## Package 'DirichletReg'

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## **R** topics documented:

	DirichletReg-package	2
	anova.DirichletRegModel	2
	ArcticLake	
	BloodSamples	4
	Dirichlet	5
	DirichletRegData	6
	DirichletRegModel	9
	DirichReg	11
	GlacialTills	14
	plot.DirichletRegData	15
	Reading Accuracy Data	16
	Rocks	16
	Simplex-Transformations	17
Index		19

DirichletReg-package The **DirichletReg** Package

## Description

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

Package: DirichletReg
Type: Package
Version: 0.7-1
Date: 2021-04-29
License: GPL (>= 2)

## Author(s)

Marco J. Maier

## **Examples**

example(plot.DirichletRegData)
example(DirichReg)

 $an ova. \verb|DirichletRegModel|$ 

Compare Dirichlet Regression Models using an LRT

ArcticLake 3

#### **Description**

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

#### Usage

```
## 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 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**

```
ALake <- ArcticLake
ALake$AL <- DR_data(ArcticLake[,1:3])
mod0 <- DirichReg(AL ~ 1, ALake)
mod1 <- DirichReg(AL ~ depth, ALake)
mod2 <- DirichReg(AL ~ depth + I(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

4 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**

Aitchison, J. (2003). *The Statistical Analysis of Compositional Data*. The Blackburn Press, Caldwell, NJ.

## **Examples**

```
head(ArcticLake)
AL <- DR_data(ArcticLake[,1:3])
plot(AL)
summary(AL)</pre>
```

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.

Albumin, Pre. Albumin, Globulin. A, Globulin. B the amounts of Albumin, Pre-Albumin, Globulin A, and Globulin B.

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

Aitchison, J. (2003). *The Statistical Analysis of Compositional Data*. The Blackburn Press, Caldwell, NJ.

Dirichlet 5

#### **Examples**

```
head(BloodSamples)
Bl <- DR_data(BloodSamples[,1:4])
summary(Bl)</pre>
```

Dirichlet

The Dirichlet Distribution

## **Description**

Density function and random number generation for the Dirichlet distribution

#### Usage

```
rdirichlet(n, alpha)

ddirichlet(x, alpha, log = FALSE, sum.up = FALSE)

ddirichlet_R(x, alpha, log = FALSE, sum.up = FALSE)
```

#### **Arguments**

n x	number of random observations to draw 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

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

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.

6 DirichletRegData

#### Value

#### Author(s)

Marco J. Maier

## **Examples**

```
X1 <- rdirichlet(100, c(5, 5, 10))
a.mat <- cbind(1:10, 5, 10:1)
a.mat
X2 <- rdirichlet(10, a.mat)
# note how the probabilities in the first an last column relate to a.mat
round(X2, 2)

ddirichlet(X1, c(5, 5, 10))
ddirichlet(X2, a.mat)

ddirichlet(X2[1:3,], c(1, 2, -1))
ddirichlet(X2[1:3,], c(1, 2, -1), sum.up = TRUE)</pre>
```

DirichletRegData

Prepare Compositional Data

## Description

This function prepares a matrix with compositional variables for further processing in the **DirichletReg** package.

## Usage

```
DR_data(Y, trafo = sqrt(.Machine$double.eps), base = 1,
    norm_tol = sqrt(.Machine$double.eps))
## S3 method for class 'DirichletRegData'
print(x, type = c("processed", "original"), ...)
## S3 method for class 'DirichletRegData'
summary(object, ...)
```

DirichletRegData 7

#### **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. There-

fore, norm\_tol is a small non-negative value (default:  $\sqrt{.\text{Machine}\$\text{double.eps}}$ ) 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  $y^* = \frac{y(n-1) + \frac{1}{d}}{n}$ .

#### 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.

8 DirichletRegData

```
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. {\tt 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

Smithson, M. & Verkuilen, J. (2006). A Better Lemon Squeezer? Maximum-Likelihood Regression With Beta-Distributed Dependent Variables. *Psychological Methods*, 11(1), 54–71.

Cribari-Neto, F. & Zeileis, A. (2010). Beta Regression in R. *Journal of Statistical Software*, 34(2), 1–24.

#### **Examples**

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

DirichletRegModel 9

DirichletRegModel

Methods for the Class DirichletRegModel

#### **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

```
## 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, ...)
```

10 DirichletRegModel

```
## 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, sort = TRUE, ...)
```

#### **Arguments**

x an object of class DirichletRegModel

object an object of class DirichletRegModel or DirichletRegConfint for printing

an object obtained by confint.DirichletRegModel

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 and 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

sort if TRUE, p-values will be sorted in decreasing order.

... further arguments

#### Author(s)

Marco J. Maier

## Examples

```
ALake <- ArcticLake
ALake$AL <- DR_data(ArcticLake[, 1:3])
mod1 <- DirichReg(AL ~ depth + I(depth^2) | depth, data = ALake, model="alternative")</pre>
```

DirichReg 11

