# Package 'cgam'

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Type Package

Title Constrained Generalized Additive Model

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Description A constrained generalized additive model is fitted by the cgam routine. Given a set of predictors, each of which may have a shape or order restrictions, the maximum likelihood estimator for the constrained generalized additive model is found using an iteratively reweighted cone projection algorithm. The ShapeSelect routine chooses a subset of predictor variables and describes the component relationships with the response. For each predictor, the user needs only specify a set of possible shape or order restrictions. A model selection method chooses the shapes and orderings of the relationships as well as the variables. The cone information criterion (CIC) is used to select the best combination of variables and shapes. A genetic algorithm may be used when the set of possible models is large. In addition, the cgam routine implements a two-dimensional isotonic regression using warped-plane splines without additivity assumptions. It can also fit a convex or concave regression surface with triangle splines without additivity assumptions. See Liao X, Meyer MC (2019)<a href="https://doi.org/10.18637/jss.v089.i05">doi:10.18637/jss.v089.i05</a> for more details.

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2 Contents

# **Contents**

Index

best.fit	3
cgam	4
cgamm	11
COforest	14
conc	17
conv	19
cubic	20
decr	21
decr.conc	22
decr.conv	24
in.or.out	26
incr	27
incr.conc	28
incr.conv	30
mental	32
Ord	33
plasma	35
plotpersp	36
plotpersp_control	38
predict.cgam	39
s	42
s.conc	43
s.conc.conc	45
s.conv	47
s.conv.conv	48
s.decr	50
s.decr.conc	52
s.decr.conv	53
s.decr.decr	55
s.decr.incr	57
s.incr	59
s.incr.conc	61
s.incr.conv	62
s.incr.decr	64
s.incr.incr	66
shapes	68
ShapeSelect	<b>7</b> 0
testpar	73
tree	76
umbrella	78

80

best.fit 3

best.fit

Extract the Best Fit Returned by the ShapeSelect Routine

# Description

This is a subroutine that only works for the ShapeSelect routine. It returns an object of the cgam class given the variables and their shapes chosen by the ShapeSelect routine.

## Usage

```
best.fit(x)
```

# **Arguments**

Х

An object of the ShapeSelect class.

## Value

The best fit returned by the ShapeSelect routine, which is an object of class cgam.

# Author(s)

Xiyue Liao

#### See Also

```
cgam, ShapeSelect
```

4

Constrained Generalized Additive Model Fitting

cgam

## **Description**

The partial linear generalized additive model is fitted using the method of maximum likelihood, where shape or order restrictions can be imposed on the non-parametrically modelled predictors with optional smoothing, and no restrictions are imposed on the optional parametrically modelled covariate.

## Usage

```
cgam(formula, cic = FALSE, nsim = 100, family = gaussian, cpar = 1.5,
data = NULL, weights = NULL, sc_x = FALSE, sc_y = FALSE, pnt = TRUE,
pen = 0, var.est = NULL, gcv = FALSE, pvf = TRUE)
```

## **Arguments**

formula

A formula object which gives a symbolic description of the model to be fitted. It has the form "response ~ predictor". The response is a vector of length n. The specification of the model can be one of the three exponential families: gaussian, binomial and poisson. The systematic component  $\eta$  is E(y), the log odds of y=1, and the logarithm of E(y) respectively. A predictor can be a non-parametrically modelled variable with or without a shape or order restriction, or a parametrically modelled unconstrained covariate. In terms of a non-parametrically modelled predictor, the user is supposed to indicate the relationship between the systematic component  $\eta$  and a predictor x in the following way:

Assume that  $\eta$  is the systematic component and x is a predictor:

**incr(x):**  $\eta$  is increasing in x. See incr for more details.

**s.incr(x):**  $\eta$  is smoothly increasing in x. See s.incr for more details.

**decr**(x):  $\eta$  is decreasing in x. See decr for more details.

**s.decr(x):**  $\eta$  is smoothly decreasing in x. See s.decr for more details.

**conc(x):**  $\eta$  is concave in x. See conc for more details.

**s.conc(x):**  $\eta$  is smoothly concave in x. See s.conc for more details.

**conv(x):**  $\eta$  is convex in x. See conv for more details.

**s.conv(x):**  $\eta$  is smoothly convex in x. See s. conv for more details.

**incr.conc(x):**  $\eta$  is increasing and concave in x. See incr.conc for more details.

**s.incr.conc(x):**  $\eta$  is smoothly increasing and concave in x. See s.incr.conc for more details.

**decr.conc(x):**  $\eta$  is decreasing and concave in x. See decr.conc for more details

**s.decr.conc(x):**  $\eta$  is smoothly decreasing and concave in x. See s.decr.conc for more details.

**incr.conv(x):**  $\eta$  is increasing and convex in x. See incr.conv for more details. **s.incr.conv(x):**  $\eta$  is smoothly increasing and convex in x. See s.incr.conv for more details.

**decr.conv(x):**  $\eta$  is decreasing and convex in x. See decr.conv for more details.

**s.decr.conv(x):**  $\eta$  is smoothly decreasing and convex in x. See s.decr.conv for more details.

 $\mathbf{s}(\mathbf{x})$ :  $\eta$  is smooth in x. See  $\mathbf{s}$  for more details.

**tree(x):**  $\eta$  has a tree-ordering in x. See tree for more details.

**umbrella(x):**  $\eta$  has an umbrella-ordering in x. See umbrella for more details. Logical flag indicating if or not simulations are used to get the cic value. The default is cic = FALSE

The number of simulations used to get the cic parameter. The default is nsim = 100.

A parameter indicating the error distribution and link function to be used in the model. It can be a character string naming a family function or the result of a call to a family function. This is borrowed from the glm routine in the stats package. There are four families used in csvy: Gaussian, binomial, poisson, and Gamma. Note that if family = Ord is specified, a proportional odds regression model with shape constraints is fitted. This is under development.

A multiplier to estimate the model variance, which is defined as  $\sigma^2 = SSR/(n-cpar*edf)$ . SSR is the sum of squared residuals for the full model and edf is the effective degrees of freedom. The default is cpar = 1.2. The user-defined value must be between 1 and 2. See Meyer, M. C. and M. Woodroofe (2000) for more details.

An optional data frame, list or environment containing the variables in the model. The default is data = NULL.

An optional non-negative vector of "replicate weights" which has the same length as the response vector. If weights are not given, all weights are taken to equal 1. The default is weights = NULL.

Logical flag indicating if or not continuous predictors are normalized. The default is  $sc_x = FALSE$ .

Logical flag indicating if or not the response variable is normalized. The default is  $sc_y = FALSE$ .

User-defined penalty parameter. It must be non-negative. It will only be used in a warped-plane spline fit or a triangle spline fit. The default is pen = 0.

Logical flag indicating if or not penalized constrained regression splines are used. It will only be used in a warped-plane spline fit or a triangle spline fit. The default is pnt = TRUE.

To do a monotonic variance function estimation, the user can set var.est = s.incr(x) or var.est = s.decr(x). See s.incr and s.decr for more details. The default is var.est = NULL.

Logical flag indicating if or not gcv is used to choose a penalty term in warpedplane surface fit. The default is gcv = FALSE.

Logical flag indicating if or not simulations are used to find the p-value of the test of linear vs double monotone in warped plane surface fit.

cic

nsim

family

cpar

data

weights

sc\_y
pen

sc\_x

pnt

var.est

gcv

pvf

## **Details**

We consider generalized partial linear models with independent observations from an exponential family of the form  $p(y_i; \theta, \tau) = exp[\{y_i\theta_i - b(\theta_i)\}\tau - c(y_i, \tau)], i = 1, \ldots, n$ , where the specifications of the functions b and c determine the sub-family of models. The mean vector  $\mu = E(y)$  has values  $\mu_i = b'(\theta_i)$ , and is related to a design matrix of predictor variables through a monotonically increasing link function  $g(\mu_i) = \eta_i, i = 1, \ldots, n$ , where  $\eta$  is the systematic component and describes the relationship with the predictors. The relationship between  $\eta$  and  $\theta$  is determined by the link function b.

For the additive model, the systematic component is specified for each observation by  $\eta_i = f_1(x_{1i}) + \ldots + f_L(x_{Li}) + z_i'\beta$ , where the functions  $f_l$  describe the relationships of the non-parametrically modelled predictors  $x_l$ ,  $\beta$  is a parameter vector, and  $z_i$  contains the values of variables to be modelled parametrically. The non-parametric components are modelled with shape or order assumptions with optional smoothing, and the solution is obtained through an iteratively re-weighted cone projection, with no back-fitting of individual components.

Suppose that  $\eta$  is a n by 1 vector. The matrix form of the systematic component and the predictor is  $\eta = \phi_1 + \ldots + \phi_L + Z\beta$ , where  $\phi_l$  is the individual component for the lth non-parametrically modelled predictor,  $l = 1, \ldots, L$ , and Z is an n by p design matrix for the parametrically modelled covariate.

To model the component  $\phi_l$ , smooth regression splines or non-smooth ordinal basis functions can be used. The constraints for the component  $\phi_l$  are in  $C_l$ . In the first case,  $C_l = \{\phi_l \in R^n : \phi_l = v_l + B_l\beta_l$ , where  $\beta_l \geq 0$  and  $v_l \in V_l\}$ , where  $B_l$  has regression splines as columns and  $V_l$  is the linear space contained in  $C_l$ , and in the second case,  $C_l = \{\phi \in R^n : A_l\phi \geq 0 \text{ and } B_l\phi = 0\}$ , for inequality constraint matrix  $A_l$  and equality constraint matrix  $B_l$ .

The set  $C_l$  is a convex cone and the set  $C = C_1 + \ldots + C_p + Z$  is also a convex cone with a finite set of edges, where the edges are the generators of C, and Z is the column space of the design matrix Z for the parametrically modelled covariate.

An iteratively re-weighted cone projection algorithm is used to fit the generalized regression model over the cone C.

See references cited in this section and the official manual (https://cran.r-project.org/package=coneproj) for the R package coneproj for more details.

