# Package 'SGB'

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Author Monique Graf
Maintainer Monique Graf <monique.p.n.graf@bluewin.ch></monique.p.n.graf@bluewin.ch>
Description Main properties and regression procedures using a generalization of the Dirichlet distribution called Simplicial Generalized Beta distribution. It is a new distribution on the simplex (i.e. on the space of compositions or positive vectors with sum of components equal to 1). The Dirichlet distribution can be constructed from a random vector of independent Gamma variables divided by their sum. The SGB follows the same construction with generalized Gamma instead of Gamma variables. The Dirichlet exponents are supplemented by an overall shape parameter and a vector of scales. The scale vector is itself a composition and can be modeled with auxiliary variables through a log-ratio transformation. Graf, M. (2017, ISBN: 978-84-947240-0-8). See also the vignette enclosed in the package.
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# Description

Package SGB contains a generalization of the Dirichlet distribution, called the Simplicial Generalized Beta (SGB). It is a new distribution on the simplex (i.e. on the space of compositions or positive vectors with sum of components equal to 1). The Dirichlet distribution can be constructed from a random vector of independent Gamma variables divided by their sum. The SGB follows the same construction with generalized Gamma instead of Gamma variables. The Dirichlet exponents are supplemented by an overall shape parameter and a vector of scales. The scale vector is itself a composition and can be modeled with auxiliary variables through a log-ratio transformation.

#### **Details**

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MarginPlots Histograms, quantile and probability plots for

the z(u)-transforms of parts

SGB-package SGB Package SGB

SGBLik SGB log-likelihood and gradient

SGBdistrib Density and random generator for the SGB

distribution

SGButil Computation of scales and z-vectors

Tabulation Tabulation of overall SGB regression results

with AIC and matrix view of regression

coefficients

arc dataset carseg dataset

covest.SGB Classical and robust asymptotic covariance

matrix

ocar ocar data set oilr oilr data set

regSGB Regression for compositions following a SGB

distribution

stepSGB Stepwise backward elimination for SGB

regression

summaryA.SGB Aitchison expectation and mode under the SGB

distribution

Further information is available in the following vignettes:

vignette SGB multivariate regression (source)

# Author(s)

Monique Graf

Maintainer: Monique Graf <monique.p.n.graf@bluewin.ch>

#### References

Graf, M. (2017). A distribution on the simplex of the Generalized Beta type. *In J. A. Martin-Fernandez (Ed.), Proceedings CoDaWork 2017*, University of Girona (Spain), 71-90.

```
## Result of a regression object:
summary(oilr)
```

4 arc

arc

# Description

39 (sand,silt,clay) compositions in an Arctic lake in function of depth.

arc dataset

# Usage

```
data("arc")
```

#### **Format**

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

```
sand sand partsilt silt partclay clay partdepth depth (m)
```

#### Source

Aitchison, J. (1986). *The Statistical Analysis of Compositional Data*. Monographs on Statistics and Applied Probability. Chapman and Hall Ltd (reprinted 2003 with additional material by the Blackburn Press, London (UK).

# References

Coakley, J.P. and Rust, B.R. (1968). Sedimentation in an Arctic lake. *J. Sed. Petrology*, **38**, 1290-1300.

```
data(arc)
str(arc)
```

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B2i

Balances to isometric log-ratio

# **Description**

Coefficients of log of parts in a balance matrix, (+1) for numerator and (-1) for denominator, are transformed into the corresponding isometric log-ratio (ilr) coefficients

# Usage

```
B2i(bal, balnames=FALSE)
```

#### **Arguments**

bal a  $(D-1 \times D)$  balance matrix with cells +1, 0 or -1.

balnames logical, if TRUE, balance names are attributed to ilr transforms; if FALSE (de-

fault) ilr transforms are numbered ilr1 to ilrD1, where D1 = D - 1 and D is

the number of parts.

#### **Details**

Two scalars multiplying positive and negative cells respectively are defined for each row of the matrix bal in such a way that the resulting matrix defines the ilr transformation to apply to the log of a compositional vector. The output transformation matrix is transposed for application to a compositional dataset where the compositions are the rows.

#### Value

```
a D \times (D-1) matrix giving the coefficients of the ilr transforms
```

# References

Pawlowsky-Glahn, V., J. J. Egozcue, and R. Tolosana-Delgado (2007). Lecture Notes on Compositional Data Analysis.

```
bal <- matrix(c(1,-1,0,1,1,-1),nrow=2, byrow=TRUE)
colnames(bal) <- paste("l.P",1:3,sep="")
bal
B2i(bal)

rownames(bal) <- paste("B",1:2,sep="")
bal
B2i(bal,balnames=TRUE)
B2i(bal)</pre>
```

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carseg

carseg dataset

#### **Description**

Segment shares of car sales in five categories according to the size of the car chassis, with explanatory variables.

# Usage

```
data("carseg")
```

#### **Format**

A data frame with 152 observations on the following 13 variables.

SA Segment share in category A

SB Segment share in category B

**SC** Segment share in category C

SD Segment share in category D

**SE** Segment share in category E

expend quarterly household expenditures

sent monthly confidence indicator made up of several branches

FBCF monthly households investment

PAC binary vector indicating the incentive period

PIB Gross domestic product

price gas oil price

rates monthly short term interest rates

month sequential month number (1 to 150)

#### **Details**

This dataset consists of simulated monthly segment market shares (SA to SE) corresponding to the 5 segments of a certain brand during 150 consecutive months (01/2003 to 08/2015). The set of explanatory variables was selected by Morais and Thomas-Agnan (2019) as being the most meaningful to explain the segment shares. Names have been simplified.

#### References

Morais, J. and Thomas-Agnan, C. (2019), Impact of economic context on automobile market segment shares: a compositional approach, *Case Studies in Business, Industry and Government Statistics*, in press.

```
data(carseg)
summary(carseg[,(6:12)])
```

covest.SGB 7

covest.SGB Classical and robust asymptotic covariance matrix
--

# Description

Computation of two covariance matrices of the estimators of parameters in a SGB regression. The first is based on the Hessian and the second is the sandwich estimator.

# Usage

```
covest.SGB(x, d, u, V, weight=rep(1,dim(d)[1]), x0 = NULL, hessian = NULL, ind = NULL, shape1 = NULL)
```

# Arguments

X	vector of parameters (shape1,coefi,shape2) where shape1 is the overall shape, coefi is the vector of regression coefficients (see initpar.SGB) and shape2 the vector of the $D$ Dirichlet shape parameters; $D$ : number of parts. shape1 and shape2 must be positive.
d	data matrix of explanatory variables (with constant vector if required in the model) $(n \times m)$ ; $n$ : sample size, $m$ : number of auxiliary variables.
u	data matrix of compositions (variables to be explained) $n \times D$ .
V	full rank transformation of log(parts) into log-ratios, matrix $D \times (D-1)$ .
weight	vector of length $n$ ; positive observation weights, default rep(1,n). Should be scaled to sum to $n$ .
×0	specification of the initial parameter vector of length $npar$ (optional), default: NULL, no specification.
hessian	Hessian matrix (optional), see regSGB, default: NULL, no specification. In this case the Hessian is computed numerically.
ind	vector of length equal to the number of fixed parameters; specifies the indices of the fixed components in the vector of parameters $\boldsymbol{x}$ (possible for shape1 and coefi (regression coefficients) only).
shape1	fixed value of the overall shape parameter, if heq = heqa . SGB or heq = heqab . SGB. Default is 1.

