Package ‘codacore’

August 29, 2022

Title Learning Sparse Log-Ratios for Compositional Data

Version 0.0.4

Description In the context of high-throughput genetic data, CoDaCoRe identifies a set of sparse biomarkers that are predictive of a response variable of interest (Gordon-Rodriguez et al., 2021) <doi:10.1093/bioinformatics/btab645>. More generally, CoDaCoRe can be applied to any regression problem where the independent variable is Compositional (CoDa), to derive a set of scale-invariant log-ratios (ILR or SLR) that are maximally associated to a dependent variable.

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Encoding UTF-8

LazyData true

RoxygenNote 7.1.1

Depends R (>= 3.6.0)

Imports tensorflow (>= 2.1), keras (>= 2.3), pROC (>= 1.17), R6 (>= 2.5), gtools(>= 3.8)

SystemRequirements TensorFlow (https://www.tensorflow.org/)

Suggests zCompositions, testthat (>= 2.1.0), knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

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R topics documented:

activeInputs.codacore ..................................................... 2
activeInputs.codacore

Description

activeInputs

Usage

activeInputs.codacore(cdc)

Arguments

cdc A codacore object.

Value

The covariates included in the log-ratios
**Description**

This function implements the codacore algorithm described by Gordon-Rodriguez et al. 2021 (https://doi.org/10.1101/2021.02.11.430695).

**Usage**

```r
codacore(
  x,
  y,
  logRatioType = "balances",
  objective = NULL,
  lambda = 1,
  offset = NULL,
  shrinkage = 1,
  maxBaseLearners = 5,
  optParams = list(),
  cvParams = list(),
  verbose = FALSE,
  overlap = TRUE,
  fast = TRUE
)
```

**Arguments**

- `x` A data.frame or matrix of the compositional predictor variables.
- `y` A data.frame, matrix or vector of the response.
- `logRatioType` A string indicating whether to use "balances" or "amalgamations". Also accepts "balance", "B", "ILR", or "amalgam", "A", "SLR". Note that the current implementation for balances is not strictly an ILR, but rather just a collection of balances (which are possibly non-orthogonal in the Aitchison sense).
- `objective` A string indicating "binary classification" or "regression". By default, it is NULL and gets inferred from the values in y.
- `lambda` A numeric. Corresponds to the "lambda-SE" rule. Sets the "regularization strength" used by the algorithm to decide how to harden the ratio. Larger numbers tend to yield fewer, more sparse ratios.
- `offset` A numeric vector of the same length as y. Works similarly to the offset in a glm.
- `shrinkage` A numeric. Shrinkage factor applied to each base learner. Defaults to 1.0, i.e., no shrinkage applied.
- `maxBaseLearners` An integer. The maximum number of log-ratios that the model will learn before stopping. Automatic stopping based on seRule may occur sooner.
optParams

A list of named parameters for the optimization of the continuous relaxation. Empty by default. User can override as few or as many of our defaults as desired. Includes adaptiveLR (learning rate under adaptive training scheme), momentum (in the gradient-descent sense), epochs (number of gradient-descent epochs), batchSize (number of observations per minibatch, by default the entire dataset), and vanillaLR (the learning rate to be used if the user does *not* want to use the 'adaptiveLR', to be used at the risk of optimization issues).

cvParams

A list of named parameters for the "hardening" procedure using cross-validation. Includes numFolds (number of folds, default=5) and maxCutoffs (number of candidate cutoff values of 'c' to be tested out during CV process, default=20 meaning log-ratios with up to 21 components can be found by codacore).

verbose

A boolean. Toggles whether to display intermediate steps.

overlap

A boolean. Toggles whether successive log-ratios found by CoDaCoRe may contain repeated input variables. TRUE by default. Changing to FALSE implies that the log-ratios obtained by CoDaCoRe will become orthogonal in the Aitchison sense, analogously to the isometric-log-ratio transformation, while losing a small amount of model flexibility.

fast

A boolean. Whether to run in fast or slow mode. TRUE by default. Running in slow mode will take ~x5 the computation time, but may help identify slightly more accurate log-ratios.

Value

A codacore object.

