Package 'simplexreg'

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Type Package

Title Regression Analysis of Proportional Data Using Simplex Distribution

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Description Simplex density, distribution, quantile functions as well as random variable generation of the simplex distribution are given. Regression analysis of proportional data using various kinds of simplex models is available. In addition, GEE method can be applied to longitudinal data to model the correlation. Residual analysis is also involved. Some subroutines are written in C with GNU Scientific Library (GSL) so as to facilitate the computation.

Depends Formula, plotrix

Imports graphics, stats

License GPL-2

NeedsCompilation yes

Repository CRAN

SystemRequirements GNU Scientific Library version >= 1.8

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R topics documented:

ot.simplexreg	 2
edict.simplexreg	 3
iduals.simplexreg	 4
inal	 6
ю	 7
nplex	 8
nplexreg	 10
nplexreg.control	
nmary.simplexreg	 14

Index

plot.simplexreg Plots for simplexreg Objects

Description

Various types of plots could be produced for simplexreg Objects, including plots of correlation structure, plots of different types of residuals and plots of partial deviance.

Usage

```
## S3 method for class 'simplexreg'
plot(x, type = c("residuals", "corr", "GOF"), res = "adjvar", lag = 1, ...)
```

Arguments

x	fitted model object of class "simplexreg"
type	character specifying types of plots: the correlation (corr), residuals (residuals), partial deviances (GOF). See 'Details'
res	character specifying types of residuals:approximate Pearson residual (appstdPerr), standard Pearson residual (stdPerr), adjusted dependent variable s_i (adjvar). See residuals.simplexreg
lag	when type = corr, this function examine the autocorrelation at lag lag
	other parameters to be passed through to the plot function

Details

This function provides graphical presentations for simplexreg objects. The plot of correlation aims examine the correlation structure of the longitudinal data set. Let r_{ij} be the standardised score residuals of the ith observation at time t_{ij} , and lag = k, then r_{ij} are plotted against r_{ik} for all i and j < k, if $|t_{ij} - t_{ik}| = k$.

Residuals can be plotted when specifying type = "residuals", The upper and lower 95 (1.96) are also lined.

Plots of partial deviance are for the goodness-of-fit test in the presence of within-subject dependence for longitudinal data. The partial deviances are defined as

$$D_j^P = \sum_{i=1}^{m_j} d(y_{ij} - \hat{\mu}_{ij}) / \sigma_{ij}^2, j \in T$$

where T denotes a collection of all distinct times on which observation are made. Cross-sectionally, y_{ij} 's are independent and hence D_j^P follows approximately χ^2 , with m_j being the total number of y_{ij} 's observed cross-sectionally at time t_j . Both observed partial deviance D_j^P statistics and the corresponding critical values are depicted and compared at each time point.

16

Author(s)

Chengchun Shi

References

Song, P. and Qiu, Z. and Tan, M. (2004) Modelling Heterogeneous Dispersion in Marginal Models for Longitudinal Proportional Data. *Biometrical Journal*, **46:** 540–553

Qiu Z. (2001) *Simplex Mixed Models for Longitudinal Proportional Data*. Ph.D. Dissertation, York University

Zhang, P. and Qiu, Z. and Shi, C. (2016) simplexreg: An R Package for Regression Analysis of Proportional Data Using the Simplex Distribution. *Journal of Statistical Software*, **71**: 1–21

See Also

summary.simplexreg,residuals.simplexreg

Examples

```
## fit the model
data("sdac", package="simplexreg")
sim.glm2 <- simplexreg(rcd~ageadj+chemo|age,
    link = "logit", data = sdac)
data("retinal", package = "simplexreg")
sim.gee2 <- simplexreg(Gas~LogT+LogT2+Level|LogT+Level|Time,
    link = "logit", corr = "AR1", id = ID, data = retinal)
## produce the plots
plot(sim.glm2, type = "residuals", res = "stdPerr", ylim = c(-3, 3))
plot(sim.gee2, type = "corr", xlab = "", ylab = "")
plot(sim.gee2, type = "GOF", xlab = "", ylab = "")
```

predict.simplexreg *Prediction Method for simplexreg Objects*

Description

Predicted values based on simplex regression object

Usage

Arguments

object	fitted model object of class "simplexreg"
newdata	an optional data frame in which to look for variables with which to predict. If omitted, original observations are used.
type	character indicating type of predictions:fitted mean of response ("response") or fitted dispersion parameter("dispersion")
na.action	function determining what should be done with missing values in newdata
	currently not used

