ćevid D, Bühlmann P (2022). "Doubly debiased lasso: High-dimensional inference under hidden confounding." *The Annals of Statistics*, **50**(3). ISSN 0090-5364, doi:10.1214/21AOS2152.

Paul D, Bair E, Hastie T, Tibshirani R (2008). ""Preconditioning" for feature selection and regression in high-dimensional problems." *The Annals of Statistics*, **36**(4). ISSN 0090-5364, doi:10.1214/009053607000000578.

Ćevid D, Bühlmann P, Meinshausen N (2020). "Spectral Deconfounding via Perturbed Sparse Linear Models." *J. Mach. Learn. Res.*, **21**(1). ISSN 1532-4435, http://jmlr.org/papers/v21/19-545.html.

#### See Also

get\_Q, get\_W, SDTree, simulate\_data\_nonlinear, regPath, stabilitySelection, prune, partDependence

```
set.seed(1)
n <- 50
X \leftarrow matrix(rnorm(n * 5), nrow = n)
y < - sign(X[, 1]) * 3 + rnorm(n)
model <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', nTree = 5, cp = 0.5)</pre>
predict(model, newdata = data.frame(X))
##### subset of predictors
# if we know, that only the first covariate has an effect on y,
# we can estimate only its effect and use the others just for deconfounding
model \leftarrow SDForest(x = X, y = y, cp = 0.5, nTree = 5, predictors = c(1))
set.seed(42)
# simulation of confounded data
sim_data <- simulate_data_nonlinear(q = 2, p = 150, n = 100, m = 2)</pre>
X <- sim_data$X
Y <- sim_data$Y
train_data <- data.frame(X, Y)</pre>
# causal parents of y
sim_data$j
# comparison to classical random forest
fit_ranger <- ranger::ranger(Y ~ ., train_data, importance = 'impurity')</pre>
fit <- SDForest(x = X, y = Y, nTree = 100, Q_type = 'pca', q_hat = 2)
fit <- SDForest(Y ~ ., nTree = 100, train_data)</pre>
```

```
fit
# we can plot the fit to see whether the number of trees is high enough
# if the performance stabilizes, we have enough trees otherwise one can fit
# more and add them
plot(fit)
# a few more might be helpfull
fit2 <- SDForest(Y ~ ., nTree = 50, train_data)</pre>
fit <- mergeForest(fit, fit2)</pre>
# comparison of variable importance
imp_ranger <- fit_ranger$variable.importance</pre>
imp_sdf <- fit$var_importance</pre>
imp_col <- rep('black', length(imp_ranger))</pre>
imp_col[sim_data$j] <- 'red'</pre>
plot(imp_ranger, imp_sdf, col = imp_col, pch = 20,
     xlab = 'ranger', ylab = 'SDForest',
     main = 'Variable Importance')
# check regularization path of variable importance
path <- regPath(fit)</pre>
# out of bag error for different regularization
plot00B(path)
plot(path)
# detection of causal parent using stability selection
stablePath <- stabilitySelection(fit)</pre>
plot(stablePath)
# pruning of forest according to optimal out-of-bag performance
fit <- prune(fit, cp = path$cp_min)</pre>
# partial functional dependence of y on the most important covariate
most_imp <- which.max(fit$var_importance)</pre>
dep <- partDependence(fit, most_imp)</pre>
plot(dep, n_examples = 100)
```