## **Details**

This function is internally called by regSGB. In this case the Hessian is the output of auglag and is numerically computed.

A design based covariance matrix of the parameters can be obtained by linearization as the covariance matrix of the scores.

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#### Value

a list with Data frame with summary Initial = x0 (if specified), Estimate = x, StdErr1 = ordinary asymptotic standard error of parameters, StdErr = robust asymptotic standard error, p.value = asymptotic normal p-value based on StdErr. For shape1,  $H_0$  is "shape1=shape1", or "shape1=1" if shape1=NULL. The other parameters are tested against 0. signif = significance code based on p.value. matrix  $n \times npar$ . Each row contains the (unweighted) derivatives of the logscores density at a data point w.r.t the parameters. ordinary asymptotic covariance matrix, inverse of minus the Hessian. vcov1 StdErr1 vector of ordinary asymptotic standard error of parameters. robust asymptotic covariance matrix.

#### References

varest2 StdErr

Huber, P. J. (1967). The behavior of maximum likelihood estimates under nonstandard conditions. In *Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability*, Volume 1, pp. 221-233.

vector of robust asymptotic standard error of parameters.

#### See Also

regSGB for creating oilr.

```
data(arc)
data(oilr)

## compositions
da <- as.matrix(log(arc[["depth"]]),ncol=1)
ua <- as.matrix(arc[,1:3])

## ilr transforms
c1 <- 1/sqrt(2)
c2 <- 1/sqrt(6)
Vilr <- matrix(c(-c1,c1,0,-c2,-c2,2*c2),nrow=3)
colnames(Vilr) <- c("ilr1","ilr2")
Vilr

covs <- covest.SGB(oilr[["par"]], da, ua, Vilr)

## Compare the ordinary and robust correlation matrices of parameters estimates.</pre>
```

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```
## (Ordinary) covariance based on inverse Hessian
vcov1 <- covs[["vcov1"]]
StdErr1 <- covs[["StdErr1"]]
## Estimated correlation matrix
vcor1 <- diag(1/StdErr1) %*% vcov1 %*% diag(1/StdErr1)
round(vcor1,2)
## Robust (Huber's sandwich estimator):
StdErr <- covs[["StdErr"]]
vcov <- covs[["vcov"]]
## Estimated correlation matrix
round(diag(1/StdErr) %*% vcov %*% diag(1/StdErr),2)</pre>
```

EqualityConstr

Equality constraints for overall shape and/or regression parameters and jacobian

# Description

Setting of equality constraints on parameters.

heqa. SGB sets the overall shape parameter to shape1.

heqb. SGB sets specified regression parameters to 0.

heqab. SGB is a combination of both.

heqa. SGB. jac, heqb. SGB. jac, heqab. SGB. jac compute the corresponding Jacobians.

# Usage

```
heqa.SGB(x, d, u, bound, shape1, ...)
heqa.SGB.jac(x, ...)
heqb.SGB(x, d, u, bound, shape1, index, ...)
heqb.SGB.jac(x, d, u, bound, shape1, index, ...)
heqab.SGB(x, d, u, bound, shape1, index, ...)
heqab.SGB.jac(x, d, u, bound, shape1, index, ...)
```

# **Arguments**

х	current vector of parameters (shape1, coefi, shape2) where shape1 is the overall shape, coefi is the vector of regression coefficients (see <code>initpar.SGB</code> ) and shape2 the vector of $D$ Dirichlet shape parameters.
d	data matrix of explanatory variables (without constant vector) $(N \times m)$ ; $N$ : sample size, $m$ : number of explanatory variables.
u	data matrix of compositions (independent variables) $(N \times D)$ ; $D$ : number of parts.
bound	not used.

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shape1 chosen fixed value of the overall shape parameter.

Default shape 1 = 1 for heqa. SGB and heqab. SGB.

shape1 is not fixed in hegb. SGB.

index vector of length equal to the number of fixed parameters; specifies the indices of

the fixed components in the vector of parameters x, such that for

heqa.SGB, heqa.SGB.jac: index=1. The fixed value of the overall shape pa-

rameter is shape1 (by default 1).

heqb.SGB, heqb.SGB.jac: index= c(...) with ... the indices of regression pa-

rameters to be set to 0.

heqab.SGB, heqab.SGB.jac: index=c(1,...); shape1 is the fixed value of the overall shape parameter, and ... the indices of the regression parameters to be

set to 0.

... not used.

#### **Details**

These functions are invoked by regSGB through the specification of the function name, shape1 and/or index.

#### Value

heqa. SGB, heqab. SGB, heqab. SGB: vector of the same length as index specifying the current value of x[index] or x[1]-shape1, where x is the current vector of parameters. It should be near zero at convergence of the regression algorithm.

heqa.SGB.jac, heqb.SGB.jac, heqab.SGB.jac: the corresponding jacobian matrices of dimensions  $length(index) \times length(x)$ .

# See Also

```
regSGB, summary.regSGB
```

```
## parameter vector for a 3 parts composition with one explanatory variable (+ intercept):
x <- c(1,3.2,0.04,0.05,6,7:9)

## shape1 fixed to 1.5:
heqa.SGB(x,d,u,bound,1.5)
heqa.SGB.jac(x)

## Parameters 3 (first slope) and 4 (second intercept) fixed to 0:
heqb.SGB(x,d,u,bound,shape1,c(3,4))
heqb.SGB.jac(x,d,u,bound,shape1,c(3,4))

## Parameters 1, 3, 4 fixed to 1.5, 0, 0 respectively:
heqab.SGB(x,d,u,bound,1.5,c(1,3,4))
heqab.SGB.jac(x,d,u,bound,1.5,c(1,3,4))</pre>
```

EZ.SGB

EZ.SGB

Expectations of Z under the SGB distribution

# Description

Expectations under Lebesgue and Aitchison measures for the transformed composition  $Z=C((U/scale)^{shape1})$  and  $C(Z^{1/shape1})$ , where C(.) is the closure operation.

## Usage

```
EZ.SGB(D, x)
```

# **Arguments**

X	vector of parameters (shape1,coefi,shape2) where shape1 is the overall shape,
	coefi is the vector of regression coefficients (see initpar. SGB) and shape 2 the
	vector of $D$ Dirichlet shape parameters
D	number of parts

## Value

A matrix with 4 rows and D columns giving on each row the expectation of parts

```
EZ E(Z), expectation under the (ordinary) Lebesgue measure, EAZ E_A(Z), expectation under the Aitchison measure, EZa E(Z^{1/shape1}), expectation under the (ordinary) Lebesgue measure, EAZa E_A(Z^{1/shape1}), expectation under the Aitchison measure.
```

# See Also

zval