Author(s)

Chengchun Shi

See Also

simplexreg

Examples

```
## fit the model
data("sdac", package="simplexreg")
sim.glm2 <- simplexreg(rcd~ageadj+chemo|age, link = "logit",
    data = sdac)
data("retinal", package = "simplexreg")
sim.gee2 <- simplexreg(Gas~LogT+LogT2+Level|LogT+Level|Time,
    link = "logit", corr = "AR1", id = ID, data = retinal)
## predict the mean
predict(sim.glm2, type = "response")
## predict the dispersion
predict(sim.gee2, type = "dispersion")
```

residuals.simplexreg Extract residuals for simplexreg Objects

Description

Methods for extracting various types of residuals from simplex regression, from approximate Pearson residuals, standard Pearson residuals and standardise score residuals to adjusted dependent variable suggested by McCullagh and Nelder (1989). The first three can be used to examine mean-variance relation while the last aims to test the link function.

residuals.simplexreg

Usage

Arguments

object	fitted model object of class "simplexreg"
type	character specifying types of residuals:approximate Pearson residual (appstdPerr), standard Pearson residual (stdPerr), adjusted dependent variable s_i (adjvar). Details are given in 'Details'
	currently not used

Details

The Pearson residual takes the form

$$r_i^P = \frac{y_i - \hat{\mu}_i}{\hat{\tau}_i}$$

where $\hat{\mu}_i$ is the fitted mean parameter and details about calculation of τ is given in Jorgensen (1997). When the dispersion parameter σ^2 (see simplex) is large the variance of response approaches to $\mu(1-\mu)$ and this leads to the approximate Pearson residual

$$r_i^a = \frac{y_i - \hat{\mu}_i}{\sqrt{\hat{\mu}_i (1 - \hat{\mu}_i)}}$$

Plot of the standardised score residuals,

$$r_i^S = \frac{u_i}{\sqrt{var(u_i)}}$$

where u_i is the score function, can also detect model assumption violation. Details can be found in Song *et al.* (2004). The adjusted dependent variable suggested by McCullagh and Nelder (1989) could be employed as an informal check for the link function,

$$s_i = g(\mu_i) + \left(\frac{3\sigma^4}{\mu_i(1-\mu_i)} + \frac{\sigma^2}{V(\mu_i)}\right)^{-1/2} u(y_i;\mu_i)$$

where $u(y_i; \mu_i)$ and $V(\mu_i)$ are the score function and variance function.

Author(s)

Chengchun Shi

References

Barndorff-Nielsen, O.E. and Jorgensen, B. (1991) Some parametric models on the simplex. *Journal of Multivariate Analysis*, **39:** 106–116

Jorgensen, B. (1997) The Theory of Dispersion Models. London: Chapman and Hall

McCullagh, P and Nelder J. (1989) Generalized Linear Models. London: Chapman and Hall

Song, P. and Qiu, Z. and Tan, M. (2004) Modelling Heterogeneous Dispersion in Marginal Models for Longitudinal Proportional Data. *Biometrical Journal*, **46**: 540–553

Zhang, P. and Qiu, Z. and Shi, C. (2016) simplexreg: An R Package for Regression Analysis of Proportional Data Using the Simplex Distribution. *Journal of Statistical Software*, **71**: 1–21

See Also

summary.simplexreg, simplex

Examples

```
## fit the model
data("sdac", package="simplexreg")
sim.glm2 <- simplexreg(rcd~ageadj+chemo|age,
    link = "logit", data = sdac)
data("retinal", package = "simplexreg")
sim.gee2 <- simplexreg(Gas~LogT+LogT2+Level|LogT+Level|Time,
    link = "logit", corr = "AR1", id = ID, data = retinal)
## extract the residuals
res <- residuals(sim.glm2, type = "stdPerr")
res <- residuals(sim.gee2, type = "adjvar")</pre>
```

retinal

Data on recorded decay of intraocular gas in complex retinal surgeries

Description

The study recorded the decay of intraocular gas C_3F_8 in complex retinal surgeries following initial injection in an ophthalmology study, reported in Meyers *et al.* (1992). The outcome variable was the percent of gas left in the eye. The gas, with three different concentration levels, 15%, 20% and 25% was injected into the eye before surgery for 31 patients. They were then followed three to eight (average of five) times over a three-month period, and the volume of gas in the eye at the follow-up times were recorded as a percentage of the initial gas volume. The primary interest was to investigate whether concentration levels of the gas injected in patients' eyes affect the decay rate of the gas.

