Package ‘DirichletMultinomial’

December 12, 2023

Type Package

Title Dirichlet-Multinomial Mixture Model Machine Learning for Microbiome Data

Version 1.45.0

Author Martin Morgan <martin.morgan@roswellpark.org>

Maintainer Martin Morgan <martin.morgan@roswellpark.org>

Description Dirichlet-multinomial mixture models can be used to describe variability in microbial metagenomic data. This package is an interface to code originally made available by Holmes, Harris, and Quince, 2012, PLoS ONE 7(2): 1-15, as discussed further in the man page for this package, ?DirichletMultinomial.

License LGPL-3

Depends S4Vectors, IRanges

Imports stats4, methods, BiocGenerics

Suggests lattice, parallel, MASS, RColorBrewer, xtable


SystemRequirements gsl

biocViews ImmunoOncology, Microbiome, Sequencing, Clustering, Classification, Metagenomics

git_url https://git.bioconductor.org/packages/DirichletMultinomial

git_branch devel

git_last_commit db95280

git_last_commit_date 2023-10-24

Repository Bioconductor 3.19

Date/Publication 2023-12-12
DirichletMultinomial-package

Table of contents:

- DirichletMultinomial-package ........................................... 2
- cvdmngroup ................................................................. 3
- data .............................................................................. 4
- dmn ............................................................................. 5
- DMN-class ..................................................................... 6
- dmmgroup ..................................................................... 7
- DMNGroup-class ............................................................. 8
- heatmapdmn ................................................................. 9
- model components ....................................................... 10
- roc ................................................................................. 11
- Utilities ........................................................................ 13

Index .................................................................................. 15

DirichletMultinomial-package

Dirichlet-Multinomial Mixture Model Machine Learning for Microbiome Data

Description

Dirichlet-multinomial mixture models can be used to describe variability in microbial metagenomic data. This package is an interface to code originally made available by Holmes, Harris, and Quince, 2012, PLoS ONE 7(2): 1-15.

Details

The estimation routine is from the LGPL-licensed (as stated on the corresponding googlecode page) source http://microbedmm.googlecode.com/files/MicrobeDMMv1.0.tar.gz, retrieved 17 February 2012.


Author(s)

Maintainer: Martin Morgan mailto:mtmorgan@fhcrc.org
Cross-validation on Dirichlet-Multinomial classifiers.

Description

Run cross-validation on Dirichlet-Multinomial generative classifiers.

Usage

\texttt{cvdmngroup(ncv, count, k, z, ..., verbose = FALSE, .lapply = \text{parallel::mclapply})}

Arguments

- \texttt{ncv}\hspace{1em}integer(1) number of cross-validation groups, between 2 and \text{nrow(count)}.
- \texttt{count}\hspace{1em}matrix of sample x taxon counts, subsets of which are used for training and cross-validation.
- \texttt{k}\hspace{1em}named integer() vector of groups and number of Dirichlet components; e.g., \text{c(Lean=1, Obese=3)} performs cross-validation for models with \text{k=1} Dirichlet components for the ‘Lean’ group, \text{k=3} Dirichlet components for ‘Obese’.
- \texttt{z}\hspace{1em}True group assignment.
- \texttt{...}\hspace{1em}Additional arguments, passed to \texttt{dmn} during each cross-validation.
- \texttt{verbose}\hspace{1em}logical(1) indicating whether progress should be reported
- \texttt{.lapply}\hspace{1em}A function used to perform the outer cross-validation loop, e.g., \text{lapply} for calculation on a single processor, \text{parallel::mclapply} for parallel evaluation.

Value

A \text{data.frame} summarizing classifications of test samples in cross-validation groups. Columns are:

- \texttt{group}\hspace{1em}The cross-validation group in which the individual was used for testing.
- \texttt{additional columns}\hspace{1em}Named after classification groups, giving the posterior probability of assignment.

Author(s)

Martin Morgan \mailto{mtmorgan@fhcrc.org}

See Also

\texttt{dmn}, \texttt{DirichletMultinomial-package}, \texttt{vignette("DirichletMultinomial")}
Examples

data(xval)  ## result of following commands
head(xval)

## Not run:
## count matrix
fl <- system.file(package="DirichletMultinomial", "extdata",
                  "Twins.csv")
count <- t(as.matrix(read.csv(fl, row.names=1)))

## phenotype
fl <- system.file(package="DirichletMultinomial", "extdata",
                  "TwinStudy.t")
pheno0 <- scan(fl)
lvls <- c("Lean", "Obese", "Overwt")
pheno <- factor(lvls[pheno0 + 1], levels=lvls)
names(pheno) <- rownames(count)

## subset
keep <- c("Lean", "Obese")
count <- count[pheno]
pheno <- factor(pheno[pheno]

## cross-validation, single Dirichlet component for Lean, 3 for Obese
xval <- cvdmngroup(nrow(count), count, c(Lean=1, Obese=3), pheno,
                   verbose=TRUE, mc.preschedule=FALSE)

## End(Not run)

Data objects used for examples and the vignette

Description

These data objects correspond to steps in a typical work flow, as described in the vignette to this package. fit corresponds to dmn fits to different values of k. bestgroup is the result of the two-group generative classifier. xval summarizes leave-one-out cross validation of the classifier.