Examples

```r
## Not run:
data("Crohn")
x <- Crohn[, -ncol(Crohn)]
y <- Crohn[, ncol(Crohn)]
x <- x + 1
model = codacore(x, y)
print(model)
plot(model)
## End(Not run)
```

Crohn

*Microbiome composition related to Crohn’s disease study*

Description

A dataset containing the number of counts of 48 different genera in a group of 975 samples (including 662 samples of patients with Crohn’s disease and 313 controls). The data.frame is composed by 48 genera and a factor variable
FranzosaMetabolite

**Format**

The data.frame is composed by 48 genera and a variable
genera The first 48 columns, from *g_Turicibacter* until *g_Bilophila* referred to different genera.
y a factor indicating if the sample corresponds to a case (*CD*) or a control (*no*).

**References**

https://qiita.ucsd.edu/

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FranzosaMetabolite  
*Metabolite relative abundances (Franzosa et al., 2019)*

**Description**

A dataset containing the relative abundances of 7156 metabolites in a group of 220 samples, together with an additional response variable indicating the corresponding Diagnosis.

**Format**

The data.frame is composed by metabolite data and Diagnosis

**Metabolites** TBD

**Diagnosis** Indicates if the sample was diagnosed with Crohn’s disease (*CD*), ulcerative colitis (*UC*), or was a control (*Control*).

**References**

https://www.nature.com/articles/s41564-018-0306-4

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FranzosaMicrobiome  
*Microbiome relative abundances (Franzosa et al., 2019)*

**Description**

A dataset containing the relative abundances of 58 bacteria in a group of 220 samples, together with an additional response variable indicating the corresponding Diagnosis.

**Format**

The data.frame is composed by microbiome data and Diagnosis

**Microbiome** The first 58 columns.

**Diagnosis** Indicates if the sample was diagnosed with Crohn’s disease (*CD*), ulcerative colitis (*UC*), or was a control (*Control*).

**References**

https://www.nature.com/articles/s41564-018-0306-4
getBinaryPartitions

description

Usage

getBinaryPartitions(cdcr)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>cdcr</td>
<td>A codacore object</td>
</tr>
</tbody>
</table>

Value

A matrix describing whether each component (as rows) is found in the numerator (1) or denominator (-1) of each learned log-ratio (as columns). This format resembles a serial binary partition matrix frequently used in balance analysis.

getDenominatorParts

description

Usage

getDenominatorParts(cdcr, baseLearnerIndex = 1, boolean = TRUE)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>cdcr</td>
<td>A codacore object</td>
</tr>
<tr>
<td>baseLearnerIndex</td>
<td>An integer indicating which of the (possibly multiple) log-ratios learned by codacore to be used.</td>
</tr>
<tr>
<td>boolean</td>
<td>Whether to return the parts in boolean form (a vector of TRUE/FALSE) or to return the column names of those parts directly.</td>
</tr>
</tbody>
</table>

Value

The covariates in the denominator of the selected log-ratio.
getLogRatios

Description
getLogRatios

Usage
getLogRatios(cdcr, x = NULL)

Arguments
  cdcr A codacore object
  x A set of (possibly unseen) compositional data. The covariates must be passed in
      the same order as for the original codacore() call.

Value
  The learned log-ratio features, computed on input x.

getNumeratorParts

Description
getNumeratorParts

Usage
getNumeratorParts(cdcr, baseLearnerIndex = 1, boolean = TRUE)

Arguments
  cdcr A codacore object.
  baseLearnerIndex An integer indicating which of the (possibly multiple) log-ratios learned by co-
                   dacore to be used.
  boolean Whether to return the parts in boolean form (a vector of TRUE/FALSE) or to
           return the column names of those parts directly.

Value
  The covariates in the numerator of the selected log-ratio.
**getSlopes**

```
getSlopes
```

**Description**

getSlopes

**Usage**

```
getSlopes(cdcr)
```

**Arguments**

<table>
<thead>
<tr>
<th>cdcr</th>
<th>A codacore object</th>
</tr>
</thead>
</table>

**Value**

The slopes (i.e., regression coefficients) for each log-ratio.