SDTree

Spectrally Deconfounded Tree

#### **Description**

Estimates a regression tree using spectral deconfounding. A regression tree is part of the function class of step functions  $f(X) = \sum_{m=1}^{M} 1_{\{X \in R_m\}} c_m$ , where  $(R_m)$  with  $m=1,\ldots,M$  are regions dividing the space of  $\mathbb{R}^p$  into M rectangular parts. Each region has response level  $c_m \in \mathbb{R}$ . For the training data, we can write the step function as  $f(\mathbf{X}) = \mathcal{P}c$  where  $\mathcal{P} \in \{0,1\}^{n \times M}$  is an indicator

matrix encoding to which region an observation belongs and  $c \in \mathbb{R}^M$  is a vector containing the levels corresponding to the different regions. This function then minimizes

$$(\hat{\mathcal{P}}, \hat{c}) = \operatorname{argmin}_{\mathcal{P}' \in \{0,1\}^{n \times M}, c' \in \mathbb{R}^M} \frac{||Q(\mathbf{Y} - \mathcal{P}'c')||_2^2}{n}$$

We find  $\hat{P}$  by using the tree structure and repeated splitting of the leaves, similar to the original cart algorithm (Breiman et al. 2017). Since comparing all possibilities for  $\mathcal{P}$  is impossible, we let a tree grow greedily. Given the current tree, we iterate over all leaves and all possible splits. We choose the one that reduces the spectral loss the most and estimate after each split all the leave estimates  $\hat{c} = \operatorname{argmin}_{c' \in \mathbb{R}^M} \frac{||Q\mathbf{Y} - Q\mathcal{P}c'||_2^2}{n}$  which is just a linear regression problem. This is repeated until the loss decreases less than a minimum loss decrease after a split. The minimum loss decrease equals a cost-complexity parameter cp times the initial loss when only an overall mean is estimated. The cost-complexity parameter cp controls the complexity of a regression tree and acts as a regularization parameter.

# **Usage**

```
SDTree(
  formula = NULL,
  data = NULL,
  x = NULL
 y = NULL
 max_leaves = NULL,
  cp = 0.01,
 min_sample = 5,
 mtry = NULL,
  fast = TRUE,
  Q_{type} = "trim",
  trim_quantile = 0.5,
  q_hat = 0,
 Qf = NULL,
 A = NULL,
  gamma = 0.5,
  gpu = FALSE,
 mem_size = 1e+07,
 max\_candidates = 100,
  Q_scale = TRUE,
  predictors = NULL
)
```

## Arguments

formula	Object of class formula or describing the model to fit of the form $y \sim x1 + x2$
	+ where y is a numeric response and x1, x2, are vectors of covariates.
	Interactions are not supported.
data	Training data of class data.frame containing the variables in the model.
X	Matrix of covariates, alternative to formula and data.
у	Vector of responses, alternative to formula and data.

max\_leaves Maximum number of leaves for the grown tree.

cp Complexity parameter, minimum loss decrease to split a node. A split is only

performed if the loss decrease is larger than cp \* initial\_loss, where initial\_loss

is the loss of the initial estimate using only a stump.

min\_sample Minimum number of observations per leaf. A split is only performed if both

resulting leaves have at least min\_sample observations.

mtry Number of randomly selected covariates to consider for a split, if NULL all co-

variates are available for each split.

fast If TRUE, only the optimal splits in the new leaves are evaluated and the previously

optimal splits and their potential loss-decrease are reused. If FALSE all possible

splits in all the leaves are reevaluated after every split.

Q\_type Type of deconfounding, one of 'trim', 'pca', 'no\_deconfounding'. 'trim' corre-

sponds to the Trim transform (Ćevid et al. 2020) as implemented in the Doubly debiased lasso (Guo et al. 2022), 'pca' to the PCA transformation(Paul et al.

2008). See get\_Q.

trim\_quantile Quantile for Trim transform, only needed for trim, see get\_Q.

q\_hat Assumed confounding dimension, only needed for pca, see get\_Q.

Qf Spectral transformation, if NULL it is internally estimated using get\_Q.

A Numerical Anchor of class matrix. See get\_W.

gamma Strength of distributional robustness,  $\gamma \in [0, \infty]$ . See get\_W.

gpu If TRUE, the calculations are performed on the GPU. If it is properly set up.

mem\_size Amount of split candidates that can be evaluated at once. This is a trade-off be-

tween memory and speed can be decreased if either the memory is not sufficient

or the gpu is to small.

max\_candidates Maximum number of split points that are proposed at each node for each covari-

ate.