Usage

data(fit)
data(bestgrp)
data(xval)

Format

fit is a list of seven DMN objects.
bestgrp is a DMNGroup object.
xval is a data.frame with columns corresponding to the cross-validation group membership and the Lean and Obese posterior probabilities.
Fit Dirichlet-Multinomial models to count data.

Description

Fit Dirichlet-Multinomial models to a sample x taxon count matrix.

Usage

dmn(count, k, verbose = FALSE, seed = runif(1, 0, .Machine$integer.max))

Arguments

count: matrix() of sample x taxon counts.
k: integer(1), the number of Dirichlet components to fit.
verbose: logical(1) indicating whether progress in fit should be reported.
seed: numeric(1) random number seed.

Details

This implements Dirichlet-multinomial mixture models describe in the package help page, DirichletMultinomial-package.

Value

An object of class dmn, with elements (elements are usually retrieved via functions defined in the package, not directly).

Group: matrix of dimension samples x k, providing the Dirichlet parameter vectors.
Mixture: Weight numeric() of length k, with relative weight of each component.
Fit: Lower matrix() of dimension taxa x k with 95% lower bounds on Dirichlet component vector estimates.
Estimate: matrix() of dimension taxa x k with Dirichlet component vector estimates.
Upper: matrix() of dimension taxa x k with 95% upper bounds on Dirichlet component vector estimates.

Author(s)

Martin Morgan mailto:mtmorgan@fhcrc.org
References


See Also

DirichletMultinomial-package, vignette("DirichletMultinomial")

Examples

data(fit)
## k = 1:7; full example in vignette
lplc <- sapply(fit, laplace)
plot(lplc, type="b")
fit[[which.min(lplc)]]

DMN-class

Class "DMN"

Description

Result from fitting a Dirichlet-Multinomial model.

Objects from the Class

Objects can be created by calls to dmn.

Slots

The contents of a slot is usually retrieved via the methods described on the mixture help page.

goodnessOfFit NLE, LogDet, Laplace, AIC, and BIC criteria assessing goodness-of-fit.

group matrix of dimension samples x k, providing the Dirichlet parameter vectors.
mixture Weight numeric() of length k, with relative weight of each component.

fit Lower matrix() of dimension taxa x k with 95% lower bounds on Dirichlet component vector estimates.

Estimate matrix() of dimension taxa x k with Dirichlet component vector estimates.

Upper matrix() of dimension taxa x k with 95% upper bounds on Dirichlet component vector estimates.

Methods

See the mixture help page.

Author(s)

Martin Morgan mailto:mtmorgan@fhcrc.org
dmngroup

See Also
dmn, mixture.

Examples
data(fit)
fit[[4]]

---

dmngroup     *Dirichlet-Multinomial generative classifiers.*

Description
Fit Dirichlet-Multinomial generative classifiers to groups (rows) within a sample x taxon count matrix.

Usage
dmngroup(count, group, k, ..., simplify = TRUE,
          .lapply = parallel::mclapply)

Arguments
count     matrix() of sample x taxon counts.
group     factor() or vector to be coerced to a factor, with as many elements as there are rows in count, indicating the group to which the corresponding sample belongs.
k         integer(), the number(s) of Dirichlet components to fit.
...        Additional arguments, passed to dmn.
simplify Return only the best-fit model for each group?
          .lapply An lapply-like function for application of group x k fits.

Details
This function divided count into groups defined by group, creates all combinations of group x k, and evaluates each using dmn. When simplify=TRUE, the best (Laplace) fit is selected for each group.

Value
An object of class dmngroup, a list of fitted models of class dmn. When simplify=TRUE, elements are named by the group to which they correspond.

Author(s)
Martin Morgan mailto:mtmorgan@fhcrc.org
References


See Also
dmn, DirichletMultinomial-package, vignette("DirichletMultinomial")

Examples

```r
## best fit for groups 'Lean' and 'Obese'; full example in vignette.
## Not run: bestgrp <- dmngroup(count, pheno, k=1:5, verbose=TRUE, 
##       mc.preschedule=FALSE)

## End(Not run)
data(bestgrp)
bestgrp
bestgrp[["Obese"]]
```

---

**DMNGroup-class**

**Class** "DMNGroup"

**Description**

Result from fitting a Dirichlet-Multinomial generative classifier.