#### Value

etahat	The fitted systematic component $\eta$ .
muhat	The fitted mean value, obtained by transforming the systematic component $\eta$ by the inverse of the link function.
vcoefs	The estimated coefficients for the basis spanning the null space of the constraint set.
xcoefs	The estimated coefficients for the edges corresponding to the smooth predictors with no shape constraint and shape-restricted predictors.
zcoefs	The estimated coefficients for the parametrically modelled covariate, i.e., the estimation for the vector $\beta$ .
ucoefs	The estimated coefficients for the edges corresponding to the predictors with an umbrella-ordering constraint.

tcoefs	The estimated coefficients for the edges corresponding to the predictors with a tree-ordering constraint.
coefs	The estimated coefficients for the basis spanning the null space of the constraint set and edges corresponding to the shape-restricted and order-restricted predictors.
cic	The cone information criterion proposed in Meyer(2013a). It uses the "null expected degrees of freedom" as a measure of the complexity of the model. See Meyer(2013a) for further details of cic.
d0	The dimension of the linear space contained in the cone generated by all constraint conditions.
edf0	The estimated "null expected degrees of freedom". It is a measure of the complexity of the model. See Meyer (2013a) and Meyer (2013b) for further details.
edf	The constrained effective degrees of freedom.
etacomps	The fitted systematic component value for non-parametrically modelled predictors. It is a matrix of which each row is the fitted systematic component value for a non-parametrically modelled predictor. If there are more than one such predictors, the order of the rows is the same as the order that the user defines such predictors in the formula argument of cgam.
у	The response variable.
xmat_add	A matrix whose columns represent the shape-restricted predictors and smooth predictors with no shape constraint.
zmat	A matrix whose columns represent the basis for the parametrically modelled covariate. The user can choose to include a constant vector in it or not. It must have full column rank.
ztb	A list keeping track of the order of the parametrically modelled covariate.
tr	A matrix whose columns represent the predictors with a tree-ordering constraint.
umb	A matrix whose columns represent the predictors with an umbrella-ordering constraint.
tree.delta	A matrix whose rows are the edges corresponding to the predictors with a tree-ordering constraint.
umbrella.delta	A matrix whose rows are the edges corresponding to the predictors with an umbrella-ordering constraint.
bigmat	A matrix whose rows are the basis spanning the null space of the constraint set and the edges corresponding to the shape-restricted and order-restricted predictors.
shapes	A vector including the shape and partial-ordering constraints in a cgam fit.
shapesx	A vector including the shape constraints in a cgam fit.
prior.w	User-defined weights.
wt	The weights in the final iteration of the iteratively re-weighted cone projections.
wt.iter	Logical flag indicating if or not iteratively re-weighted cone projections may be used. If the response is gaussian, then wt.iter = FALSE; if the response is binomial or poisson, then wt.iter = TRUE.

family	The family parameter defined in a cgam formula.
SSE0	The sum of squared residuals for the linear part.
SSE1	The sum of squared residuals for the full model.
pvals.beta	The approximate p-values for the estimation of the vector $\beta$ . A t-distribution is used as the approximate distribution.
se.beta	The standard errors for the estimation of the vector $\beta$ .
null_df	The degree of freedom for the null model of a cgam fit, i.e., the model only containing a constant vector.
df	The degree of freedom for the null space of a cgam fit.
resid_df_obs	The observed degree of freedom for the residuals of a cgam fit.
null_deviance	The deviance for the null model of a cgam fit, i.e., the model only containing a constant vector.
deviance	The residual deviance of a cgam fit.
tms	The terms objects extracted by the generic function terms from a cgam fit.
capm	The number of edges corresponding to the shape-restricted predictors.
capms	The number of edges corresponding to the smooth predictors with no shape constraint.
capk	The number of non-constant columns of zmat.
capt	The number of edges corresponding to the tree-ordering predictors.
capu	The number of edges corresponding to the umbrella-ordering predictors.
xid1	A vector keeping track of the beginning position of the set of edges in bigmat for each shape-restricted predictor and smooth predictor with no shape constraint in xmat.
xid2	A vector keeping track of the end position of the set of edges in bigmat for each shape-restricted predictor and smooth predictor with no shape constraint in xmat.
tid1	A vector keeping track of the beginning position of the set of edges in bigmat for each tree-ordering factor in tr.
tid2	A vector keeping track of the end position of the set of edges in bigmat for each tree-ordering factor in tr.
uid1	A vector keeping track of the beginning position of the set of edges in bigmat for each umbrella-ordering factor in umb.
uid2	A vector keeping track of the end position of the set of edges in bigmat for each umbrella-ordering factor in umb.
zid	A vector keeping track of the positions of the parametrically modelled covariate.
vals	A vector storing the levels of each variable used as a factor.
zid1	A vector keeping track of the beginning position of the levels of each variable used as a factor.
zid2	A vector keeping track of the end position of the levels of each variable used as a factor.

nsim The number of simulations used to get the cic parameter. A vector storing the names of the shape-restricted predictors and the smooth xnms predictors with no shape constraint in xmat. The name of the response variable. ynm znms A vector storing the names of the parametrically modelled covariate. A logical scalar showing if or not a variable is a parametrically modelled covariis\_param ate, which could be a linear term or a factor. is\_fac A logical scalar showing if or not a variable is a factor. knots A list storing the knots used for each shape-restricted predictor and smooth predictor with no shape constraint. For a smooth, constrained and a smooth, unconstrainted predictor, knots is a vector of more than 1 elements, and for a shape-restricted predictor without smoothing, knots = 0. numknots A vector storing the number of knots for each shape-restricted predictor and smooth predictor with no shape constraint. For a smooth, constrained and a smooth, unconstrainted predictor, numknots > 1, and for a shape-restricted predictor without smoothing, numknots = 0. A character vector storing the *space* parameter to create knots for each shapesps restricted predictor. The centering terms used to make edges for shape-restricted predictors. ms

cpar The cpar argument in the cgam formula

vh The estimated monotonic variance function.

kts.var The knots used in monotonic variance function estimation.

call The matched call.

#### Author(s)

Mary C. Meyer and Xiyue Liao

## References

Liao, X. and Meyer, M. C. (2019) cgam: An R Package for the Constrained Generalized Additive Model. *Journal of Statistical Software* 89(5), 1–24.

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Meyer, M. C. and M. Woodroofe (2000) On the degrees of freedom in shape-restricted regression. *Annals of Statistics* **28**, 1083–1104.

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Mammen, E. and K. Yu (2007) Additive isotonic regression. *IMS Lecture Notes-Monograph Series Asymptotics: Particles, Process, and Inverse Problems* 55, 179–195.

Huang, J. (2002) A note on estimating a partly linear model under monotonicity constraints. *Journal of Statistical Planning and Inference* **107**, 343–351.

Cheng, G.(2009) Semiparametric additive isotonic regression. *Journal of Statistical Planning and Inference* 139, 1980–1991.

Bacchetti, P. (1989) Additive isotonic models. *Journal of the American Statistical Association* 84(405), 289–294.

```
# Example 1.
 data(cubic)
 # extract x
 x <- cubic$x
 # extract y
 y <- cubic$y
 # regress y on x with no restriction with lm()
 fit.lm <- lm(y \sim x + I(x^2) + I(x^3))
 # regress y on x under the restriction: "increasing and convex"
 fit.cgam <- cgam(y ~ incr.conv(x))</pre>
 # make a plot to compare the two fits
 par(mar = c(4, 4, 1, 1))
 plot(x, y, cex = .7, xlab = "x", ylab = "y")
 lines(x, fit.cgammuhat, col = 2, lty = 2)
 lines(x, fitted(fit.lm), col = 1, lty = 1)
 legend("topleft", bty = "n", c("constrained cgam fit", "unconstrained lm fit"),
 lty = c(2, 1), col = c(2, 1)
# Example 2.
 library(MASS)
 data(Rubber)
 # regress loss on hard and tens under the restrictions:
 # "decreasing" and "decreasing"
 fit.cgam <- cgam(loss ~ decr(hard) + decr(tens), data = Rubber)</pre>
 # "smooth and decreasing" and "smooth and decreasing"
 fit.cgam.s <- cgam(loss ~ s.decr(hard) + s.decr(tens), data = Rubber)</pre>
 summary(fit.cgam.s)
 anova(fit.cgam.s)
 # make a 3D plot based on fit.cgam and fit.cgam.s
 ctl <- list(th = 120, main = "3D Plot of a Cgam Fit")</pre>
 plotpersp(fit.cgam, control = ctl)
 ctl <- list(th = 120, main = "3D Plot of a Smooth Cgam Fit")</pre>
 plotpersp(fit.cgam.s, "tens", "hard", control = ctl)
```

cgamm 11

```
# Example 3. monotonic variance estimation
 n <- 400
 x <- runif(n)</pre>
 sig < -.1 + exp(15*x-8)/(1+exp(15*x-8))
 e <- rnorm(n)
 mu < - 10*x^2
 y <- mu + sig*e
 fit <- cgam(y \sim s.incr.conv(x), var.est = s.incr(x))
 est.var <- fit$vh
 muhat <- fit$muhat</pre>
 par(mfrow = c(1, 2))
 plot(x, y)
 points(sort(x), muhat[order(x)], type = "1", lwd = 2, col = 2)
 lines(sort(x), (mu)[order(x)], col = 4)
 plot(sort(x), est.var[order(x)], col=2, lwd=2, type="1",
 lty=2, ylab="Variance", ylim=c(0, max(c(est.var, sig^2))))
 points(sort(x), (sig^2)[order(x)], col=1, lwd=2, type="1")
## Not run:
# Example 4. monotonic variance estimation with the lidar data set in SemiPar
 library(SemiPar)
 data(lidar)
 fit <- cgam(logratio ~ s.decr(range), var.est=s.incr(range), data=lidar)</pre>
 muhat <- fit$muhat</pre>
 est.var <- fit$vh
 logratio <- lidar$logratio</pre>
 range <- lidar$range</pre>
 pfit <- predict(fit, newData=data.frame(range=range), interval="confidence", level=0.95)</pre>
 upp <- pfit$upper</pre>
 low <- pfit$lower</pre>
 par(mfrow = c(1, 2))
 plot(range, logratio)
 points(sort(range), muhat[order(range)], type = "1", lwd = 2, col = 2)
 lines(sort(range), upp[order(range)], type = "1", lwd = 2, col = 4)
 lines(sort(range), low[order(range)], type = "1", lwd = 2, col = 4)
 title("Smoothly Decreasing Fit with a Point-Wise Confidence Interval", cex.main=0.5)
 plot(range, est.var, col=2, lwd=2, type="1",lty=2, ylab="variance")
 title("Smoothly Increasing Variance", cex.main=0.5)
## End(Not run)
```

12 cgamm

# Description

This routine is an addition to the main routine cgam in this package. A random-intercept component is included in a cgam model.