```
set.seed(1234)
x <- c(2,rnorm(4,0,1),1.8,3.1,4.0)
D <- 3
EZ.SGB(D,x)</pre>
```

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GenGammaDistrib

Generalized Gamma distribution

#### **Description**

Density and random generation of the generalized gamma distribution.

#### Usage

```
dggamma(x, shape1, scale, shape2)
rggamma(n, shape1, scale, shape2)
```

#### **Arguments**

x vector of positive values
 n number of simulated vectors
 shape1 overall shape parameter
 scale vector of scales. Should be of the same length as x

shape2 vector of Dirichlet parameters. Should be of the same length as x.

#### **Details**

```
\log \text{ density at } x>0:\\ \log(shape1/scale)-lgamma(shape2)+(shape1*shape2-1)*log(x/scale)-(x/scale)^{shape1}
```

#### Value

```
dggamma: Generalized gamma density evaluated at x rggamma: Generalized gamma random deviates
```

# References

Stacy, E.W. (1962). "A Generalization of the Gamma Distribution." *Annals of Mathematical Statistics* **33**(3): 1187-1192.

Johnson, N.L.; Kotz, S; Balakrishnan, N. (1994) *Continuous Univariate Distributions*, Volume 1, 2nd Edition. Wiley. ISBN 0-471-58495-9 (Section 17.8.7)

```
set.seed(12345) u1 <- rggamma(10,2,1,1.4) # 10 random deviates with scale 1 set.seed(12345) u <- rggamma(10,2,1:10,1.4) # 10 random deviates with scale 1:10, repectively u u/u1 dggamma(u,2,1:10,1.4)
```

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GoodnessFit	Goodness of fit tests on the marginal distributions of each part in a SGB model

# **Description**

Kolmogorov-Smirnov goodness of fit tests Cramer-von-Mises goodness of fit tests.

#### Usage

```
ks.SGB(u,shape1,shape2,scale,alpha=0.05)
cvm.SGB(u,shape1,shape2,scale,alpha=0.05)
## S3 method for class 'testSGB'
print(x,...)
```

## Arguments

u	data matrix of compositions (independent variables) $(N \times D)$ ; $D$ : number of parts
shape1	$positive\ number, overall\ shape\ parameter\ of\ the\ SGB\ distribution.\ See\ SGB distrib.$
shape2	vector of length $D$ , Dirichlet shape parameters of the SGB distribution. See ${\sf SGBdistrib}$ .
scale	matrix of the same dimensions as u, containing the shape compositions, or positive number if the scales of all parts are identical. See SGBdistrib.
alpha	overall level of the test, default 0.05.
х	an object of class "testSGB".
	further arguments passed to or from other methods.

#### **Details**

```
ks.SGB calls ks.test and cvm.SGB calls cvm.test.
```

Consider  $z = C[(u/scale)^{shape1}]$ , where C[.] is the closure operation. The scale compositions scale may be modelled with auxiliary variables. Under the SGB hypothesis, the components of z should be marginally beta-distributed. The functions provide D tests, one for each part.

Theoretically, the parameters should be known and not estimated on the data. Thus the test using estimated parameters is conservative.

The cutoff value is based on the false discovery rate for multiple comparisons (Benjamini and Hochberg, 1995), which is simply alpha\*i/D for the i-th ordered p-value, i=1,...,D (number of tests). Reject the null hypothesis if at least one p-value is smaller than the cutoff. The overall level is then alpha. The proof of the result does not use an independence assumption between the tests.

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#### Value

A list of class 'testSGB' with the following components:

method either "One-sample Kolmogorov-Smirnov test" or "Cramer-von Mises test of

goodness-of-fit"

Compositions name of the dataset u

tests data frame with D rows and 3 columns: test statistics for each part against the

beta distribution and corresponding p-values and cutoff. Any p-value smaller than the cutoff means that the assumption of the beta distribution for all the

margins is rejected.

A print method exists for the class "testSGB".

#### References

Benjamini, Y. and Y. Hochberg (1995). Controlling the false discovery rate: A practical and powerful approach to multiple testing. *Journal of the Royal Statistical Society*. Series B (Methodological) 57 (1), 289-300.

Birnbaum, Z. W. and Fred H. Tingey (1951), One-sided confidence contours for probability distribution functions. *The Annals of Mathematical Statistics*, **22**/4, 592-596.

Conover, William J. (1971), *Practical Nonparametric Statistics*. New York: John Wiley & Sons. Pages 295-301 (one-sample Kolmogorov test), 309-314 (two-sample Smirnov test).

Csorgo, S. and Faraway, J.J. (1996) The exact and asymptotic distributions of Cramer-von Mises statistics. *Journal of the Royal Statistical Society*, Series B **58**, 221-234.

Durbin, J. (1973), Distribution theory for tests based on the sample distribution function. SIAM.

Marsaglia, G., Wai Wan Tsang and Jingbo Wang (2003), Evaluating Kolmogorov's distribution. *Journal of Statistical Software*, **8**/18.

#### See Also

SGBdistrib for the theoretical distribution, oilr for the regression results.

```
## Generate 1000 random variates according to SGB(shape1,rep(1/3,3),shape2)
shape1 <- 0.6
shape2 <- c(10,20, 30)
rnum <- rSGB(1000,shape1,rep(1,3)/3,shape2)
ks.SGB(rnum,shape1=shape1, shape2=shape2,scale=1)
## same result as
ks.SGB(rnum,shape1=shape1,scale= matrix(rep(1/3,3000),ncol=3), shape2=shape2)
library(goftest)
cvm.SGB(rnum,shape1=shape1,scale= matrix(rep(1/3,3000),ncol=3), shape2=shape2)</pre>
```

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```
## Arctic lake data
# oilr is a SGB regression object, see \code{\link{oilr}}.
data(oilr)
                                                                  # regSGB object
data(arc)
ua <- arc[1:3]
                                                                  # compositions
## Kolmogorov-Smirnov goodness of fit test
ks.SGB(ua,shape1=oilr[["par"]][1],shape2=oilr[["par"]][4:6],scale=oilr[["scale"]])
## Rounding shape1 affects the results less than rounding shape2.
ks. SGB (ua, shape 1= round (oilr[["par"]][1], 3), shape 2= round (oilr[["par"]][4:6], 1), shape 2= round (oilr[["par"][["par"][4:6], 1), shape 2= round (oilr[["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par"][["par
   scale=oilr[["scale"]])
ks.SGB(ua,shape1=round(oilr[["par"]][1],1),shape2=round(oilr[["par"]][4:6],3),
   scale=oilr[["scale"]])
## Cramer-von-Mises goodness of fit test
library(goftest)
 cvm. SGB(ua, shape1=oilr[["par"]][1], shape2=oilr[["par"]][4:6], scale=oilr[["scale"]]) \\
```

Imputation

Imputation of missing parts in compositions from a SGB model

# **Description**

Applied to a completely missing composition, the function returns the Aitchison expectation. Applied to a partially missing composition, it returns the conditional Aitchison expectation, given the observed sub-composition.