Q\_scale Should data be scaled to estimate the spectral transformation? Default is TRUE

to not reduce the signal of high variance covariates, and we do not know of a

scenario where this hurts.

predictors Subset of colnames(X) or numerical indices of the covariates for which an effect

on y should be estimated. All the other covariates are only used for deconfound-

ing.

## Value

Object of class SDTree containing

predictions Predictions for the training set.

tree The estimated tree of class Node from (Glur 2023). The tree contains the infor-

mation about all the splits and the resulting estimates.

var\_names Names of the covariates in the training data.

var\_importance Variable importance of the covariates. The variable importance is calculated as

the sum of the decrease in the loss function resulting from all splits that use this

covariate.

#### Author(s)

Markus Ulmer

#### References

Breiman L, Friedman JH, Olshen RA, Stone CJ (2017). *Classification And Regression Trees*. Routledge. ISBN 9781315139470, doi:10.1201/9781315139470.

Glur C (2023). "data.tree: General Purpose Hierarchical Data Structure." https://CRAN.R-project.org/package=data.tree.

Guo Z, Ćevid D, Bühlmann P (2022). "Doubly debiased lasso: High-dimensional inference under hidden confounding." *The Annals of Statistics*, **50**(3). ISSN 0090-5364, doi:10.1214/21AOS2152.

Paul D, Bair E, Hastie T, Tibshirani R (2008). "Preconditioning" for feature selection and regression in high-dimensional problems." *The Annals of Statistics*, **36**(4). ISSN 0090-5364, doi:10.1214/009053607000000578.

Ćevid D, Bühlmann P, Meinshausen N (2020). "Spectral Deconfounding via Perturbed Sparse Linear Models." *J. Mach. Learn. Res.*, **21**(1). ISSN 1532-4435, http://jmlr.org/papers/v21/19-545.html.

#### See Also

simulate\_data\_nonlinear, regPath.SDTree, prune.SDTree, partDependence

```
set.seed(1)
n <- 10
X \leftarrow matrix(rnorm(n * 5), nrow = n)
y \leftarrow sign(X[, 1]) * 3 + rnorm(n)
model \leftarrow SDTree(x = X, y = y, cp = 0.5)
##### subset of predictors
# if we know, that only the first covariate has an effect on y,
# we can estimate only its effect and use the others just for deconfounding
model \leftarrow SDTree(x = X, y = y, cp = 0.5, predictors = c(1))
set.seed(42)
# simulation of confounded data
sim_data <- simulate_data_step(q = 2, p = 15, n = 100, m = 2)
X <- sim_data$X
Y <- sim_data$Y
train_data <- data.frame(X, Y)</pre>
# causal parents of y
sim_data$j
tree_plain_cv <- cvSDTree(Y ~ ., train_data, Q_type = "no_deconfounding")</pre>
```

```
tree_plain <- SDTree(Y ~ ., train_data, Q_type = "no_deconfounding", cp = 0)
tree_causal_cv <- cvSDTree(Y ~ ., train_data)
tree_causal <- SDTree(y = Y, x = X, cp = 0)

# check regularization path of variable importance
path <- regPath(tree_causal)
plot(path)

tree_plain <- prune(tree_plain, cp = tree_plain_cv$cp_min)
tree_causal <- prune(tree_causal, cp = tree_causal_cv$cp_min)
plot(tree_causal)
plot(tree_plain)</pre>
```

simulate\_data\_nonlinear

Simulate data with linear confounding and non-linear causal effect

#### Description

Simulation of data from a confounded non-linear model. The data generating process is given by:

$$Y = f(X) + \delta^{T} H + \nu$$
$$X = \Gamma^{T} H + E$$

where f(X) is a random function on the fourier basis with a subset of size m covariates  $X_j$  having a causal effect on Y.

