Package ‘DirichletReg’

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Description

This package provides a functions to analyze compositional data using Dirichlet regression methods.

| Package: | DirichletReg |
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Author(s)

Marco J. Maier

Examples

```r
example(plot.DirichletRegData)
example(DirichReg)
```

anova.DirichletRegModel

*Compare Dirichlet Regression Models using an LRT*
Description

This function allows for pairwise tests of Dirichlet regression models using a likelihood ratio test (LRT).

Usage

```r
## S3 method for class 'DirichletRegModel'
anova(object, ..., sorted = FALSE)
```

Arguments

- `object`: the model to be compared against those listed in ...
- `...`: models to be tested against the one specified as `object`
- `sorted`: should the models be sorted according to their numbers or parameters?

Details

The test statistic is computed $LR = -2 \log(L_a) - \log(L_b)$ where $L_i$ is the likelihood of model $i$ with $df$ equal to the difference of the number of parameters in the models.

Author(s)

Marco J. Maier

Examples

```r
ALake <- ArcticLake
ALake$AL <- DR_data(ArcticLake[,1:3])
mod0 <- DirichReg(AL ~ 1, ALake)
mod1 <- DirichReg(AL ~ depth, ALake)
mod2 <- DirichReg(AL ~ depth + 1(depth^2), ALake)
anova(mod1, mod0, mod2, sorted = TRUE)
```

ArcticLake

**Arctic Lake Data (Aitchison)**

Description

These data are taken from Aitchison (2003) and contain information on the relation of sediment composition with depth in an Arctic lake.

Usage

ArcticLake
**BloodSamples**

**Format**

A data frame with 39 observations on the following 4 variables:

- sand, silt, clay  relative frequencies of sand, silt, and clay
- depth  water depth in meters

**Source**


**Examples**

```r
head(BloodSamples)
res <- data.frame(BloodSamples[,1:3])
plot(res)
speed(res)
```

---

**BloodSamples**  
*Serum Protein Composition in Blood Samples*

**Description**

These data (Aitchison, 2003) list blood samples’ compositions of *Albumin*, *Pre-Albumin*, *Globulin A*, and *Globulin B* in relation to two types of diseases. 14 patients suffer from disease A, 16 from disease B and 6 are unclassified.

**Usage**

BloodSamples

**Format**

A data frame with 36 observations on the following 6 variables.

- Disease  diagnosis of disease A, B, or NA for unclassified observations.
- New  a factor indicating whether the observations are old and classified (No) or new and unclassified (Yes).

**Source**

**Dirichlet**

**Examples**

```r
defineBloodSamples()
Bl <- DR_data(BloodSamples[,1:4])
summary(Bl)
```

---

**The Dirichlet Distribution**

**Description**

Density function and random number generation for the Dirichlet distribution

**Usage**

```r
rdirichlet(n, alpha)
ddirichlet(x, alpha, log = FALSE, sum.up = FALSE)
ddirichlet_R(x, alpha, log = FALSE, sum.up = FALSE)
```

**Arguments**

- `n`: number of random observations to draw
- `x`: a matrix containing observations
- `alpha`: the Dirichlet distribution’s parameters. Can be a vector (one set of parameters for all observations) or a matrix (a different set of parameters for each observation), see “Details”
- `log`: if TRUE, logarithmic densities are returned
- `sum.up`: if TRUE, the (log-)likelihood is returned

**Details**

The Dirichlet distribution is a multidimensional generalization of the Beta distribution where each dimension is governed by an $\alpha$-parameter. Formally this is

$$D(\alpha_i) = \left[ \prod_i \Gamma(\alpha_i) \right] \prod_i y_i^{\alpha_i-1}$$

Usually, `alpha` is a vector thus the same parameters will be used for all observations. If `alpha` is a matrix, a complete set of $\alpha$-parameters must be supplied for each observation.

`log` returns the logarithm of the densities (therefore the log-likelihood) and `sum.up` returns the product or sum and thereby the likelihood or log-likelihood.