# Usage

```
cgamm(formula, nsim = 0, family = gaussian(), cpar = 1.2, data = NULL, weights = NULL, sc_x = FALSE, sc_y = FALSE, bisect = TRUE, reml = TRUE, nAGQ = 1L)
```

# **Arguments**

formula	A formula object which gives a symbolic description of the model to be fitted. It has the form "response ~ predictor + (1lid)", where id is the label for a group effect. For now, only gaussian responses are considered and this routine only includes a random-intercept effect. See cgam for more details.
nsim	The number of simulations used to get the cic parameter. The default is $nsim = 0$ .
family	A parameter indicating the error distribution and link function to be used in the model. For now, the options are family = gaussian() and family = binomial().
cpar	A multiplier to estimate the model variance, which is defined as $\sigma^2 = SSR/(n-cpar*edf)$ . SSR is the sum of squared residuals for the full model and edf is the effective degrees of freedom. The default is cpar = 1.2. The user-defined value must be between 1 and 2. See Meyer, M. C. and M. Woodroofe (2000) for more details.
data	An optional data frame, list or environment containing the variables in the model. The default is data = NULL.
weights	An optional non-negative vector of "replicate weights" which has the same length as the response vector. If weights are not given, all weights are taken to equal 1. The default is weights = NULL.
sc_x	Logical flag indicating if or not continuous predictors are normalized. The default is $sc_x = FALSE$ .
sc_y	Logical flag indicating if or not the response variable is normalized. The default is $sc_y = FALSE$ .
bisect	If bisect = TRUE, a 95 percent confidence interval will be found for the variance ratio parameter by a bisection method.
reml	If reml = TRUE, restricted maximum likelihood (REML) method will be used to find estimates instead of maximum likelihood estimation (MLE).
nAGQ	Integer scalar - the number of points per axis for evaluating the adaptive Gauss-Hermite approximation to the log-likelihood. Defaults to 1, corresponding to the Laplace approximation. Values greater than 1 produce greater accuracy in the evaluation of the log-likelihood at the expense of speed.

# Value

muhat The fitted fixed-effect term.

cgamm 13

A vector of estimated random-effect terms. ahat Estimate of the variance  $(\sigma^2)$  of between-cluster error terms. sig2hat Estimate of the variance  $(\sigma_a^2)$  of within-cluster error terms. siga2hat Estimate of the ratio  $(\theta)$  of two variances. thhat p-value of the test  $H_0: \sigma_a^2 = 0$ pv.siga2 ci.siga2 95 percent confidence interval for the variance of within-cluster error terms. ci.th 95 percent confidence interval for ratio of two variances. ci.rho 95 percent confidence interval for intraclass correlation coefficient. ci.sig2 95 percent confidence interval for the variance of between-cluster error terms. call The matched call.

## Author(s)

Xiyue Liao

```
# Example 1 (family = gaussian).
# simulate a balanced data set with 30 clusters
# each cluster has 30 data points
n <- 30
m <- 30
# the standard deviation of between cluster error terms is 1
# the standard deviation of within cluster error terms is 2
sige <- 1
siga <- 2
# generate a continuous predictor
x < -1:(m*n)
for(i in 1:m) {
x[(n*(i-1)+1):(n*i)] <- round(runif(n), 3)
# generate a group factor
group \leftarrow trunc(0:((m*n)-1)/n)+1
# generate the fixed-effect term
mu < -10*exp(10*x-5)/(1+exp(10*x-5))
# generate the random-intercept term asscosiated with each group
avals <- rnorm(m, 0, siga)
# generate the response
y <- 1:(m*n)
for(i in 1:m){
y[group == i] <- mu[group == i] + avals[i] + rnorm(n, 0, sige)</pre>
```

14 COforest

```
# use REML method to fit the model
ans <- cgamm(y ~ s.incr(x) + (1|group), reml=TRUE)</pre>
summary(ans)
anova(ans)
muhat <- ans$muhat
plot(x, y, col = group, cex = .6)
lines(sort(x), mu[order(x)], lwd = 2)
lines(sort(x), muhat[order(x)], col = 2, lty = 2, lwd = 2)
legend("topleft", bty = "n", c("true fixed-effect term", "cgamm fit"),
col = c(1, 2), lty = c(1, 2), lwd = c(2, 2))
# Example 2 (family = binomial).
# simulate a balanced data set with 20 clusters
# each cluster has 20 data points
  n <- 20
  m <- 20#
  N <- n*m
  # siga is the sd for the random intercept
  siga <- 1
# generate a group factor
  group \leftarrow trunc(0:((m*n)-1)/n)+1
  group <- factor(group)</pre>
# generate the random-intercept term asscosiated with each group
  avals <- rnorm(m,0,siga)</pre>
# generate the fixed-effect mean term: mu, systematic term: eta and the response: y
  x <- runif(m*n)</pre>
  mu <- 1:(m*n)
  y < -1:(m*n)
  eta <-2 * (1 + tanh(7 * (x - .8))) - 2
  eta0 <- eta
  for(i in 1:m){eta[group == i] \leftarrow eta[group == i] + avals[i]}
  for(i in 1:m){mu[group == i] <- 1 - 1 / (1 + exp(eta[group == i]))}
  for(i in 1:m){y[group == i] <- rbinom(n, size = 1, prob = mu[group == i])}
  dat <- data.frame(x = x, y = y, group = group)
  ansc <- cgamm(y \sim s.incr.conv(x) + (1|group),
  family = binomial(link = "logit"), reml = FALSE, data = dat)
  summary(ansc)
  anova(ansc)
```

COforest 15

## **Description**

This data set contains 9167 records of different species of live trees for 345 sampled forested plots measured in 2015.

## Usage

```
data("COforest")
```

#### **Format**

A data frame with 9167 observations on the following 19 variables.

PLT\_CN Unique identifier of plot

STATECD State code using Bureau of Census Federal Information Processing Standards (FIPS)

COUNTYCD County code (FIPS)

ELEV\_PUBLIC Elevation (ft) extracted spatially using LON\_PUBLIC/LAT\_PUBLIC

LON\_PUBLIC Fuzzed longitude in decimal degrees using NAD83 datum

LAT\_PUBLIC Fuzzed latitude in decimal degrees using NAD83 datum

ASPECT a numeric vector

SLOPE a numeric vector

SUBP Subplot number

TREE Tree number within subplot

STATUSCD Tree status (0:no status; 1:live tree; 2:dead tree; 3:removed)

SPCD Species code

DIA Current diameter (in)

HT Total height (ft): estimated when broken or missing

ACTUALHT Actual height (ft): measured standing or down

HTCD Height method code (1:measured; 2:actual measured-length estimated; 3:actual and length estimated; 4:modeled

TREECLCD Tree class code (2:growing-stock; 3:rough cull; 4:rotten cull)

CR Compacted crown ratio (percentage)

CCLCD Crown class (1:open grown; 2:domimant; 3:co-dominant; 4:intermediate; 5:overtopped)

## Source

It is provided by Forest Inventory Analysis (FIA) National Program.

## References

X. Liao and M. Meyer (2019). Estimation and Inference in Mixed-Effect Regression Models using Shape Constraints, with Application to Tree Height Estimation. (to appear in Journal of the Royal Statistical Society. Series C: Applied Statistics)

16 COforest

```
## Not run:
 library(dplyr)
 library(tidyr)
 data(COforest)
 #re-grouping classes of CCLCD:
 #combine dominant (2) and co-dominant (3)
 #combine intermediate (4) and overtopped (5)
 COforest = COforest
   mutate(CCLCD = replace(CCLCD, CCLCD == 5, 4))
 #make a list of species, each element is a small data frame for one species
 species = COforest
 #get the subset for quaking aspen, which is the 4th element in the species list
 sub = species$data[[4]]
 #for quaking aspen, there are only two crown classes: dominant/co-dominant
 #and intermediate/overtopped
 table(sub$CCLCD)
 # 3
         4
 #1400 217
 #for quaking aspen, there are only two tree clases: growing-stock and rough cull
 table(sub$TREECLCD)
 #2
       3
 #1591 26
 #fit the model
 ansc = cgamm(log(HT)~s.incr.conc(DIA)+factor(CCLCD)+factor(TREECLCD)
 +(1|PLT_CN), reml=TRUE, data=sub)
 #check which classes are significant
 summary(ansc)
 #fixed-effect 95
 newData = data.frame(DIA=sub$DIA,CCLCD=sub$CCLCD,TREECLCD=sub$TREECLCD)
 pfit = predict(ansc, newData,interval='confidence')
 lower = pfit$lower
 upper = pfit$upper
 #we need to use exp(muhat) later in the plot
 muhat = pfit$fit
 #get x and y
 x = sub\$DIA
 y = sub$HT
 #get TREECLCD and CCLCD
 z1 = sub\$TREECLCD
 z2 = sub\$CCLCD
 #plot fixed-effect confidence intervals
 plot(x, y, xlab='DIA (m)', ylab='HT (m)', ylim=c(min(y),max(exp(upper))+10),type='n')
```

conc 17

```
lines(sort(x[z2=3&z1=2]), (exp(pfit$fit)[z2=3&z1=2])[order(x[z2=3&z1=2])],
   col='slategrey', lty=1, lwd=2)
   lines(sort(x[z2==3&z1==2]), (exp(pfit$lower)[z2==3&z1==2])[order(x[z2==3&z1==2])],
   col='slategrey', lty=1, lwd=2)
   lines(sort(x[z2=3\&z1==2]), \; (exp(pfit\$upper)[z2=3\&z1==2])[order(x[z2=3\&z1==2])], \; (exp(pfit\$upper)[x2=3\&z1==2])[order(x[z2=3\&z1==2])], \; (exp(pfit\$upper)[x2=3\&z1==2])[order(x[z2=3\&z1==2])], \; (exp(pfit\$upper)[x2=3\&z1==2])[order(x[z2=3\&z1==2])], \; (exp(pfit\$upper)[x2=3\&z1==2])[order
   col='slategrey', lty=1, lwd=2)
   lines(sort(x[z2=4&z1==2]), (exp(pfit$fit)[z2=4&z1==2])[order(x[z2=4&z1==2])],
   col="blueviolet", lty=2, lwd=2)
   lines(sort(x[z2=4&z1==2]), (exp(pfit$lower)[z2=4&z1==2])[order(x[z2=4&z1==2])],
   col="blueviolet", lty=2, lwd=2)
   lines(sort(x[Cz2=+4&z1==2]), (exp(pfit$upper)[Cz2==+4&z1==2])[order(x[Cz2=+4&z1==2])], \\
   col="blueviolet", lty=2, lwd=2)
   lines(sort(x[Cz2==3&z1==3]), (exp(pfit\$fit)[Cz2==3\&z1==3])[order(x[Cz2==3\&z1==3])],
   col=3, lty=3, lwd=2)
   lines(sort(x[Cz2==3\&z1==3]), (exp(pfit\$lower)[Cz2==3\&z1==3])[order(x[Cz2==3\&z1==3])], \\
   col=3, lty=3, lwd=2)
   lines(sort(x[Cz2==3&z1==3]), (exp(pfit$upper)[Cz2==3&z1==3])[order(x[Cz2==3&z1==3])],
   col=3, lty=3, lwd=2)
   lines(sort(x[Cz2==4&z1==3]), (exp(pfit\$fit)[Cz2==4\&z1==3])[order(x[Cz2==4\&z1==3])],
   col=2, lty=4, lwd=2)
   lines(sort(x[Cz2==4&z1==3]), (exp(pfit$lower)[Cz2==4&z1==3])[order(x[Cz2==4&z1==3])],
   col=2, lty=4, lwd=2)
   lines(sort(x[Cz2==4&z1==3]), (exp(pfit$upper)[Cz2==4&z1==3])[order(x[Cz2==4&z1==3])],
   col=2, lty=4, lwd=2)
   legend('bottomright', bty='n', cex=.9,c('dominant/co-dominant and growing stock',
    \verb|'intermediate/overtopped| and growing stock', \verb|'dominant/co-dominant| and rough cull', \\
    'intermediate/overtopped and rough cull'), col=c('slategrey',"blueviolet",3,2),
   lty=c(1,2,3,4), lwd=c(2,2,2,2), pch=c(24,23,22,21))
   title('Quaking Aspen fits with 95
## End(Not run)
```

conc

Specify a Concave Shape-Restriction in a CGAM Formula

## **Description**

A symbolic routine to define that the systematic component  $\eta$  is concave in a predictor in a formula argument to cgam. This is the unsmoothed version.