$$f(x_i) = \sum_{j=1}^{p} 1_{j \in js} \sum_{k=1}^{K} (\beta_{j,k}^{(1)} \cos(0.2kx_j) + \beta_{j,k}^{(2)} \sin(0.2kx_j))$$

 $E, \nu$  are random error terms and  $H \in \mathbb{R}^{n \times q}$  is a matrix of random confounding covariates.  $\Gamma \in \mathbb{R}^{q \times p}$  and  $\delta \in \mathbb{R}^q$  are random coefficient vectors. For the simulation, all the above parameters are drawn from a standard normal distribution, except for  $\nu$  which is drawn from a normal distribution with standard deviation 0.1. The parameters  $\beta$  are drawn from a uniform distribution between -1 and 1.

### Usage

```
simulate_data_nonlinear(q, p, n, m, K = 2, eff = NULL, fixEff = FALSE)
```

# Arguments

- q number of confounding covariates in H
- p number of covariates in X
- n number of observations

simulate\_data\_step 45

m	number of covariates with a causal effect on Y
K	number of fourier basis functions K $K \in \mathbb{N}$ , e.g. complexity of causal function
eff	the number of affected covariates in $\boldsymbol{X}$ by the confounding, if NULL all covariates are affected
fixEff	if eff is smaller than p: If fixEff = TRUE, the causal parents are always affected by confounding if fixEff = FALSE, affected covariates are chosen completely at random.

#### Value

a list containing the simulated data:

X	a matrix of covariates
Υ	a vector of responses
f_X	a vector of the true function $f(X)$
j	the indices of the causal covariates in X
beta	the parameter vector for the function $f(X)$ , see $f_{four}$
Н	the matrix of confounding covariates

# Author(s)

Markus Ulmer

# See Also

f\_four

# **Examples**

```
set.seed(42)
# simulation of confounded data
sim_data <- simulate_data_nonlinear(q = 2, p = 150, n = 100, m = 2)
X <- sim_data$X
Y <- sim_data$Y</pre>
```

simulate\_data\_step

Simulate data with linear confounding and causal effect following a step-function

46 simulate\_data\_step

## **Description**

Simulation of data from a confounded non-linear model. Where the non-linear function is a random regression tree. The data generating process is given by:

$$Y = f(X) + \delta^T H + \nu$$

$$X = \Gamma^T H + E$$

where f(X) is a random regression tree with m random splits of the data. Resulting in a random step-function with m+1 levels, i.e. leaf-levels.

$$f(x_i) = \sum_{k=1}^{K} 1_{\{x_i \in R_k\}} c_k$$

 $E, \nu$  are random error terms and  $H \in \mathbb{R}^{n \times q}$  is a matrix of random confounding covariates.  $\Gamma \in \mathbb{R}^{q \times p}$  and  $\delta \in \mathbb{R}^q$  are random coefficient vectors. For the simulation, all the above parameters are drawn from a standard normal distribution, except for  $\delta$  which is drawn from a normal distribution with standard deviation 10. The leaf levels  $c_k$  are drawn from a uniform distribution between -50 and 50.

#### Usage

```
simulate_data_step(q, p, n, m, make_tree = FALSE)
```

#### **Arguments**

q number of confounding covariates in H

p number of covariates in X

n number of observations

make\_tree Whether the random regression tree should be returned.

number of covariates with a causal effect on Y

#### Value

a list containing the simulated data:

X a matrix of covariates

Y a vector of responses

 $f_X$  a vector of the true function f(X)

j the indices of the causal covariates in X

tree If make\_tree, the random regression tree of class Node from (Glur 2023)

### Author(s)

Markus Ulmer

#### References

Glur C (2023). "data.tree: General Purpose Hierarchical Data Structure." https://CRAN.R-project.org/package=data.tree.