Dirichlet (log-)densities are by default computed using C-routines (`ddirichlet_log_vector` and `ddirichlet_log_matrix`), a version only using R is provided by `ddirichlet_R`. Caution: Although `.C()` can be used to call the C routines directly, R will crash or produce wrong values, if, e.g., data types are not set properly.
Value

\texttt{rdirichlet} returns a matrix with random numbers according to the supplied alpha vector or matrix.

\texttt{ddirichlet} returns a vector of densities (if \texttt{sum.up} = \texttt{FALSE}) or the (log-)likelihood (if \texttt{sum.up} = \texttt{TRUE}) for the given data and alphas.

\texttt{ddirichlet}\_R as \texttt{ddirichlet}, only implemented purely in R.

Author(s)

Marco J. Maier

Examples

\begin{verbatim}
xQ <- rdirichlet(100, c(5, 5, 10))
amat <- cbind(1:10, 5, 10:1)
amat
X2 <- rdirichlet(10, a.mat)
# note how the probabilities in the first an last column relate to a.mat
round(X2, 2)
ddirichlet(xQ, c(5, 5, 10))
ddirichlet(xQ, a.mat)
\end{verbatim}

DirichletRegData  
Prepare Compositional Data

Description

This function prepares a matrix with compositional variables for further processing in the \texttt{DirichletReg} package.

Usage

\begin{verbatim}
DR\_data(Y, trafo = \texttt{sqrt(.Machine$double.eps)}, base = 1,
norm_tol = \texttt{sqrt(.Machine$double.eps)})

## S3 method for class 'DirichletRegData'
print(x, type = c("processed", "original"), ...)

## S3 method for class 'DirichletRegData'
summary(object, ...)
\end{verbatim}
DirichletRegData

Arguments

**Y**  
A matrix or data.frame with nonnegative values of all compositional variables (in some cases, a vector is also permissible, see “Details”).

**trafo**  
Either a logical or numeric value. Transformation of variables causes the values to shrink away from extreme values of 0 and 1, see “Details”.
If logical, it will force (TRUE) or suppress (FALSE) transformation. Suppressing transformation in the presence of extreme values (0 and 1) will result in an error.  
If trafo is numeric it is used as a “threshold”, so transformation will be applied if values in Y are $y < trafo$ or $y > (1 - trafo)$.

**base**  
The “base” component to use in the reparametrized model

**norm_tol**  
Due to numerical precision, row sums of $Y$ may not be exactly equal to 1. Therefore, norm_tol is a small non-negative value (default: $\sqrt{\text{Machine\_double\_eps}}$) which represents the tolerance when testing for “near equality” to 1 (see all.equal).

**x**  
A DirichletRegData object

**type**  
Displays either the (possibly normalized or transformed) "processed" or "original" data

**object**  
A DirichletRegData object

...  
Further arguments

Details

**Y:**
Y is a matrix or data.frame containing compositional variables. If they do not sum up to 1 for all observations, normalization is forced where each row entry is divided by the row’s sum (a warning will be issued that normalization was applied).
In case one row-entry (or more) is NA, the whole row will be returned as NA. Beta-distributed variables can be supplied as a single vector which, however, has to have values in the interval [0, 1]. The second variable will be generated ($1 - Y$) and a matrix consisting of the columns $1 - Y$ and $Y$ will be returned. A message will be issued that a beta-distributed variable was assumed and that this assumtion needs to be checked.

**trafo:**
The transformation (done if trafo = TRUE) is a generalization of that proposed by Smithson and Verkuilen (2006) that transforms each component $y$ of $Y$ by computing $y^* = \frac{y(n-1)+\frac{1}{2}}{n}$ where $n$ is the number of observations in $Y$ (this approach is also used in the package betareg, see Cribari-Neto & Zeileis, 2010).
For an arbitrary number of dimensions (or variables) $d$ the transformation is $y^* = \frac{y(n-1)+\frac{1}{2}}{n}$.

**base:**
To set the base (i.e., omitted) component of $Y$ for the “alternative” (mean/precision) model, the argument base can be used. This is by default set to the first variable in $Y$ (if a vector is be supplied, the column $1 - Y$ becomes the base component).  
Note that the definition can be overruled in DirichReg.