#### Usage

```
conc(x, numknots = 0, knots = 0, space = "E")
```

18 conc

## Arguments

X	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to smoothly constrain a predictor. The value should be 0 for a shape-restricted predictor without smoothing. The default value is 0.
knots	The knots used to smoothly constrain a predictor. The value should be 0 for a shape-restricted predictor without smoothing. The default value is 0.
space	A character specifying the method to create knots. It will not be used for a shape-restricted predictor without smoothing. The default value is "E".

#### **Details**

"conc" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "conc"; the shape attribute is 4("concave"), and according to the value of the vector itself and its shape attribute, the cone edges of the cone generated by the constraint matrix, which constrains the relationship between the systematic component  $\eta$  and "x" to be concave, will be made. The cone edges are a set of basis employed in the hinge algorithm.

Note that "conc" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 4("concave"); numknots: the numknots argument in "conc"; knots: the knots argument in "conc"; space: the space argument in "conc".

## Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

#### See Also

conv

```
# generate y
x <- seq(-1, 2, by = 0.1)
n <- length(x)
y <- - x^2 + rnorm(n, .3)</pre>
```

conv 19

```
# regress y on x under the shape-restriction: "concave"
ans <- cgam(y ~ conc(x))

# make a plot
plot(x, y)
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "concave fit", col = 2, lty = 1)</pre>
```

conv

Specify a Convex Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that the systematic component  $\eta$  is convex in a predictor in a formula argument to cgam. This is the unsmoothed version.

# Usage

```
conv(x, numknots = 0, knots = 0, space = "E")
```

# Arguments

X	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to smoothly constrain a predictor. The value should be 0 for a shape-restricted predictor without smoothing. The default value is 0.
knots	The knots used to smoothly constrain a predictor. The value should be $0$ for a shape-restricted predictor without smoothing. The default value is $0$ .
space	A character specifying the method to create knots. It will not be used for a shape-restricted predictor without smoothing. The default value is "E".

## **Details**

"conv" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "conv"; the shape attribute is 3("convex"), and according to the value of the vector itself and its shape attribute, the cone edges of the cone generated by the constraint matrix, which constrains the relationship between the systematic component  $\eta$  and "x" to be convex, will be made. The cone edges are a set of basis employed in the hinge algorithm.

Note that "conv" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

20 cubic

## Value

The vector x with five attributes, i.e., name: the name of x; shape: 3("convex"); numknots: the numknots argument in "conv"; knots: the knots argument in "conv"; space: the space argument in "conv".

#### Author(s)

Mary C. Meyer and Xiyue Liao

## References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42(5)**, 1126–1139.

## See Also

conc

## **Examples**

```
# generate y
x <- seq(-1, 2, by = 0.1)
n <- length(x)
y <- x^2 + rnorm(n, .3)

# regress y on x under the shape-restriction: "convex"
ans <- cgam(y ~ conv(x))

# make a plot
plot(x, y)
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "convex fit", col = 2, lty = 1)</pre>
```

cubic

A Data Set for Cgam

## **Description**

This data set is used for several examples in the cgam package.

# Usage

```
data(cubic)
```

# Format

A data frame with 50 observations on the following 2 variables.

- x The predictor vector.
- y The response vector.

decr 21

## **Source**

STAT640 HW 14 given by Dr. Meyer.

decr	Specify a Decreasing Shape-Restriction in a CGAM Formula
decr	Specify a Decreasing Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that the systematic component  $\eta$  is decreasing in a predictor in a formula argument to cgam. This is the unsmoothed version.

## Usage

```
decr(x, numknots = 0, knots = 0, space = "E")
```

# **Arguments**

х	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to smoothly constrain a predictor. The value should be 0 for a shape-restricted predictor without smoothing. The default value is 0.
knots	The knots used to smoothly constrain a predictor. The value should be $0$ for a shape-restricted predictor without smoothing. The default value is $0$ .
space	A character specifying the method to create knots. It will not be used for a shape-restricted predictor without smoothing. The default value is "E".

# Details

"decr" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "decr"; the shape attribute is 2("decreasing"), and according to the value of the vector itself and its shape attribute, the cone edges of the cone generated by the constraint matrix, which constrains the relationship between the systematic component  $\eta$  and "x" to be decreasing, will be made. The cone edges are a set of basis employed in the hinge algorithm.

Note that "decr" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

## Value

The vector x with five attributes, i.e., name: the name of x; shape: 2("decreasing"); numknots: the numknots argument in "decr"; knots: the knots argument in "decr"; space: the space argument in "decr".

22 decr.conc

## Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42(5)**, 1126–1139.

#### See Also

```
decr.conc, decr.conv
```

# **Examples**

```
data(cubic)

# extract x
x <- - cubic$x

# extract y
y <- cubic$y

# regress y on x with the shape restriction: "decreasing"
ans <- cgam(y ~ decr(x))

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("bottomright", bty = "n", "decreasing fit", col = 2, lty = 1)</pre>
```

decr.conc

Specify a Decreasing and Concave Shape-Restriction in a CGAM Formula

# Description

A symbolic routine to define that the systematic component  $\eta$  is decreasing and concave in a predictor in a formula argument to cgam. This is the unsmoothed version.

## Usage

```
decr.conc(x, numknots = 0, knots = 0, space = "E")
```

decr.conc 23

#### **Arguments**

X	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to smoothly constrain a predictor. The value should be $0$ for a shape-restricted predictor without smoothing. The default value is $0$ .
knots	The knots used to smoothly constrain a predictor. The value should be 0 for a shape-restricted predictor without smoothing. The default value is 0.
space	A character specifying the method to create knots. It will not be used for a shape-restricted predictor without smoothing. The default value is "E".

#### **Details**

"decr.conc" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "decr.conc"; the shape attribute is 8 ("decreasing and concave"), and according to the value of the vector itself and its shape attribute, the cone edges of the cone generated by the constraint matrix, which constrains the relationship between the systematic component  $\eta$  and "x" to be decreasing and concave, will be made. The cone edges are a set of basis employed in the hinge algorithm.

Note that "decr.conc" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 8("decreasing and concave"); numknots: the numknots argument in "decr.conc"; knots: the knots argument in "decr.conc"; space: the space argument in "decr.conc".

## Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

#### See Also

```
decr.conv, decr
```

```
data(cubic)

# extract x
x <- cubic$x</pre>
```

24 decr.conv

```
# extract y
y <- - cubic$y

# regress y on x with the shape restriction: "decreasing" and "concave"
ans <- cgam(y ~ decr.conc(x))

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "decreasing and concave fit", col = 2, lty = 1)</pre>
```

decr.conv

Specify a Decreasing and Convex Shape-Restriction in a CGAM Formula

#### **Description**

A symbolic routine to define that the systematic component  $\eta$  is decreasing and convex in a predictor in a formula argument to cgam. This is the unsmoothed version.

#### **Usage**

```
decr.conv(x, numknots = 0, knots = 0, space = "E")
```

# Arguments

X	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to smoothly constrain a predictor. The value should be $0$ for a shape-restricted predictor without smoothing. The default value is $0$ .
knots	The knots used to smoothly constrain a predictor. The value should be $0$ for a shape-restricted predictor without smoothing. The default value is $0$ .
space	A character specifying the method to create knots. It will not be used for a shape-restricted predictor without smoothing. The default value is "E".

#### **Details**

"decr.conv" returns the vector " $\mathbf{x}$ " and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "decr.conv"; the shape attribute is 6("decreasing and convex"), and according to the value of the vector itself and its shape attribute, the cone edges of the cone generated by the constraint matrix, which constrains the relationship between the systematic component  $\eta$  and "x" to be decreasing and convex, will be made. The cone edges are a set of basis employed in the hinge algorithm.

decr.conv 25

Note that "decr.conv" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 6("decreasing and convex"); numknots: the numknots argument in "decr.conv"; knots: the knots argument in "decr.conv"; space: the space argument in "decr.conv".

#### Author(s)

Mary C. Meyer and Xiyue Liao

## References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

## See Also

```
decr.conc, decr
```

```
data(cubic)
# extract x
x <- - cubic$x

# extract y
y <- cubic$y

# regress y on x with the shape restriction: "decreasing" and "convex"
ans <- cgam(y ~ decr.conv(x))

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("bottomright", bty = "n", "decreasing and convex fit", col = 2, lty = 1)</pre>
```

26 in.or.out

in.or.out  ${\it To Include \ a \ Non-Parametrically \ Modelled \ Predictor \ in \ a \ SHAPESE-LECT \ Formula}$ 

## **Description**

A symbolic routine to indicate that a predictor is included as a non-parametrically modeled predictor in a formula argument to ShapeSelect.

### Usage

```
in.or.out(z)
```

# **Arguments**

Z

A non-parametrically modelled predictor which has the same length as the response vector.

#### **Details**

To include a categorical predictor, in.or.out(factor(z)) is used, and to include a linear predictor z, in.or.out(z) is used. If in.or.out is not used, the user can include z in a model by adding z or factor(z) in a ShapeSelect formula.

#### Value

The vector z with three attributes, i.e., nm: the name of z; shape: 1 or 0 (in or out of the model); type: "fac" or "lin", i.e., z is modelled as a categorical predictor or a linear predictor.