#### See Also

```
simulate_data_nonlinear
```

## **Examples**

```
set.seed(42)
# simulation of confounded data
sim_data <- simulate_data_step(q = 2, p = 15, n = 100, m = 2)
X <- sim_data$X
Y <- sim_data$Y</pre>
```

```
stabilitySelection.SDForest
```

Calculate the stability selection of an SDForest

## **Description**

This function calculates the stability selection of an SDForest (Meinshausen and Bühlmann 2010). Stability selection is calculated as the fraction of trees in the forest that select a variable for a split at each complexity parameter.

#### Usage

```
## S3 method for class 'SDForest'
stabilitySelection(object, cp_seq = NULL, ...)
```

## **Arguments**

object an SDForest object

cp\_seq A sequence of complexity parameters. If NULL, the sequence is calculated

automatically using only relevant values.

... Further arguments passed to or from other methods.

#### Value

An object of class paths containing

cp The sequence of complexity parameters.

varImp\_path A matrix with the stability selection for each complexity parameter.

type Path type

48 toList.SDForest

#### Author(s)

Markus Ulmer

#### References

Meinshausen N, Bühlmann P (2010). "Stability Selection." *Journal of the Royal Statistical Society Series B: Statistical Methodology*, **72**(4), 417–473. ISSN 1369-7412, doi:10.1111/j.1467-9868.2010.00740.x.

#### See Also

```
plot.paths regPath prune get_cp_seq SDForest
```

## **Examples**

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + sign(X[, 2]) + rnorm(n)
model <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', nTree = 2, cp = 0.5)
paths <- stabilitySelection(model)
plot(paths)

plot(paths, plotly = TRUE)</pre>
```

toList.SDForest

SDForest toList method

# Description

Converts the trees in an SDForest object from class Node (Glur 2023) to class list. This makes it substantially easier to save the forest to disk.

#### Usage

```
## S3 method for class 'SDForest'
toList(object, ...)
```

### **Arguments**

object an SDForest object with the trees in Node format
... Further arguments passed to or from other methods.

### Value

an SDForest object with the trees in list format

toList.SDTree 49

#### Author(s)

Markus Ulmer

#### References

Glur C (2023). "data.tree: General Purpose Hierarchical Data Structure." https://CRAN.R-project.org/package=data.tree.

#### See Also

```
fromList toList.SDTree
```

# **Examples**

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n)
model <- SDForest(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5, nTree = 2)
toList(model)</pre>
```

toList.SDTree

SDTree toList method

#### **Description**

Converts the tree in an SDTree object from class Node (Glur 2023) to class list. This makes it substantially easier to save the tree to disk.

# Usage

```
## S3 method for class 'SDTree'
toList(object, ...)
```

## Arguments

object an SDTree object with the tree in Node format
... Further arguments passed to or from other methods.

#### Value

an SDTree object with the tree in list format

## Author(s)

Markus Ulmer

50 varImp.SDAM

#### References

Glur C (2023). "data.tree: General Purpose Hierarchical Data Structure." https://CRAN.R-project.org/package=data.tree.

## See Also

```
fromList
```

# **Examples**

```
set.seed(1)
n <- 10
X <- matrix(rnorm(n * 5), nrow = n)
y <- sign(X[, 1]) * 3 + rnorm(n)
model <- SDTree(x = X, y = y, Q_type = 'no_deconfounding', cp = 0.5)
toList(model)</pre>
```

varImp.SDAM

Extract Variable importance for SDAM

## **Description**

This function extracts the variable importance of an SDAM. The variable importance is calculated as the empirical squared L2 norm of fj. The measure is not standardized.