**x and object:**
Objects created by DR_data.
type:
specifies for the print method whether the original or processed data are displayed.

Value

The function returns a matrix object of class DirichletRegData with the following attributes:

- `attr(*, "dimnames")`: a list with two entries, row names (by default NULL) and column names.
- `attr(*, "Y.original")`: the original data
- `attr(*, "dims")`: number of dimensions of Y (i.e., number of columns)
- `attr(*, "dim.names")`: the number of components in Y
- `attr(*, "obs")`: number of observations of Y (i.e., number of rows)
- `attr(*, "valid_obs")`: number of valid observations
- `attr(*, "normalized")`: a logical value indicating whether the data were normalized
- `attr(*, "transformed")`: a logical value indicating whether the data were transformed
- `attr(*, "base")`: number of the variable used as the base in the reparametrized model

Author(s)

Marco J. Maier

References


Examples

```r
# create a DirichletRegData object from the Arctic Lake data
head(ArcticLake[, 1:3])
AL <- DR_data(ArcticLake[, 1:3])
summary(AL)
head(AL)
```
**Description**

These are available methods for the results of Dirichlet regression models and objects of class DirichletRegModel. These methods contain functions for print and summary of the data, generate fitted values and predicting new values using predict. Various types of residuals are implemented and confint can be used to compute confidence intervals of the parameters. Furthermore logLik extracts the log-likelihood of the model and vcov extracts the covariance matrix of the parameter estimates.

**Usage**

```r
## S3 method for class 'DirichletRegModel'
print(x, digits = max(3,getOption("digits") - 3), ...)

## S3 method for class 'DirichletRegModel'
summary(object, ...)

## S3 method for class 'DirichletRegModel'
fitted(object, mu = TRUE, alpha = FALSE, phi = FALSE, ...)

## S3 method for class 'DirichletRegModel'
predict(object, newdata, mu = TRUE, alpha = FALSE, phi = FALSE, ...)

## S3 method for class 'DirichletRegModel'
residuals(object, type = c("standardized", "composite", "raw"), ...)

## S3 method for class 'DirichletRegModel'
confint(object, parm, level, ..., type=c("all", "beta", "gamma"), exp = FALSE)

## S3 method for class 'DirichletRegConfint'
print(x, digits = 3, ...)

## S3 method for class 'DirichletRegModel'
logLik(object, ...)

## S3 method for class 'DirichletRegModel'
AIC(object, ..., k = 2)

## S3 method for class 'DirichletRegModel'
BIC(object, ...)

## S3 method for class 'DirichletRegModel'
nobs(object, ...)
```
## S3 method for class 'DirichletRegModel'
vcov(object, ...)

## S3 method for class 'DirichletRegModel'
update(object, formula, ..., evaluate = TRUE)

## S3 method for class 'DirichletRegModel'
drop1(object, scope, test = c("LRT", "none"), k = 2, ...)

**Arguments**

- `x`: an object of class `DirichletRegModel`
- `object`: an object of class `DirichletRegModel` or `DirichletRegConfint` for printing
- `alpha`: logical; returns alpha values
- `mu`: logical; returns expected values
- `phi`: logical; returns precision values
- `type`: for residuals: defines the type of residuals to be computed ("standardized" (i.e., Pearson), "composite", or "raw")
  - for `confint`: defines the type of parameter ("all", "beta", or "gamma") for which confidence values are returned
- `newdata`: a data.frame containing new observations
- `k`: number for the weighting of parameters
- `parm`: a vector containing names of the parameters to print
- `level`: (a vector of) confidence level(s), defaults to .95
- `exp`: logical; returns parameters in exponentiated form
- `digits`: the number of digits in the output
- `formula`: the new formula to be updated, see `update.Formula`
- `evaluate`: if FALSE the updated call will be returned, but not evaluated
- `scope`: defines the scope of variables to be dropped, see `drop1`
- `test`: defines the type of test for `drop1`
- `...`: further arguments

