# Package 'treeDA'

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Title Tree-Based Discriminant Analysis
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<b>Description</b> Performs sparse discriminant analysis on a combination of node and leaf predictors when the predictor variables are structured according to a tree, as described in Fukuyama et al. (2017) <doi:10.1371 journal.pcbi.1005706="">.</doi:10.1371>
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# **Description**

A package for performing sparse, tree-based discriminant analysis.

#### **Details**

This package contains functions for building sparse, tree-structured models for classification. The method is based on the idea that when our predictors are structured according to a tree, we can create an expanded feature space containing both the original leaf predictors as well as node predictors, which correspond to sums or averages across the leaves descending from them. Without some sort of regularization this problem would be unidentifiable, but with the regularization provided by sparse discriminant analysis we get stable solutions.

The package fits a sparse discriminant model in the expanded feature space and translates the results back to the leaf space, so that the interpretation can be purely in terms of the original predictors. The package also includes functions to perform cross validation to pick the sparsity level and plotting commands to visualize the tree and the fitted coefficient vectors.

The main function in this package is treeda, which fits a sparse tree-based discriminant model. Additional functions provided are treedacv, which performs cross-validation to determine the correct sparsity level, and functions to plot the resulting coefficient vectors along the tree (plot\_coefficients).

#### Author(s)

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#### See Also

Useful links:

• https://github.com/jfukuyama/treeda

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coef.treeda

Coefficients from treeda fit

#### **Description**

Returns the coefficients from a treeda fit either in terms of the leaves only or in terms of the nodes and leaves.

# Usage

```
## S3 method for class 'treeda'
coef(object, type = c("leaves", "nodes"), ...)
```

# Arguments

object An object of class treeda.

type Should the coefficients be in the leaf space or the node space?

... Not used.

#### Value

A Matrix object containing the coefficients.

# **Examples**

```
data(treeda_example)
out.treeda = treeda(response = treeda_example$response,
    predictors = treeda_example$predictors,
    tree = treeda_example$tree,
    p = 1)
coef(out.treeda, type = "leaves")
coef(out.treeda, type = "nodes")
```

 ${\tt combine\_plot\_and\_tree} \quad \textit{Method for combining two ggplots}$ 

# **Description**

This method takes a ggplot of some data along the tips of the tree and a ggplot of a tree and combines them. It assumes that you are putting the tree on top and that the x axis for the plot has the leaves in the correct position (this can be found using the function get\_leaf\_position).

#### Usage

```
combine_plot_and_tree(plot, tree.plot, tree.height = 5, print = TRUE)
```

#### **Arguments**

plot A plot of data about the leaves with the x axis corresponding to leaves.

tree.plot A plot of the tree.

tree.height The relative amount of space in the plot the tree should take up.

print If true, the function will print the combined plot to a graphics device, otherwise

it will just return the gtable object without printing.

#### Value

Returns a gtable object.

get\_leaf\_position Get leaf positions from a tree layout

## Description

Takes a tree, returns a vector with names describing the leaves and entries giving the position of that leaf in the tree layout.

#### Usage

```
get_leaf_position(tree, ladderize)
```

# **Arguments**

tree A tree of class phylo.

ladderize FALSE for a non-ladderzied layout, TRUE or "right" for a ladderized layout,

"left" for a layout ladderized the other way.

makeNodeAndLeafPredictors

Make a matrix with predictors for each leaf and node

# **Description**

Make a matrix with one predictor for each leaf and node in the tree, where the node predictors are the sum of the leaf predictors descending from them.

# Usage

makeNodeAndLeafPredictors(leafPredictors, tree)

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# Arguments

leafPredictors A predictor matrix for the leaves: rows are samples, columns are leaves.

tree A phyloger

A phylogenetic tree describing the relationships between the species/leaves.

#### Value

A predictor matrix for leaves and nodes together: rows are samples, columns are leaf/node predictors.

nodeToLeafCoefficients

Node coefficients to leaf coefficients

# Description

General-purpose function for going from a coefficient vector on the nodes to a coefficient vector on the leaves.

# Usage

```
nodeToLeafCoefficients(coef.vec, tree)
```

# **Arguments**

coef.vec A vector containing coefficients on internal nodes plus leaves.

tree The phylogenetic tree.

# Value

A vector containing coefficients on the leaves.

plot.treedacv

Plot a treedacy object

# **Description**

Plots the cross-validation error with standard error bars.

# Usage

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

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# Arguments

x An object of class treedacv.

... Not used.

#### **Examples**

```
data(treeda_example)
out.treedacv = treedacv(response = treeda_example$response,
    predictors = treeda_example$predictors,
    tree = treeda_example$tree,
    pvec = 1:10)
plot(out.treedacv)
```

plot\_coefficients

Plot the discriminating axes from treeda

#### **Description**

Plots the leaf coefficients for the discriminating axes in a fitted treeda model aligned under the tree

#### Usage

```
plot_coefficients(
  out.treeda,
  remove.bl = TRUE,
  ladderize = TRUE,
  tree.height = 2
)
```

#### **Arguments**

out.treeda The object resulting from a call to treeda.

remove.bl A logical, TRUE if the tree should be plotted after setting all branch lengths equal

to the same value or not. The plots tend to look nicer when all the branch lengths

are the same, and the branch length information is not used in the model.

ladderize Layout parameter for the tree.

tree.height The height of the tree relative to the height of the plot below.