Usage

data("retinal")

Format

A data frame with 181 observations on the following 6 variables.

Gas Percentage of the initial gas volume left

Time Time covariate of days after the gas injection

sdac

- LogT Logarithm of Time
- LogT2 Square of LogT
- Level Concentration levels of the initial intraocular gas. For each patient, Level = -1 if the gas concentration level is 15%, Level = 0 if 20%, or 1 if 25%.
- ID A factor indicating patients.

References

Meyers, S. M. and Ambler, J. S. and Tan, M. (1992) Variation of Perfluorpropane Disappearance after Vitrectomy. *Retinal*, **12**: 359–363

Zhang, P. and Qiu, Z. and Shi, C. (2016) simplexreg: An R Package for Regression Analysis of Proportional Data Using the Simplex Distribution. *Journal of Statistical Software*, **71**: 1–21

sdac

Data on Autologous Peripheral Blood Stem Cell Transplants in Alberta Health Service

Description

Autologous peripheral blood stem cell (PBSC) transplants have been widely used for rapid hematologic recovery following myeloablative therapy for various malignant hematological disorders. A study enrolled 242 patients who consented to autologous PBSC transplant after myeloablative doses of chemotherapy between year 2003 and 2008 at the Edmonton Hematopoietic Stem Cell Lab in Cross Cancer Institute - Alberta Health Services. The Data is a data frame containing information about the patients' age, gender, as well as their clinical characteristics.

Usage

data("sdac")

Format

A data frame with 239 observations on the following 5 variables.

age patients' ages

gender patients' genders

- rcd recovery rates for viable CD34+ cells
- chemo dummy variable indicating if a patient receives a chemotherapy on a one-day protocol(0) or on a 3-day protocol(1)
- ageadj adjusted age variable. age < 40 is set as the baseline age and other ages are adjusted by subtracting by 40

References

Allan, D. and Keeney, M. and Howson-Jan, K. and Popma, J. and Weir, K. and Bhatia, M. and Sutherland, D. and Chin_yee, I. (2002) Number of Viable CD34+ Cells Reinfused Predicts Engraftment in Autologous Hematopoietic Stem Cell Transplantation. *BONE MARROW TRANSPL*, **20:** 967-72

Yang, H. and Acker, J. and Cabuhat, M. and Letcher, B. and Larratt, L. and McGann, L. (2005) Association of Post_Thaw viable CD34+ Cells and CFU-GM with Time to Hematopoietic Engraftment. *BONE MARROW TRANSPL*, **35:** 881-887

Zhang, P. and Qiu, Z. and Shi, C. (2016) simplexreg: An R Package for Regression Analysis of Proportional Data Using the Simplex Distribution. *Journal of Statistical Software*, **71**: 1–21

simplex

The Simplex Distribution Functions

Description

Density, cumulative distribution function, quantile function and random variable generation for the simplex distribution with mean equal to mu and dispersion equal to sig

Usage

```
dsimplex(x, mu, sig)
psimplex(q, mu, sig)
qsimplex(p, mu, sig)
rsimplex(n, mu, sig)
psimplex.norm(q, mu, sig)
qsimplex.norm(p, mu, sig)
```

Arguments

x, q	vector of quantiles
р	vector of probabilities
n	number of observations
mu	vector of means
sig	vector of square root of dispersion parameter of simplex distribution

Details

The simplex distribution has density

$$p(y) = (2\pi\sigma^2)^{-\frac{1}{2}}(y(1-y))^{-\frac{3}{2}}\exp(-\frac{1}{2\sigma^2}d(y;\mu)), y \in (0,1)$$

where $d(y; \mu)$ is a unit deviance function

$$d(y;\mu) = \frac{(y-\mu)^2}{y(1-y)\mu^2(1-\mu)^2}$$

simplex

 μ is the mean of simplex distribution and σ^2 the dispersion parameter. qnorm provides results up to about 6 digits.

Value

dsimplex gives density function, psimplex gives the distribution function, qsimplex gives quantile function and rsimplex gives random number generated from the simplex distribution. psim.norm and qsimplex.norm gives the renormalized distribution and quantile function.