# Usage

```
## S3 method for class 'SDAM'
varImp(object)
```

# Arguments

object an SDAM object

## Value

A vector of variable importance

## Author(s)

Cyrill Scheidegger

### See Also

SDAM

varImp.SDForest 51

#### **Examples**

```
set.seed(1)
X <- matrix(rnorm(10 * 5), ncol = 5)
Y <- sin(X[, 1]) - X[, 2] + rnorm(10)
model <- SDAM(x = X, y = Y, Q_type = "trim", trim_quantile = 0.5, nfold = 2)
varImp(model)</pre>
```

varImp.SDForest

Extract variable importance of an SDForest

## Description

This function extracts the variable importance of an SDForest. The variable importance is calculated as the sum of the decrease in the loss function resulting from all splits that use a covariate for each tree. The mean of the variable importance of all trees results in the variable importance for the forest.

## Usage

```
## S3 method for class 'SDForest'
varImp(object)
```

## **Arguments**

object

an SDForest object

#### Value

A named vector of variable importance

#### Author(s)

Markus Ulmer

## See Also

```
varImp.SDTree SDForest
```

52 varImp.SDTree

varImp.SDTree

Extract variable importance of an SDTree

# Description

This function extracts the variable importance of an SDTree. The variable importance is calculated as the sum of the decrease in the loss function resulting from all splits that use this covariate.

## Usage

```
## S3 method for class 'SDTree'
varImp(object)
```

## **Arguments**

object

an SDTree object

## Value

A named vector of variable importance

## Author(s)

Markus Ulmer

#### See Also

```
varImp.SDForest SDTree
```

```
data(iris)
tree <- SDTree(Sepal.Length ~ Sepal.Width + Petal.Length + Petal.Width, iris, cp = 0.5)
varImp(tree)</pre>
```

# **Index**

```
copy, 28, 29
                                                   regPath, 10, 11, 17, 28, 39, 48
copy (copy.SDForest), 3
                                                   regPath (regPath.SDForest), 30
copy.SDForest, 3
                                                   regPath.SDForest, 19, 30, 37
copy.SDTree, 4
                                                   regPath.SDTree, 7, 30, 31, 43
cvSDTree, 5
                                                   SDAM, 20, 24, 25, 32, 50
                                                   SDForest, 16, 18, 21, 23, 26, 30, 35, 48, 51
f_four, 9, 45
                                                   SDTree, 7, 16, 19, 22, 27, 31, 39, 40, 52
fromList, 8, 49, 50
fromList(fromList.SDForest), 7
                                                   simulate_data_nonlinear, 10, 39, 43, 44,
                                                            47
fromList.SDForest, 7
                                                   simulate_data_step, 45
fromList.SDTree, 8, 8
                                                   stabilitySelection, 10, 11, 17, 39
                                                   stabilitySelection
get_cp_seq, 30, 31, 48
                                                            (stabilitySelection.SDForest),
get_cp_seq (get_cp_seq.SDForest), 10
get_cp_seq.SDForest, 10
                                                   stabilitySelection.SDForest, 47
get_cp_seq.SDTree, 10, 11
get_Q, 6, 12, 33, 34, 37, 39, 42
                                                   toList, 9
get_W, 6, 13, 37, 39, 42
                                                   toList (toList.SDForest), 48
                                                   toList.SDForest, 48
mergeForest, 14, 37
                                                   toList.SDTree, 49, 49
partDependence, 15, 16, 24, 34, 39, 43
                                                   varImp (varImp.SDForest), 51
plot.partDependence, 16, 24
                                                   varImp. SDAM, 34, 50
plot.paths, 17, 30, 31, 48
                                                   varImp.SDForest, 51, 52
plot.SDForest, 18
                                                   varImp.SDTree, 51, 52
plot.SDTree, 18
plot00B, 19, 23, 30
predict. SDAM, 20, 34
predict.SDForest, 21
predict.SDTree, 22
predict_individual_fj, 23, 34
predictOOB, 23
print.partDependence, 24
print.SDAM, 25
print.SDForest, 26
print.SDTree, 27
prune, 3, 4, 30, 31, 39, 48
prune (prune. SDForest), 28
prune.SDForest, 23, 28, 37
prune.SDTree, 7, 28, 29, 43
```