## Author(s)

Xiyue Liao

# See Also

```
shapes, ShapeSelect
```

```
## Not run:
    n <- 100
    # x is a continuous predictor
    x <- runif(n)

# generate z and to include it as a categorical predictor
    z <- rep(0:1, 50)

# y is generated as correlated to both x and z
# the relationship between y and x is smoothly increasing-convex</pre>
```

incr 27

```
y <- x^2 + 2 * I(z == 1) + rnorm(n, sd = 1)

# call ShapeSelect to find the best model by the genetic algorithm
# factor(z) may be in or out of the model
fit <- ShapeSelect(y ~ shapes(x) + in.or.out(factor(z)), genetic = TRUE)

# factor(z) isn't chosen and is included in the model
fit <- ShapeSelect(y ~ shapes(x) + factor(z), genetic = TRUE)

## End(Not run)</pre>
```

incr

Specify an Increasing Shape-Restriction in a CGAM Formula

## **Description**

A symbolic routine to define that the systematic component  $\eta$  is increasing in a predictor in a formula argument to cgam. This is the unsmoothed version.

## Usage

```
incr(x, numknots = 0, knots = 0, space = "E")
```

# Arguments

X	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to smoothly constrain a predictor. The value should be $0$ for a shape-restricted predictor without smoothing. The default value is $0$ .
knots	The knots used to smoothly constrain a predictor. The value should be $0$ for a shape-restricted predictor without smoothing. The default value is $0$ .
space	A character specifying the method to create knots. It will not be used for a shape-restricted predictor without smoothing. The default value is "E".

#### **Details**

"incr" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "incr"; the shape attribute is 1("increasing"), and according to the value of the vector itself and its attributes, the cone edges of the cone generated by the constraint matrix, which constrains the relationship between the systematic component  $\eta$  and "x" to be increasing, will be made. The cone edges are a set of basis employed in the hinge algorithm.

Note that "incr" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

28 incr.conc

## Value

The vector x with five attributes, i.e., name: the name of x; shape: 1("increasing"); numknots: the numknots argument in "incr"; knots: the knots argument in "incr"; space: the space argument in "incr".

#### Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42(5)**, 1126–1139.

#### See Also

```
incr.conc, incr.conv
```

## **Examples**

```
data(cubic)
# extract x
x <- cubic$x

# extract y
y <- cubic$y

# regress y on x with the shape restriction: "increasing"
ans <- cgam(y ~ incr(x))

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "increasing fit", col = 2, lty = 1)</pre>
```

incr.conc

Specify an Increasing and Concave Shape-Restriction in a CGAM Formula

#### **Description**

A symbolic routine to define that the systematic component  $\eta$  is increasing and concave in a predictor in a formula argument to cgam. This is the unsmoothed version.

## Usage

```
incr.conc(x, numknots = 0, knots = 0, space = "E")
```

incr.conc 29

## Arguments

X	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to smoothly constrain a predictor. The value should be $0$ for a shape-restricted predictor without smoothing. The default value is $0$ .
knots	The knots used to smoothly constrain a predictor. The value should be 0 for a shape-restricted predictor without smoothing. The default value is 0.
space	A character specifying the method to create knots. It will not be used for a shape-restricted predictor without smoothing. The default value is "E".

#### **Details**

"incr.conc" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "incr.conc"; the shape attribute is 7("increasing and concave"), and according to the value of the vector itself and its attributes, the cone edges of the cone generated by the constraint matrix, which constrains the relationship between the systematic component  $\eta$  and "x" to be increasing and concave, will be made. The cone edges are a set of basis employed in the hinge algorithm.

Note that "incr.conc" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 7("increasing and concave"); numknots: the numknots argument in "incr.conc"; knots: the knots argument in "incr.conc"; space: the space argument in "incr.conc".

## Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

#### See Also

```
incr.conv
```

```
data(cubic)
# extract x
x <- - cubic$x</pre>
```

30 incr.conv

```
# extract y
y <- - cubic$y

# regress y on x with the shape restriction: "increasing" and "concave"
ans <- cgam(y ~ incr.conc(x))

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "increasing and concave fit", col = 2, lty = 1)</pre>
```

incr.conv

Specify an Increasing and Convex Shape-Restriction in a CGAM Formula

## **Description**

A symbolic routine to define that the systematic component  $\eta$  is increasing and convex in a predictor in a formula argument to cgam. This is the unsmoothed version.

#### **Usage**

```
incr.conv(x, numknots = 0, knots = 0, space = "E")
```

# Arguments

x	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to smoothly constrain a predictor. The value should be $0$ for a shape-restricted predictor without smoothing. The default value is $0$ .
knots	The knots used to smoothly constrain a predictor. The value should be $0$ for a shape-restricted predictor without smoothing. The default value is $0$ .
space	A character specifying the method to create knots. It will not be used for a shape-restricted predictor without smoothing. The default value is "E".

#### **Details**

"incr.conv" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "incr.conv"; the shape attribute is 5("increasing and convex"), and according to the value of the vector itself and its attributes, the cone edges of the cone generated by the constraint matrix, which constrains the relationship between the systematic component  $\eta$  and "x" to be increasing and convex, will be made. The cone edges are a set of basis employed in the hinge algorithm.

incr.conv 31

Note that "incr.conv" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 5("increasing and convex"); numknots: the numknots argument in "incr.conv"; knots: the knots argument in "incr.conv"; space: the space argument in "incr.conv".

#### Author(s)

Mary C. Meyer and Xiyue Liao

## References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

# See Also

```
incr.conc, incr
```

```
data(cubic)
# extract x
x <- cubic$x

# extract y
y <- cubic$y

# regress y on x with the shape restriction: "increasing" and "convex"
ans <- cgam(y ~ incr.conv(x))

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "increasing and convex fit", col = 2, lty = 1)</pre>
```

32 mental

mental

Alachua County Study of Mental Impairment

## **Description**

The date set is from a study of mental health for a random sample of 40 adult residents of Alachua County, Florida. Mental impairment is an ordinal response with 4 categories: well, mild symptom formation, moderate symptom formation, and impaired, which are recorded as 1, 2, 3, and 4. Life event index is a composite measure of the number and severity of important life events that occurred with the past three years, e.g., birth of a child, new job, divorce, or death of a family member. It is an integer from 0 to 9. Another covariate is socio-economic status and it is measured as binary: high = 1, low = 0.

## Usage

```
data(mental)
```

#### **Format**

```
mental Mental impairment. It is an ordinal response with 4 categories recorded as 1, 2, 3, and 4. ses Socio-economic status measured as binary: high = 1, low = 0. life Life event index. It is an integer from 0 to 9.
```

## References

Agresti, A. (2010) Analysis of Ordinal Categorical Data, 2nd ed. Hoboken, NJ: Wiley.

## See Also

**Ord** 

```
# proportional odds model example
data(mental)

# model the relationship between the latent variable and life event index as increasing
# socio-economic status is included as a binary covariate
fit.incr <- cgam(mental ~ incr(life) + ses, data = mental, family = Ord)

# check the estimated probabilities P(mental = k), k = 1, 2, 3, 4
probs.incr <- fitted(fit.incr)
head(probs.incr)</pre>
```

Ord 33

0rd

Specify an Ordered Categorical Family in a CGAM Formula

# **Description**

This is a subroutine to specify an ordered catergorical family in a cgam formula. It set things up to a routine called cgam.polr. This is learned from the polr routine in the MASS package, which fits a logistic or probit regression model to an ordered categorical response. Currently only the logistic regression model is allowed.

# Usage

```
Ord(link = "identity")
```

# **Arguments**

link

The link function. Users don't need specify this term.

# **Details**

See the polr section in the official manual of the MASS package (https://cran.r-project.org/package=MASS) for details.

# Value

muhat The estimated expected value of a latent variable.

zeta Estimated cut-points defining the intervals of a latent variable such that the la-

tent variable is between two adjacent cut-points is equivalent to that the ordered

categorical response is in a category.

## Author(s)

Xiyue Liao

#### References

Agresti, A. (2002) Categorical Data. Second edition. Wiley.

## See Also

mental

34 Ord

```
## Not run:
# Example 1.
# generate the predictor and the latenet variable
n <- 500
set.seed(123)
x \leftarrow runif(n, 0, 1)
yst <-5*x^2 + rlogis(n)
# generate observed ordered response, which has levels 1, 2, 3.
cts <- quantile(yst, probs = seq(0, 1, length = 4))</pre>
yord <- cut(yst, breaks = cts, include.lowest = TRUE, labels = c(1:3), Ord = TRUE)
y <- as.numeric(levels(yord))[yord]</pre>
# regress y on x under the shape-restriction: the latent variable is "increasing-convex"
# w.r.t x
ans <- cgam(y \sim s.incr.conv(x), family = Ord)
# check the estimated cut-points
ans$zeta
# check the estimated expected value of the latent variable
head(ans$muhat)
# check the estimated probabilities P(y = k), k = 1, 2, 3
head(fitted(ans))
# check the estimated latent variable
plot(x, yst, cex = 1, type = "n", ylab = "latent variable")
cols <- topo.colors(3)</pre>
for (i in 1:3) {
points(x[y == i], yst[y == i], col = cols[i], pch = i, cex = 0.7)
for (i in 1:2) {
abline(h = (ans$zeta)[i], lty = 4, lwd = 1)
lines(sort(x), (5*x^2)[order(x)], lwd = 2)
lines(sort(x), (ans*muhat)[order(x)], col = 2, lty = 2, lwd = 2)
legend("topleft", bty = "n", col = c(1, 2), lty = c(1, 2),
c("true latent variable", "increasing-convex fit"), lwd = <math>c(1, 1)
## End(Not run)
## Not run:
# Example 2. mental impairment data set
# mental impairment is an ordinal response with 4 categories recorded as 1, 2, 3, and 4
# two covariates are life event index and socio-economic status (high = 1, low = 0)
data(mental)
table(mental$mental)
# model the relationship between the latent variable and life event index as increasing
# socio-economic status is included as a binary covariate
fit.incr <- cgam(mental ~ incr(life) + ses, data = mental, family = Ord)</pre>
```

plasma 35

```
# check the estimated probabilities P(mental = k), k = 1, 2, 3, 4
probs.incr <- fitted(fit.incr)
head(probs.incr)
## End(Not run)</pre>
```

plasma

A Data Set for Cgam

## **Description**

This data set is used for the routine plotpersp. It contains 314 observations of blood plasma, beta carotene measurements along with several covariates. High levels of blood plasma and beta carotene are believed to be protective against cancer, and it is of interest to determine the relationships with covariates.

## Usage

data(plasma)

#### **Format**

logplasma A numeric vector of the logarithm of plasma levels.

betacaro A numeric vector of dietary beta carotene consumed mcg per day.

bmi A numeric vector of BMI values.

cholest A numeric vector of cholesterol consumed mg per day.

dietfat A numeric vector of the logarithm of grams of diet fat consumed per day.

fiber A numeric vector of grams of fiber consumed per day.

retinol A numeric vector of retinol consumed per day.

smoke A numeric vector of smoking status (1=Never, 2=Former, 3=Current Smoker).

vituse A numeric vector of vitamin use (1=Yes, fairly often, 2=Yes, not often, 3=No).