**Author(s)**

Marco J. Maier

**Examples**

```r
ALake <- ArcticLake
ALake$AL <- DR_data(ArcticLake[, 1:3])

mod1 <- DirichReg(AL ~ depth + I(depth^2) | depth, data = ALake, model="alternative")

update(mod1, . ~ . | . + I(depth^2), evaluate = FALSE)
```
mod1

drop1(mod1)  ### issues a caveat when used for the first time in an R session
summary(mod1)

head(fitted(mod1))
predict(mod1, newdata = data.frame("depth" = seq(10, 100, 10)))

head(residuals(mod1))
confint(mod1)
confint(mod1, exp = TRUE)

logLik(mod1)
round(vcov(mod1), 5)

---

**DirichReg**

*Fitting a Dirichlet Regression*

**Description**

This function allows for fitting Dirichlet regression models using two different parametrizations.

**Usage**

```r
DirichReg(formula, data, model = c("common", "alternative"),
          subset, sub.comp, base, weights, control, verbosity = 0)
```

**Arguments**

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>formula</td>
<td>the model formula (for different specifications see “Details”)</td>
</tr>
<tr>
<td>data</td>
<td>a data.frame containing independent and dependent variables</td>
</tr>
<tr>
<td>model</td>
<td>specifies whether the &quot;common&quot; (αs) or &quot;alternative&quot; (μ/φ) parametrization</td>
</tr>
<tr>
<td></td>
<td>is employed (see “Details”)</td>
</tr>
<tr>
<td>subset</td>
<td>estimates the model for a subset of the data</td>
</tr>
<tr>
<td>sub.comp</td>
<td>analyze a subcomposition by selecting specific components (see “Details”)</td>
</tr>
<tr>
<td>base</td>
<td>redefine the base variable</td>
</tr>
<tr>
<td>weights</td>
<td>frequency weights</td>
</tr>
<tr>
<td>control</td>
<td>a list containing control parameters used for the optimization</td>
</tr>
<tr>
<td>verbosity</td>
<td>prints information about the function’s progress, see Details</td>
</tr>
</tbody>
</table>
Details

**Formula Specification and Models:** formula determines the used predictors. The responses must be prepared by DR_data and can be optionally stored in the object containing all covariates which is then specified as the argument data. (Although “on-the-fly” processing of DR_data in a formula works, it is only intended for testing purposes and may be removed at any time – use at your own risk.)

There are two different parametrization (controlled by the argument model, see below):

- the “common” param. that models each \( \alpha \) by an (possibly individual) set of predictors, and
- the “alternative” param. that models expected values (\( \mu \); as in multinomial logistic regression) and precision parameters (\( \phi \)) with two sets of predictors.

As the two models offer different modeling strategies, the specification of their formulae differ:

**Formulae for the “Common” Model:** The simplest possible model here is to include only an intercept for all components. If \( DV \) is the ‘dependent variable’ (i.e., compositional data) with three components, we can request this null-model by \( DV \sim 1 \). We always have at least two dependent variables, so simple formulae as the one given above will be expanded to \( DV \sim 1 \mid 1 \mid 1 \), because \( DV \) hast three components. Likewise, it is possible to specify a common set of predictors for all components, as in \( DV \sim pQ \ast pR \), where \( pQ \) and \( pR \) are predictors.

If the covariates of the components shall differ, one has to set up a complete formula for each subcomposition, using | as separators between the components, for example, \( DV \sim p1 \mid p1 + p2 \mid p1 \ast p2 \) will lead to a model where the first response in \( DV \) will be modeled using \( p1 \), the second will be predicted by \( p1 + p2 \) and the third by \( p1 \ast p2 \). Note that if you use the latter approach, the predictors have to be stated explicitly for all response variables.

**Formulae for the “Alternative” Model:** The simplest possible model here is to include an intercept for all components (except the base) and an intercept for precision. This can be achieved by \( DV \sim 1 \), which is expanded to \( DV \sim 1 \mid 1 \). The part modeling the ‘mean’ (first element on the right-hand side) is mandatory, if no specification for precision is included, an intercept will be added. Note that you need to set model = “alternative” to use this parametrization!