Applied to a complete case, it returns the complete case.

#### Usage

```
impute.regSGB(obj, dsup, usup)
```

# **Arguments**

obj list, output of regSGB.

dsup data frame with explanatory variables for the incomplete compositions. Missing

values not allowed.

usup compositions corresponding to dsup. On each row, the non-missing parts sum

to 1.

## Value

data frame with imputed compositions instead of missing or partially missing compositions. Complete cases are also returned.

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# **Examples**

```
## Arctic lake
data(arc)
arcmis <- arc
arc[11:13.]
## Introduce NA alues
                        # "core" observation
arcmis[11,2] <- NA
arcmis[12,3] <- NA
                        # outlying clay value
arcmis[13,1:3] <- NA  # totally missing observation</pre>
umis <- arcmis[,1:3]</pre>
umis <- umis/rowSums(umis,na.rm=TRUE)</pre>
umis[11:13,]
d <- data.frame(depth=arc[["depth"]])</pre>
## original compositions
arc[11:13,1:3]
## unconditional predicted value
MeanA.SGB(oilr[["par"]][1],oilr[["scale"]],oilr[["par"]][4:6])[11:13,]
## predicted value given the sub-composition (sand,clay) for 11, (sand,silt) for 12
impute.regSGB(oilr,arcmis,umis)[11:13, ]
impute.regSGB(oilr,arcmis[11:13, ],umis[11:13, ]) # same result.
```

InequalityConstr

Inequality constraints and jacobian

# Description

Setting of inequality constraints on shape parameters.

hin. SGB sets inequality constraints on the shape parameters in a SGB regression.

hin. SGB. jac defines the corresponding Jacobian.

# Usage

```
hin.SGB(x, d, u, bound, ...)
hin.SGB.jac(x, d, u, ...)
```

#### **Arguments**

x vector of parameters (shape1, coefi, shape2) where shape1 is the overall shape, coefi is the vector of regression coefficients (see initpar.SGB) and shape2 the vector of D Dirichlet shape parameters.

d data matrix of explanatory variables (without constant vector)  $(N \times m)$ ; N: sample size, m: number of auxiliary variables.

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u	data matrix of compositions (independent variables) $(N \times D)$ ; $D$ : number of parts.
bound	the estimates of shapes are constrained by shape1*shape2[i] > bound, i=1, , D. By default bound = 2.1.
	not used.

#### **Details**

These functions are invoked internally by regSGB with bound specified by the user.

shape1 is constrained to be larger than 0.1, in order to avoid numerical problems and shape2 must be positive.

Moments of ratios of parts only exist up to bound. Thus bound = 2.1 guarantees the existence of variances of ratios of parts.

#### Value

```
hin. SGB: vector of length D+1 with the current value of c(shape1-0.1, shape1*shape2-bound). It should be non-negative at convergence of the regression algorithm.
hin. SGB. jac: corresponding jacobian matrix of dimensions (D+1)\times length(x).
```

## **Examples**

```
## Parameter vector for a 3 parts composition with one explanatory variable (+ intercept): x <- c(1,3.2,0.04,0.05,6,7:9) bound <- 2.1 u <- t(c(0.1,0.5,0.4)) # only used to compute the number of parts. hin.SGB(x, d, u, bound) # = c(shape1-0.1, shape1*shape2-bound,shape2) # all must be positive.
```

**InitialParameters** 

*Initial parameters estimates and comparison* 

# **Description**

initpar. SGB computes an initial vector of parameters.

condshape2 computes the shape2 parameters by the same method as initpar.SGB, but from an arbitrary set of parameters (shape1,coefi) (e.g. the result of a SGB regression fit). These approximations are compared with the shape2 estimates.

compushape2 is internally called by initpar. SGB and condshape2. It computes shape2 parameters in function of shape1 and given regression parameters coefi.

#### **Usage**

```
initpar.SGB(d, u, V, weight = rep(1, dim(u)[1]), shape1 = 1, Mean2 = TRUE) condshape2(x,d,u,V) compushape2(shape1, coefi, d, u, V)
```

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#### **Arguments**

d	data matrix of explanatory variables (without constant vector) $(n \times m)$ ; $n$ : sample size, $m$ : number of auxiliary variables
u	data matrix of compositions (independent variables) $(n\times D);D$ : number of parts
V	full rank transformation of log(parts) into log-ratios, matrix $D \times (D-1)$
weight	vector of length $n$ ; positive observation weights, default rep(1,n). Should be scaled to sum to $n$ .
shape1	positive number, overall shape parameter
Mean2	logical, if TRUE (default), the computed shape2 parameters are each replaced by their average.
coefi	vector of regression coefficients of length $(m+1)*(D-1)$ , resp. $D-1$ constants, then $D-1$ coef. of the 1st expl. variable,, $D-1$ coef. of the $m$ -th expl. variable
X	fitted SGB regression parameters, see regSGB.

#### **Details**

The main function here is initpar. SGB. The initial value of shape1 must be specified by the user; by default, it takes the value 1. In the initial regression model, each column of  $\log(u)$  % \* % V is regressed by OLS on the columns of d. coefi is the vector of regression parameters, first the D-1 terms associated with the first explanatory variable in d, and so on similarily for each explanatory variable. The initial scale compositions are computed by back-transforming the predicted values to the simplex and used to compute the vector  $z = C[(u/scale)^{shape1}]$ , where C[.] is the closure operation. Wicker et al. (2008), see also Ng et al. (2011) p.74-75, describe a procedure to find initial values for the shape parameters in a Dirichlet distribution. Their method is used on the (approximate) Dirichlet vector z.

## Value

```
initpar.SGB:
```

vector of length (1 + (D-1)\*(m+1) + D) containing initial values for (shape1,coefi,shape2). condshape2:

list with two components: 1. title and 2. data-frame with 2 columns: fitted shape2 and Wicker's approximation.

#### References

Wicker, N., J. Muller, R. K. R. Kalathur, and O. Poch (2008). A maximum likelihood approximation method for Dirichlet's parameter estimation. *Computational Statistics & Data Analysis* **52** (3), 1315-1322.

Kai Wang Ng, Guo-Liang Tian, Man-Lai Tang (2011). *Dirichlet and Related Distributions: Theory, Methods and Applications*. Wiley Series in Probability and Statistics.

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#### **Examples**

```
## Explanatory variable
da <- data.frame(l.depth=log(arc[["depth"]]))</pre>
damat <- as.matrix(da)</pre>
## Compositions
ua <- arc[,1:3]
## alr transforms
Va \leftarrow matrix(c(1,0,-1,0,1,-1),nrow=3)
colnames(Va) <- c("alr1","alr2")</pre>
## Initial values
initpar.SGB(damat,ua,Va)
initpar.SGB(damat,ua,Va,Mean2=FALSE)
## Conditional shape2 values; same as parameters computed with initpar
condshape2(initpar.SGB(damat,ua,Va,Mean2=FALSE),damat,ua,Va)
## Comparison with fitted parameters
oa <- regSGB(damat, as.matrix(ua), Va)
condshape2(oa[["par"]],damat,ua,Va)
```

MarginPlots

Histograms, quantile and probability plots for the z(u)-transforms of parts

#### **Description**

These functions draw a plot for each part in the dataset.