Author(s)

Peng Zhang and Zhenguo Qiu

References

Barndorff-Nielsen, O.E. and Jorgensen, B. (1991) Some parametric models on the simplex. *Journal of Multivariate Analysis*, **39:** 106–116

Jorgensen, B. (1997) The Theory of Dispersion Models. London: Chapman and Hall

Song, P. and Qiu, Z. and Tan, M. (2004) Modelling Heterogeneous Dispersion in Marginal Models for Longitudinal Proportional Data. *Biometrical Journal*, **46:** 540–553

```
# simplex distribution function
dsimplex(seq(0.01,0.99,0.01), 0.5, 1)
psimplex(seq(0.01,0.99,0.01), 0.5, 1)
qsimplex(seq(0.01,0.99,0.01), 0.5, 1)
# random variable generation
n <- 200
ga0 <- 1.5
ga1 <- 0.5
ga2 <- -0.5
sigma <- 4
T <- c(rep(0, n/2), rep(1, n/2))
S <- runif(n, 0, 5)</pre>
eta <- ga0 + ga1 * T + ga2 * S
mu <- exp(eta)/(1+exp(eta))</pre>
Y \leq rep(0, n)
for (i in 1:n){
  Y[i] <- rsimplex(1, mu[i], sigma)</pre>
}
```

simplexreg

Description

Regression Analysis of Proportional Data Using Various Types of Simplex Models

Usage

```
simplexreg(formula, data, subset, na.action,
    link = c("logit", "probit", "cloglog", "neglog"), corr = "Ind", id = NULL,
    control = simplexreg.control(...), model = TRUE, y = TRUE, x = TRUE, ...)
simplexreg.fit(y, x, z = NULL, t = NULL, link = "logit", corr = "Ind",
    id = NULL, control = simplexreg.control())
```

Arguments

formula	a symbolic description of the model to be fitted(of type $y \sim x$ or $y \sim x z t$. The Details are given under 'Details').
data	an optional data frame, list or environment containing variables in formula and id.
subset, na.act:	ion
	arguments controlling formula processing via model.frame
link	type of link function to the mean. Currently, "logit" (logit function), "probit" (probit function), "cloglog" (complementary log-log function), "neglog" (negative log function) are supported.
corr	the covariance structure, chosen from "Ind"(independent structure), "Exc"(exchangeability) and "AR1"(AR(1)), see Details
id	a factor identifies the clusters when gee = TRUE. The length of id should be the same as the number of observations. y, x, z, t are assumed to be sorted in accordance with clusters specified by id
control	a list of control argument via simplexreg.control
model	a logical value indicating whether <i>model frame</i> should be included as a compo- nent of the return value
у, х	For simplexreg:logical values indicating whether response vector and covari- ates modelling the mean parameter should be returned as components of the returned value For simplexreg.fit:x is the design matrix and y is the response vector
Z	regressor matrix modelling the dispersion parameter
t	time covariate in the correlation structure, see Details
	argument passed to simplexreg.control

simplexreg

Details

Outcomes of continuous proportions arise in many applied areas. Such data could be properly modelled using simplex regression. See also simplex. The mean and dispersion parameters are linked to set of regressors. Regression analysis of the simplex model is implemented in simplexreg. If corr = "Ind", simplex generalized regression model is employed. Estimations is performed by maximum likelihood via Fisher scoring technique.

Apart from including generalized simplex regression models, this function also provides users with generalized estimating equations (GEE) techniques to model longitudinal proportional response. Exchangeability and AR(1) structures are available. Parameter estimation and residual analysis are involved.

We employ the specification approach designed in the fitting model function betareg of beta regression in the package **betareg**. As for simplex regression models, assuming the dispersion is homogeneous, the response is linked to a linear predictor described by $y \sim x1 + x2$ using a link function. Four types of function are available linking the regressors to the mean. However, for dispersion, the link function is restricted to logarithm function. When modeling dispersion, the regressor modelling the dispersion parameter should be specified in a formula form of type $y \sim x1 + x2$ where z1 and z2 are linked to the dispersion parameter σ^2 .

Model specification is a bit complicated when it comes to modelling longitudinal proportional response. Song *et. al* (2004) proposed a marginal simplex model consists of three components, the population-average effects, the pattern of dispersion and the correlation structure. Let the percentage responses for the *i*th subject be y_{ij} , observed at time t_{ij} . If corr = "AR1", the working covariance matrix of y_{ij} , $j = 1, 2, ..., n_i$, is

$$\exp(\alpha * |t_{ik} - t_{ij}|)_{ki}$$

where $\alpha < 0$ and $\exp(\alpha)$ is the lag-1 autocorrelation. If corr = "Exc", the covariance matrix will be $(1 - exp(\alpha))I + exp(\alpha)1$ where I is the identity matrix while 1 the matrix with all elements being equal to one.