The alternative parametrization consists of two parts: modeled expected values (\( \mu \)) and their ‘precision’ (\( \phi \)). As in multinomial logistic regression, one response variable is omitted (by default the first, but this can be changed by the base argument in DR_data or DirichReg) and for the rest a set of predictors is used with a multinomial logit-link. For precisions, a different set of predictors can be set up using a log-link. \( DV \sim p1 \ast p2 \mid p1 + p2 \) will set up a model where the expected values are predicted by \( p1 \ast p2 \) and precision are modeled using \( p1 + p2 \).

**Data Preparation:** The data argument accepts a data.frame that must include the dependent variable as a named element (see examples how to do this).

**Changing the Base Component and Analyzing Subcompositions:** The base-component (i.e., omitted component) is initially set during the stage of data preparation DR_data, but can easily be changed using the argument base which takes integer values from 1 to the maximum number of components.

If a data set contains a large number of components, of which only a few are relevant, the latter can be ‘sorted out’ and the irrelevant (i.e., not selected) components will be aggregated into a single variable (row sums) that automatically becomes the base category for the model, unless specified otherwise by base. The positioning of variables will necessarily change: the aggregated variable takes the first column and the others are appended in their order of selection.
Subsets and Weights: Using subset, the model can be fitted only to a part of the data, for more information about this functionality, see subset. Note that, unlike in glm, weights are not treated as prior weights, but as frequency weights!

Optimization and Verbosity: Using the control argument, the settings passed to the optimizers can be altered. This argument takes a named list. To supply user-defined starting values, use control = list(sv=c(...)) and supply a vector containing initial values for all parameters. Optimizer-specific options include the number of iterations (iterlim = 1000) and convergence criteria for the BFGS- and NR-optimization ((tol1 = 1e-5) and (tol2 = 1e-10)). Verbosity takes integer values from 0 to 4. 0, no information is printed (default). 1 prints information about 3 stages (preparation, starting values, estimation). 2 prints little information about optimization (verbosity values greater than one are passed to print.default = verbosity - 1 of maxBFGS and maxNR). 3 prints more information about optimization. 4 prints all information about optimization.

Value

- call [language] function call
- parametrization [character] used parametrization
- varnames [character] components’ names
- n.vars [numeric] vector with the number of parameters per set of predictors
- dims [numeric] number of components
- Y [numeric] used components
- X [numeric list] sets of predictors
- Z [numeric list] sets of predictors (only for the alternative parametrization)
- sub.comp [numeric] vector of single components
- base [numeric] base (only for the alternative parametrization)
- weights [numeric] vector of frequency weights
- orig.resp [DirichletRegData] the original response
- data [data.frame] original data
- d [data.frame] used data
- formula [Formula] expanded formula
- mf_formula [language] expression for generating the model frame
- npar [numeric] number of parameters
- coefficients [numeric] named vector of parameters
- coefnames [character] names of the parameters
- fitted.values [list of matrices] list containing alpha’s, mu’s, phi’s for the observations
- logLik [numeric] the log-likelihood
- vcov [matrix] covariance-matrix of parameter estimates
- hessian [matrix] (observed) Hessian
- se [numeric] vector of standard errors
- optimization [list] contains details about the optimization process provided by maxBFGS and maxNR
Author(s)

Marco J. Maier

Examples

```R
ALake <- ArcticLake
ALake$Y <- DR_data(ALake[,1:3])

# fit a quadratic Dirichlet regression models ("common")
res1 <- DirichReg(Y ~ depth + I(depth^2), ALake)

# fit a Dirichlet regression with quadratic predictor for the mean and
# a linear predictor for precision ("alternative")
res2 <- DirichReg(Y ~ depth + I(depth^2) | depth, ALake, model="alternative")

# test both models
anova(res1, res2)
res1
summary(res2)
```

GlacialTills

Description

Data from Aitchison (2003)

Usage

GlacialTills

Format

A data frame with 92 observations on the following 5 variables.