#### References

Nierenberg, D., Stukel, T., Baron, J., Dain, B., and Greenberg, E. (1989) Determinants of plasma levels of beta-carotene and retinol. *American Journal of Epidemiology* 130, 511–521.

# **Examples**

data(plasma)

36 plotpersp

plotpersp	Create a 3D Plot for a CGAM Object	

## **Description**

Given an object of the cgam class, which has at least two non-parametrically modelled predictors, this routine will make a 3D plot of the fit with a set of two non-parametrically modelled predictors in the formula being the x and y labs. If there are more than two non-parametrically modelled predictors, any other such predictor will be evaluated at the largest value which is smaller than or equal to its median value.

If there is any categorical covariate and if the user specifies the argument categ to be a character representing a categorical covariate in the formula, then a 3D plot with multiple parallel surfaces, which represent the levels of a categorical covariate in an ascending order, will be created; otherwise, a 3D plot with only one surface will be created. Each level of a categorical covariate will be evaluated at its mode.

This routine is extended to make a 3D plot for an object fitted by warped-plane splines or triangle splines. Note that two non-parametrically modelled predictors specified in this routine must both be modelled as additive components, or a pair of predictors forming an isotonic or convex surface without additivity assumption.

This routine is an extension of the generic R graphics routine persp. See the documentation below for more details.

## Usage

```
plotpersp(object,...)
```

# **Arguments**

object An object of the cgam class with at least two non-parametrically modelled pre-

dictors.

.. Additional arguments passed to the plotting method, such as x1, x2, and control. These include:

x1 Optional; either a character string or a vector matching the first nonparametric predictor. If omitted, the first predictor's name is used.

x2 Optional; either a character string or a vector matching the second nonparametric predictor. If omitted, the second predictor's name is used.

control A list of graphical control parameters, typically created with plotpersp\_control. Controls aspects such as colors, axis limits, rotation angles, and grid resolution.

## Value

The routine plotpersp returns a 3D plot of an object of the cgam class. The x lab and y lab represent a set of non-parametrically modelled predictors used in a cgam formula, and the z lab represents the estimated mean value or the estimated systematic component value.

plotpersp 37

### Author(s)

Mary C. Meyer and Xiyue Liao

```
# Example 1.
 data(FEV)
 # extract the variables
 y <- FEV$FEV
 age <- FEV$age
 height <- FEV$height
 sex <- FEV$sex
 smoke <- FEV$smoke
 fit <- cgam(y ~ incr(age) + incr(height) + factor(sex) + factor(smoke), nsim = 0)</pre>
 fit.s <- cgam(y \sim s.incr(age) + s.incr(height) + factor(sex) + factor(smoke), nsim = 0)
 ctl <- list(ngrid = 10, main = "Cgam Increasing Fit",</pre>
 sub = "Categorical Variable: Sex", categ = "factor(sex)")
 plotpersp(fit, age, height, control = ctl)
 ctl <- list(ngrid = 10, main = "Cgam Smooth Increasing Fit",</pre>
 sub = "Categorical Variable: Smoke", categ = "factor(smoke)")
 plotpersp(fit.s, age, height, control = ctl)
# Example 2.
 data(plasma)
 fit <- cgam(logplasma ~ s.decr(bmi) + s.decr(logdietfat) + s.decr(cholest) + s.incr(fiber)</pre>
+ s.incr(betacaro) + s.incr(retinol) + factor(smoke) + factor(vituse), data = plasma)
 ctl <- list(ngrid = 15, th = 120, ylab = "log(dietfat)",
            zlab = "est mean of log(plasma)", main = "Cgam Fit with the Plasma Data Set",
            sub = "Categorical Variable: Vitamin Use", categ = "factor(vituse)")
 plotpersp(fit, "bmi", "logdietfat", control = ctl)
# Example 3.
 data(plasma)
 addl <- 1:314*0 + 1
 addl[runif(314) < .3] <- 2
 addl[runif(314) > .8] <- 4
 addl[runif(314) > .8] <- 3
 plasma$addl <- addl</pre>
 ans <- cgam(logplasma ~ s.incr(betacaro, 5) + s.decr(bmi) +
                s.decr(logdietfat) + as.factor(addl), data = plasma)
 ctl <- list(th = 240, random = TRUE, categ = "as.factor(addl)")</pre>
 plotpersp(ans, "betacaro", "logdietfat", control = ctl)
```

38 plotpersp\_control

```
# Example 4.
## Not run:
    n <- 100
    set.seed(123)
    x1 <- sort(runif(n))
    x2 <- sort(runif(n))
    y <- 4 * (x1 - x2) + rnorm(n, sd = .5)

# regress y on x1 and x2 under the shape-restriction: "decreasing-increasing"
# with a penalty term = .1
    ans <- cgam(y ~ s.decr.incr(x1, x2), pen = .1)

# plot the constrained surface
    plotpersp(ans)

## End(Not run)</pre>
```

plotpersp\_control

Control Parameters for plotpersp.cgam

# **Description**

Constructs a list of control parameters to customize the appearance of perspective plots created by plotpersp.cgam.

# Usage

```
plotpersp_control(surface = "mu", x1nm = NULL, x2nm = NULL, categ = NULL,
  col = NULL, random = FALSE, ngrid = 12, xlim = NULL, ylim = NULL, zlim = NULL,
  xlab = NULL, ylab = NULL, zlab = NULL, th = NULL, ltheta = NULL,
  main = NULL, sub = NULL, ticktype = "simple")
```

# **Arguments**

surface	Character string indicating the surface type to plot. Options are "mu" for fitted means or "eta" for systematic component.
x1nm	Optional character strings specifying names of the predictors for the x axis.
x2nm	Optional character strings specifying names of the predictors for the y axis.
categ	Optional character string naming a categorical covariate in the $\operatorname{cgam}$ fit to stratify surfaces. Default is NULL.
col	Colors used for the surface(s). If $NULL$ , defaults are applied automatically depending on the number of surfaces.
random	$Logical; if \ TRUE, colors \ are \ randomized \ for \ multiple \ surfaces. \ Default \ is \ FALSE.$
ngrid	Integer; number of grid points along each axis. Default is 12.
${\tt xlim,ylim,zlim}$	Optional numeric vectors of length 2 specifying limits for the x, y, and z axes.

predict.cgam 39

xlab, ylab, zlab Axis labels for x, y, and z axes. Default is based on the predictor names and

surface type.

th Angle defining the azimuthal direction for viewing the plot (theta).

1theta Angle defining the direction of lighting (light theta).

main Main title of the plot. sub Subtitle of the plot.

ticktype Character string indicating type of tick marks: "simple" (default) or "detailed".

## Value

A named list of control settings for use with plotpersp.

## Author(s)

Mary C. Meyer and Xiyue Liao

#### See Also

```
plotpersp, persp
```

## **Examples**

```
ctrl <- plotpersp_control(col = "topo", ngrid = 20, th = 45)
# Then used inside plotpersp:
# plotpersp(fit, control = ctrl)</pre>
```

predict.cgam

Predict Method for CGAM Fits

# **Description**

Predicted values based on a cgam object

# Usage

```
## S3 method for class 'cgam'
predict(object, newdata, interval = c("none", "confidence", "prediction"),
type = c("response", "link"), level = 0.95, n.mix = 500,...)
```

# Arguments

object A cgam object.

newdata A data frame in which to look for variables with which to predict. If omitted,

the fitted values are used.

interval Type of interval calculation. A prediction interval is only implemented for Gaus-

sian response for now.

40 predict.cgam

type	If the response is Gaussian, type = "response" gives the predicted mean; if the response is binomial, type = "response" gives the predicted probabilities, and type = "link" gives the predicted systematic component.
level	Tolerance/confidence level.
n.mix	Number of simulations to get the mixture distribution. The default is $n.mix = 500$ .
	Further arguments passed to the routine.

#### **Details**

Constrained spline estimators can be characterized by projections onto a polyhedral convex cone. Point-wise confidence intervals for constrained splines are constructed by estimating the probabilities that the projection lands on each of the faces of the cone, and using a mixture of covariance matrices to estimate the standard error of the function estimator at any design point.

Note that currently predict.cgam only works when all components in a cgam formula are additive.

See references cited in this section for more details.

#### Value

fit	A vector of predictions.
lower	A vector of lower bound if interval is set to be "confidence".
upper	A vector of upper bound if interval is set to be "confidence".

# Author(s)

Mary C. Meyer and Xiyue Liao

# References

Meyer, M. C. (2017) Constrained partial linear regression splines. Statistical Sinica in press.

Meyer, M. C. (2017) Confidence intervals for regression functions using constrained splines with application to estimation of tree height

Meyer, M. C. (2012) Constrained penalized splines. Canadian Journal of Statistics 40(1), 190-206.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* **2**(3), 1013–1033.

```
# Example 1.
# generate data
n <- 100
set.seed(123)
x <- runif(n)
y <- 4*x^3 + rnorm(n)
# regress y on x under the shape-restriction: "increasing-convex"
fit <- cgam(y ~ s.incr.conv(x))</pre>
```

predict.cgam 41

```
# make a data frame
x0 < - seq(min(x), max(x), by = 0.05)
# predict values in new.Data based on the cgam fit without a confidence interval
pfit <- predict(fit, newdata = data.frame(x = x0))</pre>
# make a plot to check the prediction
plot(x, y, main = "Predict Method for CGAM")
lines(sort(x), (fitted(fit)[order(x)]))
points(x0, pfitfit, col = 2, pch = 20)
# predict values in newdata based on the cgam fit with a 95 percent confidence interval
pfit \leftarrow predict(fit, newdata = data.frame(x = x0), interval = "confidence", level = 0.95)
# make a plot to check the prediction
plot(x, y, main = "Pointwise Confidence Bands (Gaussian Response)")
lines(sort(x), (fitted(fit)[order(x)]))
lines(sort(x0), (pfit$lower)[order(x0)], col = 2, lty = 2)
lines(sort(x0), (pfitper)[order(x0)], col = 2, lty = 2)
points(x0, pfitfit, col = 2, pch = 20)
# Example 2. binomial response
n <- 200
x \leftarrow seq(0, 1, length = n)
eta <- 4*x^2 - 2
mu <- exp(eta)/(1+exp(eta))</pre>
set.seed(123)
y <- 1:n*0
y[runif(n) < mu] = 1
fit <- cgam(y \sim s.incr.conv(x), family = binomial)
muhat <- fitted(fit)</pre>
 # predict values in new.Data based on the cgam fit with a 95 percent confidence interval
  xinterp <- seq(min(x), max(x), by = 0.05)
pfit <- predict(fit, newdata = data.frame(x = xinterp),</pre>
  interval = "confidence", level = 0.95)
pmu <- pfit$fit
lwr <- pfit$lower</pre>
upp <- pfit$upper</pre>
# make a plot to check the prediction
plot(x, y, type = "n", ylim = c(0, 1),
main = "Pointwise Confidence Bands (Binomial Response)")
rug(x[y == 0])
    rug(x[y == 1], side = 3)
lines(x, mu)
lines(x, muhat, col = 5, lty = 2)
points(xinterp, pmu, pch = 20)
lines(xinterp, upp, col = 5)
```

42 s

```
points(xinterp, upp, pch = 20)
lines(xinterp, lwr, col = 5)
points(xinterp, lwr, pch = 20)
```

Specify a Smooth Shape-Restriction in a CGAM Formula

# Description

s

A symbolic routine to define that the systematic component  $\eta$  is smooth in a predictor in a formula argument to cgam. This is the smooth version.