For homogeneous dispersion, the formula is supposed to be of the form $y \sim x1 + x2 \mid 1 \mid t$ where *t* is the time covariate. Otherwise, the formula will be of the form $y \sim x1 + x2 \mid z1 + z2 \mid t$.

Value

fixef	estimates of coefficients modelling the mean as well as the standard deviation
dispar	estimates of coefficients modelling dispersion as well as the standard deviation
Dispersion	estimate of the dispersion parameter
appstdPerr	approximated standard deviations of the regression coefficients
stdPerr	exact standard deviations of the regression coefficients
meanmu	estimate of mean parameter
adjvar	adjusted dependent variable s_i . Details could be found in McCullagh and Nelder (1989)
stdscor	standardised score residuals. Details can be found in Song et al. (2004)
predict	predicted values of $g(\mu_i)$ where g is the link function and μ_i the mean parameter
loglike	value of maximum log-likelihood function

exreg

deviance	value of deviance
call	the original function call
formula	the original formula
terms	a list with elements "mean" and "dispersion" containing term object for the model
levels	a list with elements "mean" and "dispersion" containing levels of categorical regressors
link	type of function linking to the mean
type	type = "homo" for homogeneous dispersion while type = "hetero" for hetero- geneous dispersion
model	the full model frame (if model = TRUE)
У	response vector (if $y = TRUE$)
X	a list with elements mean, dispersion, time and id containing corresponding variables
n	number of proportional observations
iter	number of Fisher iterations
	argument passed to simplexreg.control

Author(s)

Zhenguo Qiu, Peng Zhang and Chengchun Shi

References

Barndorff-Nielsen, O.E. and Jorgensen, B. (1991) Some parametric models on the simplex. *Journal of Multivariate Analysis*, **39:** 106–116

Jorgensen, B. (1997) The Theory of Dispersion Models. London: Chapman and Hall

McCullagh, P and Nelder J. (1989) Generalized Linear Models. London: Chapman and Hall

Song, P. and Qiu, Z. and Tan, M. (2004) Modelling Heterogeneous Dispersion in Marginal Models for Longitudinal Proportional Data. *Biometrical Journal*, **46:** 540–553

Zhang, P. and Qiu, Z. and Shi, C. (2016) simplexreg: An R Package for Regression Analysis of Proportional Data Using the Simplex Distribution. *Journal of Statistical Software*, **71:** 1–21

See Also

simplex

```
# GLM models
data("sdac", package = "simplexreg")
sim.glm1 <- simplexreg(rcd~ageadj+chemo, link = "logit",
    data = sdac)
sim.glm2 <- simplexreg(rcd~ageadj+chemo|age, link = "logit",
    data = sdac)</pre>
```

simplexreg.control

```
# GEE models
data("retinal", package = "simplexreg")
sim.gee1 <- simplexreg(Gas~LogT+LogT2+Level|1|Time, link = "logit",
    corr = "Exc", id = ID, data = retinal)
sim.gee2 <- simplexreg(Gas~LogT+LogT2+Level|LogT+Level|Time,
    link = "logit", corr = "AR1", id = ID, data = retinal)</pre>
```

simplexreg.control Control Parameters for Simplex Regression

Description

Various parameters that control fitting of simplex regression models using simplexreg.

Usage

```
simplexreg.control(maxit = 200, beta = NULL, gamma = NULL, alpha = NULL,
tol = 1e-6, ...)
```

Arguments

maxit	maximum number of iterations
beta	start value for beta modelling the mean parameter
gamma	start value for gamma modelling the dispersion
alpha	start value for alpha modelling correlation structure using GEEs, see Song <i>et.al</i> (2004)
tol	numeric tolerance for convergence in Fisher scoring
	currently not used

Value

A list with the arguments specified.