---

**getNumLogRatios**

```
getNumLogRatios
```

**Description**

getNumLogRatios

**Usage**

```
getNumLogRatios(cdcr)
```

**Arguments**

<table>
<thead>
<tr>
<th>cdcr</th>
<th>A codacore object</th>
</tr>
</thead>
</table>

**Value**

The number of log-ratios that codacore found. Typically a small integer. Can be zero if codacore found no predictive log-ratios in the data.
getTidyTable

**Description**

getTidyTable

**Usage**

getTidyTable(cdc)

**Arguments**

- **cdcr** A codacore object

**Value**

A table displaying the log-ratios found.

---

**HIV Microbiome, HIV infection and MSM factor**

**Description**

A dataset containing the number of counts of 60 different genera in a group of 155 samples (including HIV - infected and non-infected patients). The data.frame is composed by 60 genera and two variables.

**Format**

The data.frame is composed by 60 genera and 2 variables

- **genera** The first 60 columns, from g_Prevotella until o_NB1-n_g_unclassified referred to different genera.

- **MSM** a factor determining if the individual is MSM (*Men Sex with Men*) or not (*nonMSM*).

- **HIV_Status** a factor specifying if the individual is infected (*Pos*) or not (*Neg*).

**References**

**plotROC**

Description

Plots a summary of a fitted codacore model. Credit to the authors of the selbal package (Rivera-Pinto et al., 2018), from whose package these plots were inspired.

Usage

```r
## S3 method for class 'codacore'
plot(x, index = 1, ...)
```

Arguments

- `x` A codacore object.
- `index` The index of the log-ratio to plot.
- `...` Not used.

**plotROC**

Description

`plotROC`

Usage

```r
plotROC(cdcdr)
```

Arguments

- `cdcr` A codacore object.
**predict.codacore**

**Description**

predict

**Usage**

```r
## S3 method for class 'codacore'
predict(object, newx, asLogits = TRUE, numLogRatios = NA, ...)
```

**Arguments**

- **object**: A codacore object.
- **newx**: A set of inputs to our model.
- **asLogits**: Whether to return outputs in logit space (as opposed to probability space). Should always be set to TRUE for regression with continuous outputs, but can be toggled for classification problems.
- **numLogRatios**: How many predictive log-ratios to include in the prediction. By default, includes the effects of all log-ratios that were obtained during training. Setting this parameter to an integer k will restrict to using only the top k log-ratios in the model.
- **...**: Not used.

**print.codacore**

**Description**

print

**Usage**

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

**Arguments**

- **x**: A codacore object.
- **...**: Not used.
Microbiome and sCD14 inflammation parameter

Description
A dataset containing the number of counts of 60 different genera in a group of 151 samples (including HIV-infected and non-infected patients). The data.frame is composed by 60 genera and a numeric variable

Format
The data.frame is composed by 60 genera and a variable

- genera The first 60 columns, from g_Prevotella until o_NB1-n_g_unclassified referred to different genera.
- sCD14 a numeric variable with the value of the inflammation parameter sCD14 for each sample.

References
doi: 10.1016/j.ebiom.2016.01.032

 simulateHTS

Description
This function simulates a set of (x, y) pairs. The covariates x are compositional, meaning they only carry relative information. The response y is a binary indicator. The rule linking x and y can be a balance or an amalgamation.

Usage
simulateHTS(n, p, outputType = "binary", logratio = "simple")

Arguments
- n Number of observations.
- p Number of covariates.
- outputType A string indicating 'binary' or 'continuous'.
- logratio A string indicating 'simple', 'balance', or 'amalgamation'.

Value
A list containing a matrix of inputs and a vector of outputs
Index

* data
  Crohn, 4
  FranzosaMetabolite, 5
  FranzosaMicrobiome, 5
  HIV, 9
  sCD14, 12

activeInputs.codacore, 2

codacore, 3
Crohn, 4
  FranzosaMetabolite, 5
  FranzosaMicrobiome, 5

getBinaryPartitions, 6
getDenominatorParts, 6
getLogRatios, 7
getNumeratorParts, 7
getNumLogRatios, 8
getSlopes, 8
getTidyTable, 9

HIV, 9

plot.codacore, 10
plotROC, 10
predict.codacore, 11
print.codacore, 11

sCD14, 12
simulateHTS, 12