#### Usage

```
hzbeta(u, obj, weight = rep(1,dim(u)[1]) )
qzbeta(u, obj, weight = rep(1,dim(u)[1]) )
pzbeta(u, obj, weight = rep(1,dim(u)[1]) )
```

### **Arguments**

```
u data matrix of compositions (independent variables) (N \times D); D: number of parts

obj list, result of regSGB. See regSGB.

weight vector of length n; positive observation weights, default rep(1,n).
```

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#### **Details**

Let U follow a SGB(shape1, scale, shape2) distribution. Then the composition

$$Z = C[(U/scale)^{shape1}]$$

is called the z(u)-transform of U.

Z follows a Dirichlet(shape2) distribution and each part  $Z_i, i = 1, ..., D$  is Beta-distributed with parameters (shape2[i], sum(shape2)-shape2[i]).

Goodness of fit plots are produced for the parts of the z(u)-transforms against the Beta distribution. Each function creates D plots, where D is the number of parts.

hzbeta: histograms and the corresponding Beta-densities,

qzbeta: marginal quantile plots,

pzbeta: marginal probability plots.

If weight is specified, weighted histgrams, quantile and probability plots are drawn.

#### Value

D plots are produced comparing the marginal distribution of the parts of the z(u) compositions with the theoretical Beta distribution.

# **Examples**

```
## Arctic lake data
data(arc)
# Compositions
ua <- arc[,1:3]

# SGB regression
data(oilr)

# plot
par(mfrow=c(3,3))
hzbeta(ua,oilr)
qzbeta(ua,oilr)
pzbeta(ua,oilr)</pre>
```

ocar

ocar data set

#### **Description**

Car segment shares SGB regression with formula

# Usage

```
data("ocar")
```

#### Format

List of 25 items, see regSGB.

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#### **Details**

ocar is the same regression as object3 in regSGB, Example 3.

#### **Examples**

```
data(ocar)
ocar
summary(ocar) # regSGB summary
ocar[["kkt1"]] # first KKT condition
ocar[["V"]]
             # matrix of log-ratio transformation
## ocar has been created by the following commands:
## Car segment shares
data(carseg)
## Extract the compositions
uc <- as.matrix(carseg[,(1:5)])</pre>
## Define the log-ratio transformation matrix
Vc <- matrix(c( 1, 0, 0, 0,
             -1, 1, 0, 0,
              0,-1, 1, 0,
              0, 0,-1, 1,
              0, 0, 0,-1),ncol=4,byrow=TRUE)
colnames(Vc) <- c("AB", "BC", "CD", "DE")</pre>
rownames(Vc) <- colnames(uc)</pre>
۷c
## Formula
Form <- Formula(AB | BC | CD | DE \sim log(expend) + I(PAC*log(expend)) + log(sent) + log(FBCF) +
               log(price) + rates)
ocar <- regSGB(Form, data = list(carseg, uc, Vc), shape10=4.4)
```

oilr

oilr data set

# **Description**

Arctic lake SGB regression based on isometric log-ratio transforms

# Usage

```
data("oilr")
```

# **Format**

List of 25 items, see regSGB.

#### **Examples**

```
data(oilr)
oilr
summary(oilr) # regSGB summary
oilr[["kkt1"]] # first KKT condition
              # matrix of log-ratio transformation
oilr[["V"]]
## oilr has been created by the following commands:
## Arctic lake data
data(arc)
# Compositions
ua <- arc[,1:3]
## ilr transforms
c1 <- 1/sqrt(2)
c2 <- 1/sqrt(6)
Vilr \leftarrow matrix(c(-c1,c1,0,-c2,-c2,2*c2),nrow=3)
colnames(Vilr) <- c("ilr1","ilr2")</pre>
Vilr
## Formula
F1 <- Formula(ilr1 | ilr2 ~ -1 + log(depth) )
# SGB regression object
oilr <- regSGB(F1, data= list(arc, ua, Vilr), shape10=0.5, bound=2.1)
```

regSGB

Regression for compositions following a SGB distribution

#### **Description**

Explanatory variables may influence the scale vector through a linear model applied to a log-ratio transform of the compositions. The shape parameters do not depend on explanatory variables. The overall shape parameter shape1 is common to all parts, whereas the Dirichlet shape parameters vector shape2 are specific to each part, i.e. shape2[j] is the Dirichlet parameter for u[i,j],  $i=1,\ldots,n$ , (n=number of compositions in the dataset u).

# Usage

```
regSGB(d, ...)
## Default S3 method:
regSGB(d, u, V, weight=rep(1,dim(d)[1]),
    shape10 = 1, bound = 2.1, ind = NULL, shape1 = NULL, Mean2 = TRUE,
    control.optim = list(trace=0,fnscale=-1),
    control.outer = list(itmax=1000,ilack.max=200,trace=TRUE, kkt2.check =TRUE,
    method = "BFGS"),...)
```

```
## S3 method for class 'formula'
regSGB(Formula, data= list(), weight=rep(1,dim(d)[1]),
    shape10 = 1, bound = 2.1, ind = NULL, shape1 = 1, Mean2=TRUE,
    control.optim = list(trace=0,fnscale=-1),
    control.outer = list(itmax=1000,ilack.max=200,trace=TRUE,kkt2.check =TRUE,
    method = "BFGS"),...)
## S3 method for class 'regSGB'
print(x, ...)
## S3 method for class 'regSGB'
summary(object, digits=3,...)
```

# **Arguments**

Formula	formula of class Formula, see Formula.
d	data matrix of explanatory variables (without constant vector) $(n \times m)$ ; $n$ : sample size, $m$ : number of auxiliary variables.
u	data matrix of compositions (independent variables) $(n \times D)$ ; $D$ : number of parts.
V	log-ratio transformation matrix $(D \times (D-1))$ .
data	a list with 3 components d, u and V.
weight	vector of length $n$ ; positive observation weights, default rep(1,n). Should be scaled to sum to $n$ .
shape10	positive number, initial value of the overall shape parameter, default 1.
bound	<pre>inequality constraints on the estimates of shapes: shape1*shape2[i] &gt; bound, i=1,,D. By default bound = 2.1, see InequalityConstr.</pre>
ind	vector of length equal to the number of fixed parameters; see index in EqualityConstr. Default ind = NULL (no fixed parameters).
shape1	fixed value of the overall shape parameter if min(ind)=1. Default is 1.
Mean2	logical, if TRUE (default), the computed shape2 parameters are each replaced by their average. See initpar.SGB.
control.optim	list of control parameters for optim, see optim. Default is from auglag, except list(fnscale = -1). Always specify fnscale = -1.
control.outer	list of control parameters to be used by the outer loop in constrOptim.nl, see auglag. Default is from auglag, except list(itmax = 1000, ilack.max = 200.
object	an object of class "regSGB".
digits	number of decimal places for print, default 3.
x	an object of class "regSGB".
	not used.