See Also

simplexreg

```
# GLM models
data("sdac", package = "simplexreg")
sim.glm1 <- simplexreg(rcd~ageadj+chemo, link = "logit",
    data = sdac, beta = c(1.115, 0.013, 0.252))
sim.glm2 <- simplexreg(rcd~ageadj+chemo|age, link = "logit",
    data = sdac, beta = c(1.115, 0.013, 0.252), gamma = c(2.61, -0.015))</pre>
```

```
# GEE models
data("retinal", package = "simplexreg")
sim.gee1 <- simplexreg(Gas~LogT+LogT2+Level|1|Time, link = "logit",
    corr = "Exc", id = ID, data = retinal, beta = c(2.72, 0.034, -0.329, 0.409),
    alpha = -0.3)
sim.gee2 <- simplexreg(Gas~LogT+LogT2+Level|LogT+Level|Time,
    link = "logit", corr = "AR1", id = ID, data = retinal, alpha = -0.3,
    beta = c(2.72, 0.034, -0.329, 0.409))</pre>
```

summary.simplexreg Extracting Information from Objects simplexreg

Description

Methods for extracting information from fitted simplex regression model objects of class "simplexreg"

Usage

```
## S3 method for class 'simplexreg'
## S3 method for class 'simplexreg'
summary(object, type = "stdPerr", ...)
## S3 method for class 'simplexreg'
## S3 method for class 'simplexreg'
coef(object, ...)
## S3 method for class 'simplexreg'
## S3 method for class 'simplexreg'
vcov(object, ...)
```

Arguments

object	fitted model object of class "simplexreg"
type	$character\ specifying\ type\ of\ residuals\ to\ be\ included,\ see\ residuals\ .\ simplex reg$
	currently not used

Details

These functions make it possible to extract information from objects of class "simplexreg". Wald statistics as well as the p-values of regression coefficients are given in the summary output. If GEE = FALSE, based on the fitted coefficients, a χ^2 test is performed and the p-value is reported in the output. Otherwise, coefficients of the autocorrelation α , ρ , (see Song *et. al* (2004)), are also involved.

Model coefficients and their covariance matrix could be extracted by the coef, and vcov, respectively. For simplex GLM models (GEE = FALSE), Akaike Information Criterion and Bayesian Information Criterion could be calculated using generic functions AIC and BIC, respectively.

Author(s)

Chengchun Shi

References

Barndorff-Nielsen, O.E. and Jorgensen, B. (1991) Some parametric models on the simplex. *Journal of Multivariate Analysis*, **39:** 106–116

Jorgensen, B. (1997) The Theory of Dispersion Models. London: Chapman and Hall

Song, P. and Qiu, Z. and Tan, M. (2004) Modelling Heterogeneous Dispersion in Marginal Models for Longitudinal Proportional Data. *Biometrical Journal*, **46:** 540–553

Zhang, P. and Qiu, Z. and Shi, C. (2016) simplexreg: An R Package for Regression Analysis of Proportional Data Using the Simplex Distribution. *Journal of Statistical Software*, **71**: 1–21

See Also

simplexreg, residuals.simplexreg

```
## fit the model
data("sdac", package = "simplexreg")
sim.glm2 <- simplexreg(rcd~ageadj+chemo|age, link = "logit",</pre>
  data = sdac)
data("retinal", package = "simplexreg")
sim.gee2 <- simplexreg(Gas~LogT+LogT2+Level|LogT+Level|Time,</pre>
  link = "logit", corr = "AR1", id = ID, data = retinal)
## extract information
summary(sim.glm2, type = "appstdPerr")
coef(sim.glm2)
vcov(sim.glm2)
AIC(sim.glm2)
BIC(sim.glm2)
summary(sim.gee2, type = "stdscor")
coef(sim.gee2)
vcov(sim.glm2)
```

Index

*Topic **distribution** simplex, 8*Topic random variable simplex, 8 *Topic simplex regression simplexreg, 10 AIC, 14 AIC.simplexreg(summary.simplexreg), 14 BIC, 14 BIC.simplexreg(summary.simplexreg), 14 coef, 14 coef.simplexreg(summary.simplexreg), 14 dsimplex (simplex), 8 logLik.simplexreg(summary.simplexreg), 14 model.frame, 10 nobs.simplexreg(summary.simplexreg), 14 plot.simplexreg, 2 predict.simplexreg, 3 print.simplexreg(simplexreg), 10 print.summary.simplexreg (summary.simplexreg), 14 psimplex (simplex), 8 qsimplex (simplex), 8 residuals.simplexreg, 2, 3, 4, 14, 15 retinal, 6 rsimplex (simplex), 8 sdac.7 simplex, *5*, *6*, 8, *11*, *12* simplexreg, 4, 10, 13, 15 simplexreg.control, 10, 12, 13

summary.simplexreg, 3, 6, 14

vcov, 14
vcov.simplexreg(summary.simplexreg), 14