**Objects from the Class**

Objects can be created by calls to `dmngroup`.

**Slots**

All slots in this class are inherited from `SimpleList`; see 'Methods', below, for information on how to manipulate this object.

**Extends**


**Methods**

See the `mixture` help page for functions that operate on DMNGroup and DMN.

DMNGroup can be manipulated as a list; see `SimpleList` for a description of typical list-like functions.

**Author(s)**

Martin Morgan mailto:mtmorgan@fhcrc.org
See Also
mixture, DMN, SimpleList.

Examples
```
data(bestgrp)
bestgrp
bestgrp[[1]]
```

```
<table>
<thead>
<tr>
<th>heatmapdmn</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Heatmap representation of samples assigned to Dirichlet components.</td>
</tr>
</tbody>
</table>

Description
Produce a heat map summarizing count data, grouped by Dirichlet component.

Usage
```
heatmapdmn(count, fit1, fitN, ntaxa = 30, ..., 
            transform = sqrt, lblwidth = 0.2 * nrow(count), col = .gradient)
```

Arguments
- **count**: A matrix of sample x taxon counts, as supplied to `dmn`.
- **fit1**: An instance of class `dmn`, from a model fit to a single Dirichlet component, \( k=1 \) in `dmn`.
- **fitN**: An instance of class `dmn`, from a model fit to \( N \neq 1 \) components, \( k=N \) in `dmn`.
- **ntaxa**: The `ntaxa` most numerous taxa to display counts for.
- **...**: Additional arguments, ignored.
- **transform**: Transformation to apply to count data prior to visualization; this does not influence mixture membership or taxonomic ordering.
- **lblwidth**: The proportion of the plot to dedicate to taxonomic labels, as a fraction of the number of samples to be plotted.
- **col**: The colors used to display (possibly transformed, by `transform`) count data, as used by `image`.

Details
Columns of the heat map correspond to samples. Samples are grouped by Dirichlet component, with average (Dirichlet) components summarized as a separate wide column. Rows correspond to taxonomic groups, ordered based on contribution to Dirichlet components.

Author(s)
Martin Morgan `mailto:mtmorgan@fhcrc.org`
Examples

```r
## counts
fl <- system.file(package="DirichletMultinomial", "extdata", "Twins.csv")
count <- t(as.matrix(read.csv(fl, row.names=1)))

## all and best-fit clustering
data(fit)
lplc <- sapply(fit, laplace)
best <- fit[[which.min(lplc)]]

heatmapdmn(count, fit[[1]], best, 30)
```

Description

The accessors `mixture` and `mixturewt` return information about the estimated Dirichlet components of the fitted model. Return values are described in the Values section, below.

Usage

```r
mixture(object, ..., assign=FALSE)
mixturewt(object, ...)
goodnessOfFit(object, ...)
laplace(object, ...)  
## S4 method for signature 'DMN'
AIC(object, ..., k = 2) 
## S4 method for signature 'DMN'
BIC(object, ...)