#### **Details**

It is advisable to use the formula to specify the model for easy comparison between models. Without formula, the d matrix of explanatory variables must contain exactly the variables used in the model, whereas with formula other variables can be included as well. Variable transformations can be utilized within the formula, see Example 4 below with the indicator I and the log.

Constraints on parameters can be introduced, see example 5 and EqualityConstr for more details. Use weight for pseudo-likelihood estimation. weight is scaled to n, the sample size.

A design based covariance matrix of the parameters can be obtained by linearization as the covariance matrix of the scores.

#### Value

A list of class 'regSGB' with the following components:

The first 13 form the output from auglag.

par Vector of length npar. Parameters that optimize the nonlinear objective func-

tion, satisfying constraints, if convergence is successful.

value The value of the objective function at termination.

counts A vector of length 2 denoting the number of times the objective and its gradient

were evaluated, respectively.

convergence An integer code indicating the type of convergence. 0 indicates successful con-

vergence. Positive integer codes indicate failure to converge.

message A character string giving any additional information on convergence returned by

optim, or NULL.

outer.iteration

Number of outer iterations.

lambda Values of the Lagrangian parameter. This is a vector of the same length as the

total number of inequalities and equalities. It must be zero for inactive inequalities are proportionally for a children and some boxes are size for a conditional and the conditional and

ities; non-negative for active inequalities; and can have any sign for equalities.

sigma Value of augmented penalty parameter for the quadratic term.

gradient Gradient of the augmented Lagrangian function at convergence. It should be

small.

hessian Hessian of the augmented Lagrangian function at convergence. It should be

negative definite for maximization.

ineq Values of inequality constraints at convergence. All of them must be non-

negative.

equal Values of equality constraints at convergence. All of them must be close to zero.

kkt1 A logical variable indicating whether or not the first-order KKT conditions were

satisfied (printed 1 if conditions satisfied and 0 otherwise).

kkt2 A logical variable indicating whether or not the second-order KKT conditions

were satisfied (printed 1 if conditions satisfied and 0 otherwise).

scale  $n \times D$  matrix, the estimated scale compositions, see bval.

meanA Aitchison expectation at estimated parameters.

fitted.values  $(n \times (D-1))$  matrix, estimated log-ratio transforms.

residuals Observed minus estimated log-ratio transforms.

scores matrix  $n \times npar$ . Each row contains the (unweighted) derivatives of the log-

density at a data point w.r.t the parameters.

Rsquare ratio of total variation of meanA and total variation of compositions u.

vcov The robust covariance matrix of parameters estimates, see covest. SGB.

StdErr1 Ordinary asymptotic standard errors of parameters.

StdErr Robust asymptotic standard errors of parameters.

fixed.par Indices of the fixed parameters.

summary The summary from covest.SGB.

AIC AIC criterion.

V log-ratio transformation matrix (same as corresponding input parameter V)

call Arguments for calling regSGB.

Formula Expression for formula.

#### References

Graf, M. (2017). A distribution on the simplex of the Generalized Beta type. *In J. A. Martin-Fernandez (Ed.)*, *Proceedings CoDaWork 2017*, University of Girona (Spain), 71-90.

Hijazi, R. H. and R. W. Jernigan (2009). Modelling compositional data using Dirichlet regression models. *Journal of Applied Probability and Statistics*, **4** (1), 77-91.

Kotz, S., N. Balakrishnan, and N. L. Johnson (2000). *Continuous Multivariate Distributions*, Volume 1, Models and Applications. John Wiley & Sons.

Madsen, K., H. Nielsen, and O. Tingleff (2004). Optimization With Constraints. *Informatics and Mathematical Modelling*, Technical University of Denmark.

Monti, G. S., G. Mateu-Figueras, and V. Pawlowsky-Glahn (2011). Notes on the scaled Dirichlet distribution. In V. Pawlowsky-Glahn and A. Buccianti (Eds.), Compositional data analysis. Theory and applications. Wiley.

Varadhan, R. (2015). alabama: Constrained Nonlinear Optimization. R package version 2015.3-1.

Wicker, N., J. Muller, R. K. R. Kalathur, and O. Poch (2008). A maximum likelihood approximation method for Dirichlet parameter estimation. Computational Statistics & Data Analysis 52 (3), 1315-1322.

Zeileis, A. and Y. Croissant (2010). Extended model formulas in R: Multiple parts and multiple responses. *Journal of Statistical Software* **34** (1), 1-13.

#### See Also

stepSGB, for an experimental stepwise descending regression, initpar. SGB, for the computation of initial parameters. This function uses Formula, auglag.

```
## Regression for car segment shares
data(carseg)
## Extract the compositions
uc <- as.matrix(carseg[,(1:5)])</pre>
## Extract the explanatory variables
attach(carseg)
## Example 1: without formula
## -----
## Change some variables
dc <- data.frame(1.exp1=log(expend)*PAC,1.exp0=log(expend)*(1-PAC), 1.sent=log(sent),</pre>
1.FBCF=log(FBCF), l.price=log(price), rates)
## Define the log-ratio transformation matrix
Vc <- matrix(c( 1,0,0,0,</pre>
               -1,1,0,0,
               0, -1, 1, 0,
               0,0,-1,1,
               0,0,0,-1),ncol=4,byrow=TRUE)
colnames(Vc) <- c("AB", "BC", "CD", "DE")</pre>
rownames(Vc) <- colnames(uc)</pre>
۷c
# 2 next rows only necessary when calling regSGB without a formula.
dc1 <- cbind("(Intercept)"= 1 , dc)</pre>
dc1 <- as.matrix(dc1)</pre>
object10 <- regSGB(dc1,uc, Vc,shape10=4.4)
summary(object10)
## Example 2: same with formula
## -----
## Define the formula
Form <- Formula(AB | BC | CD | DE ~ 1.exp1 + 1.exp0 + 1.sent + 1.FBCF + 1.price + rates)
## Regression with formula
object1 <- regSGB(Form, data= list(dc, uc, Vc), shape10=4.4)
summary(object1)
## Example 3: Usage of I()
## -----
Form2 <- Formula(AB | BC | CD | DE \sim I(l.exp1 + l.exp0) + l.exp1 +l.sent +
                1.FBCF + 1.price + rates )
object2 <- regSGB(Form2,data= list(dc, uc, Vc),shape10=4.4)
object2
## Example 4: Usage of variable transformations on the original file
```