- RedSandstone  a numeric vector
- GraySandstone  a numeric vector
- Crystalline  a numeric vector
- Miscellaneous  a numeric vector
- Pcount  a numeric vector

Source

plot.DirichletRegData  

**Plot Dirichlet-Distributed Data**

**Description**

With this function you can plot Dirichlet-distributed data in 2, 3 and 4 dimensions.

**Usage**

```r
## S3 method for class 'DirichletRegData'
plot(x, dims, ticks = TRUE, ref.lines = NULL, dim.labels, a2d = list(colored = TRUE, c.grid = TRUE, col.scheme = c("dims", "entropy"), entropy.contours = FALSE, entropy.colors = FALSE), a3d = list(rgl = TRUE, ...), rug = TRUE, reset_par = TRUE, ...)
```

**Arguments**

- `x`: data prepared with `DR_data`
- `dims`: select two, three, or four Dimensions of your data `x` to plot
- `ticks`: display ticks?
- `ref.lines`: .
- `dim.labels`: a character vector giving labels for the dimensions/variables
- `a2d`: a named list of settings for ternary plots (3 variables), see Details
- `a3d`: a named list of settings for quaternary plots (4 variables), see Details
- `rug`: display a rug for a one-dimensional plot (2 variables)
- `reset_par`: reset graphical parameters of `DR_data` after creating a two-dimensional plot (2 variables), see Details
- `...`: further graphical arguments as `col`, `pch`, `cex`, ...

**Author(s)**

Marco J. Maier

**Examples**

```r
# plot of "Sand" in the Arctic Lake data set
plot(DR_data(ReadingSkills[, 1]), main="Reading Accuracy")

# ternary plot of Arctic Lake data
plot(DR_data(ArcticLake[, 1:3]), a2d = list(colored = FALSE))
```
Rocks

Reading Accuracy Data  Pammer and Kevan’s Data on Reading Skills

Description
These data provide transformed reading accuracy scores predicted by IQ and diagnosed dyslexia.

Usage
ReadingSkills
ReadDisc

Format
A data frame containing 44 observations on 3 variables.
accuracy  reading accuracy score transformed to fit into (0, 1)
dyslexia  a factor with the diagnosis of dyslexia (“yes” or “no”)
iq  non-verbal IQ (z-scores; $\mu = 0, \sigma^2 = 1$)

Source
(no longer valid)

Rocks  Aitchison’s Rock Data

Description
A compilation of four datasets listed in Aitchison (2003)
Each type of rock has 25 observations – to use only a certain type of rock, see “Details”.

Usage
Rocks

Format
A data frame with 100 observations on the following 8 variables.
Albite, Blandite, Cornite, Daubite, Endite  numeric vectors
depth  a numeric vector
porosity  a numeric vector
type  a factor with levels Boxite Coxite Hongite Kongite
Source

Simplex-Transformations

*Transform Compositional Data for a Simplex*

Description
These functions transform a matrix with three or four components to fit into a two- or three-dimensional simplex (triangle or tetrahedron).

Usage
tosimplex(x)
toTernary(abc)
toTernaryVectors(c1, c2, c3)
toQuaternary(abcd)
toQuaternaryVectors(c1, c2, c3, c4)

Arguments
x a matrix-like object with 3 or 4 columns.
abc a matrix-like object with 3 columns.
abcd a matrix-like object with 4 columns.
c1 a numeric vector with values of the first component.
c2 a numeric vector with values of the second component.
c3 a numeric vector with values of the third component.
c4 a numeric vector with values of the fourth component.

Details
Most of these functions are only used internally, but sometimes it might be useful to plot “custom” ternary or quaternary graphics.
Note that, apart from toSimplex(), functions do not have any checks, so it is advisable to use this function if elements are added to plots or own graphics are created.

Value
The function returns a matrix object with coordinates in two or three dimensions.
Simplex-Transformations

Note

In prior versions (up to 0.5-0), an unexported function coord-trafo() was used internally and could also be accessed via DirichletReg::coord-trafo().

If you have used this in your code, you will get a message that the function is now deprecated and will become defunct in the future. Use toSimplex() instead.

Author(s)

Marco J. Maier

Examples

# create a DirichletRegData object from the Arctic Lake data
"to be added"
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