## S4 method for signature 'DMN'
fitted(object, ..., scale=FALSE) 
## S4 method for signature 'DMN'
predict(object, newdata, ..., logevidence=FALSE) 
## S4 method for signature 'DMNGroup'
fitted(object, ...) 
## S4 method for signature 'DMNGroup'
predict(object, newdata, ..., assign=FALSE) 
## S4 method for signature 'DMNGroup'
summary(object, ...)
```

Arguments

- `object` An instance of class `dmn`.
- `newdata` A matrix of new sample x taxon data to be fitted to the model of `object`. 
roc

... Additional arguments, available to methods, when applicable.

assign logical(1) indicating whether the maximum per-sample mixture component should be returned (assign=FALSE), or the full mixture matrix (assign=TRUE).

scale logical(1) indicating whether fitted values should be returned unscaled (default, scaled=FALSE) or scaled by the variability of mixturewt parameter theta.

logevidence logical(1) indicating whether posterior probability (default, logevidence=FALSE) or log evidence logical=TRUE should be returned.

k ignored.

Value

mixture with assign=FALSE returns a matrix of sample x Dirichlet component estimates. With assign=TRUE mixture returns a named vector indexing the maximal Dirichlet component of each sample.

mixturewt returns a matrix with rows corresponding to mixture components, and columns pi (component weight) and theta (component variability). Small values of theta correspond to highly variable components.

goodnessOfFit returns a named numeric vector of measures of goodness of fit.

laplace, AIC, and BIC return the corresponding measures of goodness of fit.

Author(s)

Martin Morgan mailto:mtmorgan@fhcrc.org

Examples

data(fit)
best <- fit[[4]]
mixturewt(best)
head(mixture(best), 3)
head(mixture(best, assign=TRUE), 3)
goodnessOfFit(best)

fl <- system.file(package="DirichletMultinomial", "extdata", "Twins.csv")

count <- t(as.matrix(read.csv(fl, row.names=1)))
data(bestgrp)
bestgrp
head(predict(bestgrp, count))

roc Summarize receiver-operator characteristics

Description

Returns a data.frame summarizing the cummulative true- and false-positive probabilities from expected and observed classifications.
Usage

roc(exp, obs, ...)

Arguments

exp logical() vector of expected classifications to a particular group.
obs Predicted probability of assignment to the group identified by TRUE values in exp. The length of exp and obs must be identical.
...
Additional arguments, available to methods.

Value

A data.frame with columns

TruePositive Cummulative probability of correct assignment.
FalsePositive Cummulative probability of incorrect assignment.

Author(s)

Martin Morgan mailto:mtmorgan@fhcrc.org

Examples

library(lattice)

## count matrix
fl <- system.file(package="DirichletMultinomial", "extdata", "Twins.csv")
count <- t(as.matrix(read.csv(fl, row.names=1)))

## phenotype
fl <- system.file(package="DirichletMultinomial", "extdata", "TwinStudy.t")
pheno0 <- scan(fl)
lvls <- c("Lean", "Obese", "Overwt")
pheno <- factor(lvls[pheno0 + 1], levels=lvls)
names(pheno) <- rownames(count)

## count data used for cross-validation, and cross-validation
count <- csubset(c("Lean", "Obese"), count, pheno)
data(bestgrp)

## true, false positives from single-group classifier
bst <- roc(pheno[rownames(count)] == "Obese",
predict(bestgrp, count)[,"Obese"])
head(bst)

## lattice plot
xyplot(TruePostive ~ FalsePositive, bst, type="l",
  xlab="False Positive", ylab="True Positive")
Utilities

Helpful utility functions

Description

csubset creates a subset of a count matrix, based on identity of column phenotypes to a specified value.

Usage

csubset(val, x, pheno, cidx = TRUE)

Arguments

val character(1) specifying the subset of phenotype to select.

x A matrix of counts, with rows corresponding to samples and columns to taxonomic groups.

pheno A character() vector of length equal to the number of rows in count, indicating the phenotype of the corresponding sample.

cidx A logical(1) indicating whether columns (taxa) with zero counts in the count matrix following removal of taxa not satisfying pheno %in% val should be removed. cidx=FALSE removes the 0-count columns.

Value

A matrix of counts, with rows satisfying pheno %in% val and with columns equal either to ncol(x) (when cidx=TRUE) or the number of columns with non-zero counts after row subsetting (cidx=FALSE).

Author(s)

Martin Morgan mailto:mtmorgan@fhcrc.org

Examples

## count matrix
fl <- system.file(package="DirichletMultinomial", "extdata", "Twins.csv")
count <- t(as.matrix(read.csv(fl, row.names=1)))

## phenotype
fl <- system.file(package="DirichletMultinomial", "extdata", "TwinStudy.t")
pheno0 <- scan(fl)
lvls <- c("Lean", "Obese", "Overwt")
pheno <- factor(lvls[pheno0 + 1], levels=lvls)
names(pheno) <- rownames(count)

## subset
dim(count)
sum("Lean" == pheno)
dim(csubset("Lean", count, pheno))
dim(csubset("Lean", count, pheno, cidx=FALSE))
Index

* classes
  DMN-class, 6
  DMNGroup-class, 8
* datasets
  data, 4
* manip
  dmn, 5
  dmngroup, 7
  heatmapdmn, 9
  model components, 10
  Utilities, 13
* package
  DirichletMultinomial-package, 2
* stats
  cvdmngroup, 3
  roc, 11
  AIC, DMN-method (model components), 10
  Annotated, 8
  bestgrp (data), 4
  BIC, DMN-method (model components), 10
  csubset (Utilities), 13
  cvdmngroup, 3
  data, 4
  DirichletMultinomial-package, 2, 3, 5, 6, 8
  DMN, 4, 9
  dmn, 3, 5, 6–10
  DMN-class, 6
  DMNGroup, 4
  dmngroup, 7, 8
  DMNGroup-class, 8

  fit (data), 4
  fitted, DMN-method (model components), 10
  fitted, DMNGroup-method (model components), 10
  goodnessOfFit (model components), 10
  heatmapdmn, 9
  image, 9
  laplace (model components), 10
  List, 8
  mixture, 6–9
  mixture (model components), 10
  mixturewt, 11
  mixturewt (model components), 10
  model components, 10
  predict, DMN-method (model components), 10
  predict, DMNGroup-method (model components), 10
  roc, 11
  show, DMN-method (model components), 10
  show, DMNGroup-method (model components), 10
  SimpleList, 8, 9
  summary, DMNGroup-method (model components), 10
  Utilities, 13
  Vector, 8
  xval (data), 4