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```
Form3 <- Formula(AB | BC | CD | DE ~ log(expend) + I(PAC*log(expend)) + log(sent) + log(FBCF) +
                 log(price) + rates)
object3 <- regSGB(Form3, data=list(carseg, uc, Vc),shape10=4.4)</pre>
object3
object2[["par"]]-object3[["par"]]
                                      # same results
## Example 5: Fixing parameter values
## 1. In the following regression we condition on shape1 = 2.36.
object4 <- regSGB(Form3,data=list(carseg, uc, Vc),</pre>
                  shape10 = 4.4, bound = 2.0, ind = 1, shape1 = 2.36)
summary(object4)
## 2. In the following regression we condition on shape1 = 2.36 and the coefficient of
## log(FBCF).BC = 0. Notice that it is the 19th parameter.
object5 <- regSGB(Form3,data=list(carseg, uc, Vc),</pre>
                  shape10 = 4.4, bound = 2.0, ind = c(1,19) , shape1 = 2.36)
summary(object5)
object3[["AIC"]]
object4[["AIC"]] # largest AIC
object5[["AIC"]]
```

SGBdistrib

Density and random generator for the SGB distribution

# Description

dSGB computes the density for a given argument u (a composition) and given parameters. rSGB generates n compositions for given parameters.

#### Usage

```
dSGB(u, shape1, scale, shape2) rSGB(n, shape1, scale, shape2)
```

## **Arguments**

u	vector of length $D$ containing the composition
shape1	overall shape parameter. shape $1 = 1$ for a Dirichlet composition.
scale	vector of the same length as u containing the scales of parts. If missing, scales are set to 1.
shape2	vector of length $D$ containing the (Dirichlet) shapes for each part.
n	number of observations.

#### **Details**

The number of columns in u and the number of components in shape2 must match.

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# Value

dSGB gives the density, rSGB generates a ( $n \times D$  - matrix with random compositions on each row.

#### See Also

```
bval,zval
```

# **Examples**

```
u1 <- c(0.2,0.3,0.5)
scale1 <- c(0.25,0.33,0.32)
shape1 <- 1
shape2 <- c(0.8,3,0.9)
dSGB(u1,shape1,scale1,shape2)
rSGB(10,shape1,scale1,shape2)

## with equal scales
dSGB(u1,shape1,shape2=shape2)
rSGB(10,shape1,shape2=shape2)</pre>
```

 ${\tt SGBLik}$ 

SGB log-likelihood and gradient

# Description

fn. SGB gives the log-likelihood and gr. SGB the gradient vector of the log-likelihood.

# Usage

```
fn.SGB(x, d, u, V, weight, ...) gr.SGB(x, d, u, V, weight, ...)
```

# **Arguments**

Х	vector of parameters (shape1, coefi, shape2) where shape1 is the overall shape, coefi is the vector of regression coefficients (see initpar.SGB) and shape2 the vector of $D$ Dirichlet shape parameters.
d	data matrix of explanatory variables (without constant vector) $(nxm)$ ; $n$ : sample size, $m$ : number of auxiliary variables
u	data matrix of compositions (independent variables) $(nxD)$ ; $D$ : number of parts
V	full rank transformation of log(parts) into log-ratios, matrix $(Dx(D-1))$
weight	vector of length $n$ ; positive observation weights, default rep(1,n). Should be scaled to sum to $n$ .
	others parameters that might be introduced.

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#### **Details**

The analytical expression for fn. SGB is found in the vignette "SGB regression", Section 3.2. More details in Graf(2017).

#### Value

```
fn.SGB: value of the log-likelihood at parameter x gr.SGB: gradient vector at parameter x.
```

#### References

Graf, M. (2017). A distribution on the simplex of the Generalized Beta type. *In J. A. Martin-Fernandez (Ed.), Proceedings CoDaWork 2017*, University of Girona (Spain), 71-90.

#### See Also

```
regSGB
```

# **Examples**

```
## Explanatory variable
da <- data.frame(l.depth=log(arc[["depth"]]))
damat <- as.matrix(da)

## Compositions
ua <- as.matrix(arc[,1:3])

## alr transforms
Va <- matrix(c(1,0,-1,0,1,-1),nrow=3)
colnames(Va) <- c("alr1","alr2")
Va

## Initial values
x <- initpar.SGB(damat,ua,Va)
fn.SGB(x, damat, ua, Va,weight=rep(1,dim(da)[1]))
gr.SGB(x, damat, ua, Va,weight=rep(1,dim(da)[1]))</pre>
```

SGButil

Computation of scales and z-vectors

# Description

bval computes the scale for each observed composition from the parameters and auxiliary variables for that observation.

zval computes the z-vector for each observed composition, i.e. the transform that is Dirichlet distributed under the SGB model for the observed composition.

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#### Usage

```
bval(D, x, d, V)
zval(u, x, d, V)
```

#### **Arguments**

D	number of parts
Х	vector of parameters (shape1,coefi,shape2) where shape1 is the overall shape, coefi is the vector of regression coefficients (see initpar. SGB) and shape2 the vector of $D$ Dirichlet shape parameters
d	$(n \times m)$ - data matrix of explanatory variables (variables corresponding to coefi); $n$ : sample size, $m$ : number of auxiliary variables
u	$(n\times D)$ - data matrix of compositions (independent variables); $D\!\!:$ number of parts
V	$D\times (D-1)$ - matrix specifying the full rank transformation of log(parts) into log-ratios

#### **Details**

See Graf (2017), Equation (8), or the vignette "SGB regression", Equation (1).

# Value

transformed composition of length D.

#### References

Graf, M. (2017). A distribution on the simplex of the Generalized Beta type. *In J. A. Martin-Fernandez (Ed.), Proceedings CoDaWork 2017*, University of Girona (Spain), 71-90.

```
## Example with 2 compositions
u <- matrix(c(0.2,0.4,0.5,0.5,0.3,0.2),nrow=2,byrow=TRUE)
u
D <- NCOL(u) # number of parts

## auxiliary variable
d <- matrix(c(3.2,4.6),ncol=1)

## log-ratio transformation
V <- matrix(c(c(1,-1,0)/sqrt(2),c(1,1,-2)/sqrt(6)),ncol=2)

## vector of parameters:
shape1 <- 2.00
coefi <- c(-0.78,  0.06,  0.96, -0.11)
shape2 <- c(1.80,  3.10,  4.00)
x <-c(shape1, coefi, shape2)</pre>
```

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```
bval(D,x,d,V)
zval(u,x,d,V)
```

stepSGB

Stepwise backward elimination for SGB regression

# Description

Stepwise elimination of the non significant regression parameters. Possibility to assign a fixed value shape1 to the overall shape parameter.