# Usage

```
s(x, numknots = 0, knots = 0, space = "Q")
```

#### **Arguments**

x	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to constrain $x$ . It will not be used if the user specifies the <i>knots</i> argument. The default is numknots = $0$ .
knots	The knots used to constrain $x$ . User-defined knots will be used when given. Otherwise, $numknots$ and $space$ will be used to create knots. The default is knots = $0$ .
space	A character specifying the method to create knots. It will not be used if the user

A character specifying the method to create knots. It will not be used if the user specifies the *knots* argument. If space == "E", then equally spaced knots will be created; if space == "Q", then a vector of equal x quantiles will be created based on x with duplicate elements removed. The number of knots is *numknots* when *numknots* > 0. Otherwise it is of the order  $n^{1/7}$ . The default is space = "Q".

## **Details**

"s" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s"; the shape attribute is 17("smooth"). According to the value of the vector itself and its shape, numknots, knots and space attributes, the cone edges will be made by C-spline basis functions in Meyer (2008). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 17("smooth"); numknots: the numknots argument in "s"; knots: the knots argument in "s"; space: the space argument in "s".

s.conc 43

### Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* **2(3)**, 1013–1033.

## See Also

```
s.incr, s.decr, s.conc, s.conv, s.incr.conc, s.incr.conv, s.decr.conc, s.decr.conv
```

# **Examples**

```
# generate y
x <- seq(-1, 2, by = 0.1)
n <- length(x)
y <- - x^2 + rnorm(n, .3)

# regress y on x under the shape-restriction: "smooth"
ans <- cgam(y ~ s(x))
knots <- ans$knots[[1]]

# make a plot
plot(x, y)
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "smooth fit", col = 2, lty = 1)
legend(1.6, 1.8, bty = "o", "knots", pch = "X")
points(knots, 1:length(knots)*0+min(y), pch = "X")</pre>
```

s.conc

Specify a Smooth and Concave Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that the systematic component  $\eta$  is smooth and concave in a predictor in a formula argument to cgam. This is the smooth version.

## Usage

```
s.conc(x, numknots = 0, knots = 0, space = "Q")
```

44 s.conc

### **Arguments**

x A numeric predictor which has the same length as the response vector.

number of knots used to constrain x. It will not be used if the user specifies

the *knots* argument. The default is numknots = 0.

knots The knots used to constrain x. User-defined knots will be used when given.

Otherwise, numknots and space will be used to create knots. The default is

knots = 0.

space A character specifying the method to create knots. It will not be used if the user

specifies the *knots* argument. If space == "E", then equally spaced knots will be created; if space == "Q", then a vector of equal x quantiles will be created based on x with duplicate elements removed. The number of knots is *numknots* when *numknots* > 0. Otherwise it is of the order  $n^{1/7}$ . The default is space = "Q".

#### **Details**

"s.conc" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.conc"; the shape attribute is 12("smooth and concave"). According to the value of the vector itself and its shape, numknots, knots and space attributes, the cone edges will be made by C-spline basis functions in Meyer (2008). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.conc" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 12("smooth and concave"); numknots: the numknots argument in "s.conc"; knots: the knots argument in "s.conc"; space: the space argument in "s.conc".

## Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* **2**(3), 1013–1033.

# See Also

conc

s.conc.conc 45

## **Examples**

```
# generate y
x <- seq(-1, 2, by = 0.1)
n <- length(x)
y <- - x^2 + rnorm(n, .3)

# regress y on x under the shape-restriction: "smooth and concave"
ans <- cgam(y ~ s.conc(x))
knots <- ans$knots[[1]]

# make a plot
plot(x, y)
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "smooth and concave fit", col = 2, lty = 1)
legend(1.6, 1.8, bty = "o", "knots", pch = "X")
points(knots, 1:length(knots)*0+min(y), pch = "X")</pre>
```

s.conc.conc

Specify a Doubly-Concave Shape-Restriction in a CGAM Formula

# Description

A symbolic routine to define that a surface is concave in two predictors in a formula argument to cgam.

#### Usage

```
s.conc.conc(x1, x2, numknots = c(0, 0), knots = list(k1 = 0, k2 = 0), space = c("E", "E"))
```

## **Arguments**

x1 A numeric predictor which has the same length as the response vector.

A numeric predictor which has the same length as the response vector.

numknots A vector of the number of knots used to constrain  $x_1$  and  $x_2$ . It will not be used

if the user specifies the knots argument and each predictor is within the range of

its knots. The default is numknots = c(0, 0).

knots A list of two vectors of knots used to constrain  $x_1$  and  $x_2$ . User-defined knots

will be used if each predictor is within the range of its knots. Otherwise, *num-knots* and *space* will be used to create knots. The default is knots = list(k1 = 0, knots)

k2 = 0).

space A vector of the character specifying the method to create knots for  $x_1$  and  $x_2$ .

It will not be used if the user specifies the *knots* argument. If "E" is used, then equally spaced knots will be created; if "Q" is used, then a vector of equal quantiles will be created with duplicate elements removed. The number of knots is numknots when numknots is a positive integer > 4. Otherwise it is of the order

 $n^{1/3}$ . The default is space = c("E", "E").

46 s.conc.conc

#### **Details**

"s.conc.conc" returns the vectors "x1" and "x2", and imposes on each vector six attributes: name, shape, numknots, knots, space and cvs.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.conc.conc"; the shape attribute is "tri\_cvs"(doubly-concave); the cvs values for both vectors are FALSE. According to the value of the vector itself and its shape, numknots, knots, space and cvs attributes, the cone edges will be made by triangle spline basis functions in Meyer (2017). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.conc.conc" does not make the corresponding cone edges itself. It sets things up to a subroutine called trispl.fit

See references cited in this section for more details.

#### Value

The vectors  $x_1$  and  $x_2$ . Each of them has six attributes, i.e., name: names of  $x_1$  and  $x_2$ ; shape: "tri\_cvs"(doubly-concave); numknots: the numknots argument in "s.conc.conc"; knots: the knots argument in "s.conc.conc"; space: the space argument in "s.conc.conc"; cvs: two logical values indicating the monotonicity of the isotonically-constrained surface with respect to  $x_1$  and  $x_2$ , which are both FALSE.

#### Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2017) Estimation and inference for regression surfaces using shape-constrained splines.

# See Also

```
s.conv.conv, cgam
```

```
# generate data
n <- 200
set.seed(123)
x1 <- runif(n); x2 <- runif(n)
y <- -(x1 - 1)^2 - (x2 - 3)^2 + rnorm(n)

# regress y on x1 and x2 under the shape-restriction: "doubly-concave"
ans <- cgam(y ~ s.conc.conc(x1, x2), nsim = 0)
# make a 3D plot of the constrained surface
plotpersp(ans)</pre>
```

s.conv 47

s.conv

Specify a Smooth and Convex Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that the systematic component  $\eta$  is smooth and convex in a predictor in a formula argument to cgam. This is the smooth version.

# Usage

```
s.conv(x, numknots = 0, knots = 0, space = "Q")
```

# **Arguments**

x A numeric predictor which has the same length as the response vector.

numknots The number of knots used to constrain x. It will not be used if the user specifies

the *knots* argument. The default is numknots = 0.

knots The knots used to constrain x. User-defined knots will be used when given.

Otherwise, *numknots* and *space* will be used to create knots. The default is

knots = 0.

space A character specifying the method to create knots. It will not be used if the user

specifies the *knots* argument. If space == "E", then equally spaced knots will be created; if space == "Q", then a vector of equal x quantiles will be created based on x with duplicate elements removed. The number of knots is *numknots* when *numknots* > 0. Otherwise it is of the order  $n^{1/7}$ . The default is space = "Q".

#### **Details**

"s.conv" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.conv"; the shape attribute is 11("smooth and convex"). According to the value of the vector itself and its shape, numknots, knots and space attributes, the cone edges will be made by C-spline basis functions in Meyer (2008). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.conv" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

# Value

The vector x with five attributes, i.e., name: the name of x; shape: 11("smooth and convex"); numknots: the numknots argument in "s.conv"; knots: the knots argument in "s.conv"; space: the space argument in "s.conv".

48 s.conv.conv

## Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* **2(3)**, 1013–1033.

## See Also

conv

# **Examples**

```
# generate y
x <- seq(-1, 2, by = 0.1)
n <- length(x)
y <- x^2 + rnorm(n, .3)

# regress y on x under the shape-restriction: "smooth and convex"
ans <- cgam(y ~ s.conv(x))
knots <- ans$knots[[1]]

# make a plot
plot(x, y)
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "smooth and convex fit", col = 2, lty = 1)
legend(1.6, -1, bty = "o", "knots", pch = "X")
points(knots, 1:length(knots)*0+min(y), pch = "X")</pre>
```

s.conv.conv

Specify a Doubly-convex Shape-Restriction in a CGAM Formula

## **Description**

A symbolic routine to define that a surface is convex in two predictors in a formula argument to cgam.

## Usage

```
s.conv.conv(x1, x2, numknots = c(0, 0), knots = list(k1 = 0, k2 = 0), space = c("E", "E"))
```

s.conv.conv 49

#### **Arguments**

A numeric predictor which has the same length as the response vector.
 A numeric predictor which has the same length as the response vector.

numknots A vector of the number of knots used to constrain  $x_1$  and  $x_2$ . It will not be used

if the user specifies the knots argument and each predictor is within the range of

its knots. The default is numknots = c(0, 0).

knots A list of two vectors of knots used to constrain  $x_1$  and  $x_2$ . User-defined knots

will be used if each predictor is within the range of its knots. Otherwise, num-knots and space will be used to create knots. The default is knots = list(k1 = 0,

k2 = 0).

space A vector of the character specifying the method to create knots for  $x_1$  and  $x_2$ .

It will not be used if the user specifies the *knots* argument. If "E" is used, then equally spaced knots will be created; if "Q" is used, then a vector of equal quantiles will be created with duplicate elements removed. The number of knots is numknots when numknots is a positive integer > 4. Otherwise it is of the order

 $n^{1/3}$ . The default is space = c("E", "E").

