Package ‘DirichletMultinomial’

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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 This package is an interface to code originally made available by Holmes, Harris, and Quince, 2012, PLoS ONE 7(2): 1-15, as discussed further in the man page for this package, ?DirichletMultinomial.
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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 This package is an interface to code originally made available by Holmes, Harris, and Qunice, 2012, PLoS ONE 7(2): 1-15.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
**cvdmngroup**  
*Cross-validation on Dirichlet-Multinomial classifiers.*

**Description**
Run cross-validation on Dirichlet-Multinomial generative classifiers.

**Usage**

```
cvdmngroup(ncv, count, k, z, ..., verbose = FALSE,  
.lapply = parallel::mclapply)
```

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

**Value**
A `data.frame` summarizing classifications of test samples in cross-validation groups. Columns are:
- `group` The cross-validation group in which the individual was used for testing.
- `additional columns` Named after classification groups, giving the posterior probability of assignment.

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

**See Also**
`dmn`, `DirichletMultinomial-package`, 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 <- cvdmgroup(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 workflow, 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.
Examples

data(fit); fit[1:2]
plot(sapply(fit, laplace), type="b")
data(bestgrp); bestgrp
data(xval); head(xval, 3)

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).

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.

Author(s)

Martin Morgan mailto:mtmorgan@fhcrc.org
References

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

Examples
```r
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

```r
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 divides 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

## 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]]

heatmapdmn        *Heatmap representation of samples assigned to Dirichlet components.*

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 != 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`. 
... 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)**

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**Examples**

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

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

---

**roc**

*Summarize receiver-operator characteristics*

**Description**

Returns a `data.frame` summarizing the cumulative 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(TruePositive ~ 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)
levels <- c("Lean", "Obese", "Overwt")
pheno <- factor(levels[pheno0 + 1], levels=levels)
names(pheno) <- rownames(count)

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