#### Value

A plot of the tree and the coefficients.

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#### **Examples**

```
data(treeda_example)
out.treeda = treeda(response = treeda_example$response,
    predictors = treeda_example$predictors,
    tree = treeda_example$tree,
    p = 1)
plot_coefficients(out.treeda)
```

predict.treeda

Predict using new data

#### **Description**

Given a fitted treeda model, get the predicted classes and projections onto the discriminating axes for new data.

#### Usage

```
## S3 method for class 'treeda'
predict(object, newdata, newresponse = NULL, check.consist = TRUE, ...)
```

#### **Arguments**

object Output from treeda function.

newdata New predictor matrix in the same format as the predictor argument to treeda.

A matrix of predictor variables corresponding to the leaves of the tree and in the

same order as the leaves of the tree.

newresponse New response vector, not required.

check.consist Check the consistency between the tree and predictor matrix?

. . . Not used.

#### Value

A list containing the projections of the new data onto the discriminating axes (projections), the predicted classes (classes), and the rss (rss, only included if the ground truth for the responses is available).

#### **Examples**

```
data(treeda_example)
out.treeda = treeda(response = treeda_example$response,
    predictors = treeda_example$predictors,
    tree = treeda_example$tree,
    p = 1)
## Here we are predicting on the training data, in general this
## would be done on a held out test set
preds = predict(out.treeda, newdata = treeda_example$predictors,
```

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```
newresponse = treeda_example$response)
## make a confusion matrix
table(preds$classes, treeda_example$response)
```

print.treeda

Print a treeda object

# Description

Print a treeda object

# Usage

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

# Arguments

x treeda object.

... Not used.

print.treedacv

Print treedacy objects

# Description

Print treedacy objects

# Usage

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

# Arguments

x treedacv object.

... Not used

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treeda

Tree-based sparse discriminant analysis

# **Description**

Performs tree-structured sparse discriminant analysis using an augmented predictor matrix with additional predictors corresponding to the nodes and then translating the parameters back in terms of only the leaves.

# Usage

```
treeda(
  response,
  predictors,
  tree,
  p,
  k = nclasses - 1,
  center = TRUE,
  scale = TRUE,
  class.names = NULL,
  check.consist = TRUE,
  A = NULL,
  ...
)
```

# Arguments

predictors A matrix of predictor variables corresponding to the leaves of the tree and in the

same order as the leaves of the tree.

tree A tree of class phylo.

p The number of predictors to use.

k The number of components to use.

center Center the predictor variables?
scale Scale the predictor variables?

class.names Optional argument giving the class names.

check.consist Check consistency of the predictor matrix and the tree.

A matrix describing the tree structure. If it has been computed before it can be

passed in here and will not be recomputed.

. . . Additional arguments to be passed to sda

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# Value

An object of class treeda. Contains the coefficients in the original predictor space (leafCoefficients), the number of predictors used in the node + leaf space (nPredictors), number of leaf predictors used (nLeafPredictors), the projections of the samples onto the discriminating axes (projections), and the sparse discriminant analysis object that was used in the fit (sda).

# **Examples**

```
data(treeda_example)
out.treeda = treeda(response = treeda_example$response,
    predictors = treeda_example$predictors,
    tree = treeda_example$tree,
    p = 1)
out.treeda
```

treedacv

treeda cross validation

# **Description**

Performs cross-validation of a treeda fit.

#### Usage

```
treedacv(
  response,
  predictors,
  tree,
  folds = 5,
  pvec = 1:tree$Nnode,
  k = nclasses - 1,
  center = TRUE,
  scale = TRUE,
  class.names = NULL,
  ...
)
```

# **Arguments**

response The classes to be predicted.

predictors A matrix of predictors corresponding to the tips of the tree.

tree A tree object of class phylo.

folds Either a single number corresponding to the number of folds of cross-validation

to perform or a vector of integers ranging from 1 to the number of folds desired

giving the partition of the dataset.

pvec The values of p to use.

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Additional arguments to be passed to treeda.

k The number of discriminating axes to keep.
 center Center the predictors?
 scale Scale the predictors?
 class.names A vector giving the names of the classes.

#### Value

A list with the value of p with minimum cv error (p.min), the minimum value of p with in 1 se of the minimum cv error (p.1se), and a data frame containing the loss for each fold, mean loss, and standard error of the loss for each value of p (loss.df).

# **Examples**

```
data(treeda_example)
out.treedacv = treedacv(response = treeda_example$response,
    predictors = treeda_example$predictors,
    tree = treeda_example$tree,
    pvec = 1:10)
out.treedacv
```

treeda\_example

Example dataset

# Description

A small example dataset with three components, stored as a list with a vector containing the classes (response), a matrix containing the predictor variables (predictors), and a tree describing the relationships between the predictor variables (tree). The dataset consists of 50 samples divided into two classes and 100 taxa/predictor variables, related to each other by a random tree (generated with ape::rtree). A set of 42 taxa descending from one internal node are all over-represented in one class and under-represented in the other. The predictors element in the list contains real numbers, not counts, and is supposed to reflect normalized taxon abundances (e.g., normalization using the variance-stabilizing transformation in DESeq2).

#### **Format**

A list containing response variables, predictor variables, and a tree describing the relationship between the predictor variables.

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