```
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

## **Arguments**

formula	the model formula (for different specifications see "Details")
data	a data.frame containing independent and dependent variables
model	specifies whether the "common" $(\alpha s)$ or "alternative" $(\mu/\phi)$ parametrization is employed (see "Details")
subset	estimates the model for a subset of the data
sub.comp	analyze a subcomposition by selecting specific components (see "Details")
base	redefine the base variable
weights	frequency weights
control	a list containing control parameters used for the optimization
verbosity	prints information about the function's progress, see Details

#### **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 | 1 | 1, because DV hast three components. Likewise, it is possible to specify a common set of predictors for all components, as in DV  $\sim$  p1  $\star$  p2, where p1 and p2 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,  $DV \sim p1 | p1 + p2 | p1 * p2$  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 \* 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 ~ 1, which is expanded to DV ~ 1 | 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 ~ p1 \* p2 | p1 + p2 will set up a model where the expected values are predicted by p1 \* 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.

DirichReg 13

**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

varnames

[character] used parametrization [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

14 GlacialTills

#### Author(s)

Marco J. Maier

## **Examples**

```
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

Glacial Tills

#### **Description**

Data from Aitchison (2003)

#### Usage

GlacialTills

## Format

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

Red.Sandstone a numeric vector Gray.Sandstone a numeric vector Crystalline a numeric vector Miscellaneous a numeric vector Pcount a numeric vector

## Source

Aitchison, J. (2003). *The Statistical Analysis of Compositional Data*. The Blackburn Press, Caldwell, NJ.

plot.DirichletRegData 15

```
\verb"plot.DirichletRegData" \textit{Plot Dirichlet-Distributed Data}
```

## **Description**

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

## Usage

```
## 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**

```
# 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))
```

16 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

#### **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**

Example 3 from http://www.michaelsmithson.online/stats/betareg/betareg.html

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**

Aitchison, J. (2003). *The Statistical Analysis of Compositional Data*. The Blackburn Press, Caldwell, NJ.

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.
<b>c</b> 3	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

#### 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

 $\mbox{\tt\#}$  create a DirichletRegData object from the Arctic Lake data "to be added"

# **Index**

* datasets	DirichReg, 7, 11
ArcticLake, 3	DR_data, <i>12</i> , <i>15</i>
BloodSamples, 4	<pre>DR_data(DirichletRegData), 6</pre>
GlacialTills, 14	drop1, <i>10</i>
Reading Accuracy Data, 16	drop1.DirichletRegModel
Rocks, 16	(DirichletRegModel), 9
* hplot	
plot.DirichletRegData, 15	fitted.DirichletRegModel (DirichletRegModel),9
* manip	(DITICHTE the griodet), 9
DirichletRegData, 6	GlacialTills, 14
Simplex-Transformations, 17	glm, 13
* models	8±111, 13
DirichReg, 11	lines.DirichletRegData
* multivariate	(plot.DirichletRegData), 15
DirichReg, 11	logLik.DirichletRegModel
* package	(DirichletRegModel),9
DirichletReg-package, 2	(* * * * * * * * * * * * * * * * * * *
* regression	maxBFGS, 13
DirichReg, 11	maxNR, <i>13</i>
AIC.DirichletRegModel	nobs.DirichletRegModel
(DirichletRegModel), 9	(DirichletRegModel), 9
all.equal, $7$	
anova.DirichletRegModel, 2	plot.DirichletRegData, 15
ArcticLake, 3	<pre>predict.DirichletRegModel</pre>
	(DirichletRegModel), 9
BIC.DirichletRegModel	<pre>print.DirichletRegConfint</pre>
(DirichletRegModel), 9	(DirichletRegModel), 9
BloodSamples, 4	<pre>print.DirichletRegData</pre>
	(DirichletRegData), 6
confint.DirichletRegModel	<pre>print.DirichletRegModel</pre>
(DirichletRegModel),9	(DirichletRegModel),9
ddirichlet(Dirichlet), 5	rdirichlet (Dirichlet), 5
ddirichlet_R (Dirichlet), 5	Reading Accuracy Data, 16
Dirichlet, 5	ReadingSkills (Reading Accuracy Data)
DirichletReg(DirichletReg-package), 2	16
DirichletReg-package, 2	residuals.DirichletRegModel
DirichletRegData, 6	(DirichletRegModel), 9
DirichletRegModel, 9	Rocks, 16

20 INDEX

```
{\tt Simplex-Transformations,\,17}
subset, 13
summary.DirichletRegData
        (DirichletRegData), 6
summary.DirichletRegModel
       (DirichletRegModel), 9
toQuaternary (Simplex-Transformations),
       17
toQuaternaryVectors
       (Simplex-Transformations), 17
toSimplex (Simplex-Transformations), 17
toTernary (Simplex-Transformations), 17
toTernaryVectors
       (Simplex-Transformations), 17
update.DirichletRegModel
       (DirichletRegModel), 9
update.Formula, 10
update.formula, 10
vcov.DirichletRegModel
```