# Usage

```
stepSGB(obj0, d, u, weight = rep(1, dim(d)[1]), shape10 = obj0[["par"]][1],
bound = 2.1, shape1 = NULL, Mean2 = TRUE, maxiter = 10,
control.optim = list(fnscale = -1),
control.outer = list(itmax = 1000, ilack.max = 200, trace = TRUE,
    kkt2.check = TRUE, method = "BFGS") )
```

# **Arguments**

obj0	object of class regSGB, see regSGB.
d	data matrix of explanatory variables (without constant vector) $(n \times m)$ ; $n$ : sample size, $m$ : number of auxiliary variables.
u	data matrix of compositions (independent variables) $(n \times D)$ ; $D$ : number of parts.
weight	vector of length $n$ ; positive observation weights, default rep(1,n). Should be scaled to sum to $n$ .
shape10	positive number, initial value of the overall shape parameter, default obj $0[["par"]][1]$ .
bound	<pre>inequality constraints on the estimates of shapes: shape1*shape2[i] &gt; bound, i=1,,D. By default bound = 2.1, see InequalityConstr.</pre>
shape1	fixed value of the overall shape parameter. Default is NULL (no fixed value).
Mean2	logical, if TRUE (default), the initial shape2 parameters are each replaced by their average. See initpar. SGB.
maxiter	maximum number of iterations, i.e. attempts to set a parameter to 0.
control.optim	list of control parameters for optim, see optim. Default is from auglag, except list(fnscale = -1). Always specify fnscale = -1.
control.outer	list of control parameters to be used by the outer loop in constrOptim.nl, see auglag. Default is from auglag, except list(itmax = 1000, ilack.max = 200).
• • •	not used.

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#### **Details**

This is an experimental procedure for searching a set of non-significant parameters that will be set to zero. The shape parameters are excluded from the elimination procedure. The algorithm starts with obj0, output of regSGB. The p-values for the regression parameters in summary(obj0) are taken in decreasing order. The parameter with the largest p-value is set to zero and regSGB computes the regression with this constraint. If the AIC value is smaller than the AIC in obj0, the parameter with the next largest p-value in obj0 is set to zero and the regression with the two constraints is computed. The process iterates until either a larger AIC is found or maxiter is attained.

The initial value of the overall shape parameter is set to the estimated value in the full model obj0. The other initial values are computed as in regSGB.

There is the possibility to fix the value of the overvall shape parameter, if shape1 is given a positive number  $a_0$  (default NULL, no fixed value).

If regSGB was called without Formula, the data-frame with auxiliary variables for stepSGB follows the same rules as for the initial regSGB object, see Example 1 in regSGB.

#### Value

A list of class 'stepSGB' with the following 5 components:

reg A list with the following components:

full Object of class regSGB, same as obj0, see regSGB. iter1 Object of class regSGB obtained at iteration 1.

...

iterk Object of class regSGB obtained at iteration k.

Formula The original formula, or NULL iter Value of k, the last iteration.

tab Data frame with k+1 columns, overall results and k iterations. The rows are

value Log-likelihood

n.par Total number of parameters (including the shape2 param.)

n.par.fixed Number of fixed parameters.

AIC Value of the AIC criterion. convergence 0 if converged.

kkt1 1 if first Karush-Kuhn-Tucker criterion fulfilled, zero otherwise. kkt2 1 if second Karush-Kuhn-Tucker criterion fulfilled, zero otherwise.

counts. function Number of times the objective function (the log-likelihood)

was evaluated.

counts.gradient Number of times the gradient was evaluated. \

call Arguments for calling stepSGB.

#### References

```
vignette("SGB regression", package = "SGB")
```

#### See Also

```
regSGB, initpar.SGB, auglag.
```

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#### **Examples**

```
data(carseg)
## Extract the compositions
uc <- as.matrix(carseg[,(1:5)])
## Initial regression
data(ocar)

step_ocar <- stepSGB(ocar, carseg, uc, bound=2.1, control.outer=list(trace=FALSE))
summary(step_ocar[["reg"]][["full"]])
summary(step_ocar[["reg"]][["iter4"]])
step_ocar[["tab"]]</pre>
```

summaryA.SGB

Aitchison expectation and mode under the SGB distribution

## Description

The expectation and mode in the log-ratio space, transformed back to the simplex.

# Usage

```
MeanA.SGB(shape1, scale, shape2)
ModeA.SGB(shape1, scale, shape2)
MeanAobj.SGB(obj)
ModeAobj.SGB(obj)
```

# Arguments

shape1	overall shape parameter. shape1 = 1 for a Dirichlet composition.
scale	vector of length $\boldsymbol{D}$ or matrix with $\boldsymbol{D}$ columns containing the scales of parts.
shape2	vector of length $D$ containing the (Dirichlet) shapes for each part.
obj	list, result of regSGB. See regSGB.

#### **Details**

MeanA, ModeA compute Aitchison expectation and mode in function of the SGB distribution parameters, whereas MeanAobj, ModeAobj compute Aitchison expectation and mode in function of the model variables in an SGB regression object.

#### Value

A matrix or vector of dimensions  $(n \times D)$ . Each row gives the Aitchison expectation for compositions having the corresponding set of auxiliary variables.

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#### References

Aitchison, J. (1986). *The Statistical Analysis of Compositional Data*. Monographs on Statistics and Applied Probability. Chapman and Hall Ltd (reprinted 2003 with additional material by the Blackburn Press, London (UK).

#### See Also

oilr.

# **Examples**

```
set.seed(1234)
   x \leftarrow c(2, rnorm(4, 0, 1), 1.8, 3.1, 4.0)
   d <- c(3.2, 4.6)
   V \leftarrow t(matrix(c(1/sqrt(2),-1/sqrt(2),0,
                  1/sqrt(6),1/sqrt(6),-2/sqrt(6)),
                  nrow=2,byrow=TRUE))
   D <- 3
   shape1 <- x[1]
   scale <- bval(D,x,d,V)</pre>
   shape2 <- x[(length(x)-D+1):length(x)]
# Expectation
   MeanA.SGB(shape1,scale,shape2)
# Mode
   ModeA.SGB(shape1, scale, shape2)
## Arctic lake data
# oilr is a SGB regression object
data(oilr)
MeanAobj.SGB(oilr)
                      # is the same as oilr[["meanA"]]
ModeAobj.SGB(oilr)
```

Tabulation

Tabulation of overall SGB regression results with AIC and matrix view of regression coefficients

# Description

table.regSGB: Value of the log-likelihood, number of parameters, AIC criterion, optimality tests and iterations counts.

coefmat: regression coefficients in matrix form with significance level.

# Usage

```
table.regSGB(object)
coefmat(object,digits=3)
```

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# **Arguments**

object an object of class regSGB

digits number of decimal places for the coefficients

#### Value

table.regSGB: Data frame with one column, with the overall statistics results.

value the maximum log-likelihood
n.par the number of parameters
n.par.fixed the number of fixed parameters

AIC the AIC criterion

Rsquare total variance of estimated over total variance of observed compositions

convergence the convergence code (0: converged, others, see auglag).

kkt1 the first Karush-Kuhn-Tucker conditions (1=TRUE, 0=FALSE), see auglag.
kkt2 the second Karush-Kuhn-Tucker conditions (1=TRUE, 0=FALSE), see auglag.

counts.function

number of times the log-likelihood was evaluated.

counts.gradient

number of times the gradient was evaluated.

coefmat: character matrix with the regression coefficients arranged in columns, one for each logratio transform. Each coefficient is followed by the significance level.

#### See Also

```
regSGB, oilr, auglag.
```

```
## Overall model statistics
table.regSGB(oilr)
##
print(coefmat(oilr),quote=FALSE)
## it is a subset of
summary(oilr)
```

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