#### **Details**

"s.conv.conv" returns the vectors "x1" and "x2", and imposes on each vector six attributes: name, shape, numknots, knots, space and cvs.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.conv.conv"; the shape attribute is "tri\_cvs"(doubly-convex); the cvs values for both vectors are TRUE. According to the value of the vector itself and its shape, numknots, knots, space and cvs attributes, the cone edges will be made by triangle spline basis functions in Meyer (2017). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.conv.conv" does not make the corresponding cone edges itself. It sets things up to a subroutine called trispl.fit

See references cited in this section for more details.

#### Value

The vectors  $x_1$  and  $x_2$ . Each of them has six attributes, i.e., name: names of  $x_1$  and  $x_2$ ; shape: "tri\_cvs"(doubly-convex); numknots: the numknots argument in "s.conv.conv"; knots: the knots argument in "s.conv.conv"; space: the space argument in "s.conv.conv"; cvs: two logical values indicating the monotonicity of the isotonically-constrained surface with respect to  $x_1$  and  $x_2$ , which are both TRUE.

#### Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2017) Estimation and inference for regression surfaces using shape-constrained splines.

s.decr

# See Also

```
s.conv.conv, cgam
```

# **Examples**

```
# generate data
n <- 200
set.seed(123)
x1 <- runif(n); x2 <- runif(n)
y <- (x1 - 1)^2 + (x2 - 3)^2 + rnorm(n)

# regress y on x1 and x2 under the shape-restriction: "doubly-convex"
ans <- cgam(y ~ s.conv.conv(x1, x2), nsim = 0)
# make a 3D plot of the constrained surface
plotpersp(ans)</pre>
```

s.decr

Specify a Smooth and Decreasing Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that the systematic component  $\eta$  is smooth and decreasing in a predictor in a formula argument to cgam. This is the smooth version.

# Usage

```
s.decr(x, numknots = 0, knots = 0, var.knots = 0, space = "Q", db.exp = FALSE)
```

# **Arguments**

Х	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to constrain $x$ . It will not be used if the user specifies the <i>knots</i> argument. The default is numknots = $0$ .
knots	The knots used to constrain $x$ . User-defined knots will be used when given. Otherwise, $numknots$ and $space$ will be used to create knots. The default is knots = $0$ .
var.knots	The knots used in variance function estimation. User-defined knots will be used when given. The default is var.knots = $0$ .
space	A character specifying the method to create knots. It will not be used if the user specifies the <i>knots</i> argument. If space == "E", then equally spaced knots will be created; if space == "Q", then a vector of equal $x$ quantiles will be created based on $x$ with duplicate elements removed. The number of knots is $numknots$ when $numknots > 0$ . Otherwise it is of the order $n^{1/7}$ . The default is space = "Q".
db.exp	The parameter will be used in variance function estimation. If db.exp = TRUE, then the errors are assumed to follow a normal distribution; otherwise, the errors are assumed to follow a double-exponential distribution. The default is db.exp = FALSE.

s.decr 51

#### **Details**

"s.decr" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots, space, var.knots and db.exp.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.decr"; the shape attribute is 10("smooth and decreasing"). According to the value of the vector itself and its shape, numknots, knots and space attributes, the cone edges will be made by I-spline basis functions in Meyer (2008). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.decr" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

var.knots and db.exp will be used for monotonic variance function estimation.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e, name: the name of x; shape: 10("smooth and decreasing"); numknots: the numknots argument in "s.decr"; knots: the knots argument in "s.decr"; space: the space argument in "s.decr".

#### Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* **2(3)**, 1013–1033.

## See Also

decr

```
data(cubic)
# extract x
x <- - cubic$x

# extract y
y <- cubic$y

# regress y on x under the shape-restriction: "smooth and decreasing"
ans <- cgam(y ~ s.decr(x))
knots <- ans$knots[[1]]</pre>
```

52 s.decr.conc

```
# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "smooth and decreasing fit", col = 2, lty = 1)
legend(-.3, 8, bty = "o", "knots", pch = "X")
points(knots, 1:length(knots)*0+min(y), pch = "X")
```

s.decr.conc

Specify a Smooth, Decreasing and Concave Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that the systematic component  $\eta$  is smooth, decreasing and concave in a predictor in a formula argument to cgam. This is the smooth version.

# Usage

```
s.decr.conc(x, numknots = 0, knots = 0, space = "Q")
```

# **Arguments**

space

A numeric predictor which has the same length as the response vector.

The number of knots used to constrain x. It will not be used if the user specifies the *knots* argument. The default is numknots = 0.

knots

The knots used to constrain x. User defined knots will be used when given. Otherwise, *numknots* and *space* will be used to create knots. The default is knots = 0.

A character specifying the method to create knots. It will not be used if the user specifies the *knots* argument. If space == "E", then equally spaced knots will be created; if space == "Q", then a vector of equal x quantiles will be created based on x with duplicate elements removed. The number of knots is numknots when numknots > 0. Otherwise it is of the order  $n^{1/7}$ . The default is space = "Q".

## **Details**

"s.decr.conc" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.decr.conc"; the shape attribute is 16("smooth, decreasing and concave"). According to the value of the vector itself and its shape, numknots, knots and space attributes, the cone edges will be made by C-spline basis functions in Meyer (2008). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.decr.conc" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

s.decr.conv 53

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 16("smooth, decreasing and concave"); numknots: the numknots argument in "s.decr.conc"; knots: the knots argument in "s.decr.conc"; space: the space argument in "s.decr.conc".

#### Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42(5)**, 1126–1139.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* **2(3)**, 1013–1033.

## See Also

```
decr.conv, decr
```

```
data(cubic)

# extract x
x <- cubic$x

# extract y
y <- - cubic$y

# regress y on x under the shape-restriction: "smooth, decreasing and concave"
ans <- cgam(y ~ s.decr.conc(x))
knots <- ans$knots[[1]]

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "smooth, decreasing and concave fit", col = 2, lty = 1)
legend(1.7, 4, bty = "o", "knots", pch = "X")
points(knots, 1:length(knots)*0+min(y), pch = "X")</pre>
```

54 s.decr.conv

# **Description**

A symbolic routine to define that the systematic component  $\eta$  is smooth, decreasing and convex in a predictor in a formula argument to cgam. This is the smooth version.

# Usage

```
s.decr.conv(x, numknots = 0, knots = 0, space = "Q")
```

# **Arguments**

x A numeric predictor which has the same length as the response vector.

numknots The number of knots used to constrain x. It will not be used if the user specifies

the *knots* argument. The default is numknots = 0.

knots The knots used to constrain x. User-defined knots will be used when given.

Otherwise, numknots and space will be used to create knots. The default is

knots = 0.

space A character specifying the method to create knots. It will not be used if the user

specifies the *knots* argument. If space == "E", then equally spaced knots will be created; if space == "Q", then a vector of equal x quantiles will be created based on x with duplicate elements removed. The number of knots is *numknots* when numknots > 0. Otherwise it is of the order  $n^{1/7}$ . The default is space = "Q".

#### **Details**

"s.decr.conv" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.decr.conv"; the shape attribute is 15("smooth, decreasing and convex"). According to the value of the vector itself and its shape, numknots, knots and space attributes, the cone edges will be made by C-spline basis functions in Meyer (2008). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.decr.conv" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 15("smooth, decreasing and convex"); numknots: the numknots argument in "s.decr.conv"; knots: the knots argument in "s.decr.conv"; space: the space argument in "s.decr.conv".

#### Author(s)

Mary C. Meyer and Xiyue Liao

s.decr.decr 55

## References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* 2(3), 1013–1033.

#### See Also

```
decr.conv
```

# **Examples**

```
data(cubic)

# extract x
x <- - cubic$x

# extract y
y <- cubic$y

# regress y on x under the shape-restriction: "smooth, decreasing and convex"
ans <- cgam(y ~ s.decr.conv(x))
knots <- ans$knots[[1]]

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "smooth, decreasing and convex fit", col = 2, lty = 1)
legend(-.3, 9.2, bty = "o", "knots", pch = "X")
points(knots, 1:length(knots)*0+min(y), pch = "X")</pre>
```

s.decr.decr

Specify a Doubly-Decreasing Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that a surface is decreasing in two predictors in a formula argument to cgam.

## Usage

```
s.decr.decr(x1, x2, numknots = c(0, 0), knots = list(k1 = 0, k2 = 0), space = c("E", "E"))
```

56 s.decr.decr

#### **Arguments**

x1 A numeric predictor which has the same length as the response vector. x2 A numeric predictor which has the same length as the response vector.

numknots A vector of the number of knots used to constrain  $x_1$  and  $x_2$ . It will not be used

if the user specifies the knots argument and each predictor is within the range of

its knots. The default is numknots = c(0, 0).

knots A list of two vectors of knots used to constrain  $x_1$  and  $x_2$ . User-defined knots

will be used if each predictor is within the range of its knots. Otherwise, num-knots and space will be used to create knots. The default is knots = list(k1 = 0,

k2 = 0).

space A vector of the character specifying the method to create knots for  $x_1$  and  $x_2$ .

It will not be used if the user specifies the *knots* argument. If "E" is used, then equally spaced knots will be created; if "Q" is used, then a vector of equal quantiles will be created with duplicate elements removed. The number of knots is numknots when numknots is a positive integer > 4. Otherwise it is of the order

 $n^{1/6}$ . The default is space = c("E", "E").

#### **Details**

"s.decr.decr" returns the vectors "x1" and "x2", and imposes on each vector six attributes: name, shape, numknots, knots, space and decreasing.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.decr.decr"; the shape attribute is "wps\_dd"(doubly-decreasing); the decreasing values for both vectors are TRUE. According to the value of the vector itself and its shape, numknots, knots, space and decreasing attributes, the cone edges will be made by warped-plane spline basis functions in Meyer (2016). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.decr.decr" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta\_wps.

See references cited in this section for more details.

#### Value

The vectors  $x_1$  and  $x_2$ . Each of them has six attributes, i.e., name: names of  $x_1$  and  $x_2$ ; shape: "wps\_dd"(doubly-decreasing); numknots: the numknots argument in "s.decr.decr"; knots: the knots argument in "s.decr.decr"; space: the space argument in "s.decr.decr"; decreasing: two logical values indicating the monotonicity of the isotonically-constrained surface with respect to  $x_1$  and  $x_2$ , which are both TRUE.

#### Author(s)

Mary C. Meyer and Xiyue Liao

# References

Meyer, M. C. (2017) Estimation and inference for regression surfaces using shape-constrained splines.

s.decr.incr 57

## See Also

```
s.incr.incr, s.decr.incr, s.incr.decr, cgam
```

## **Examples**

```
## Not run:
    # generate data
    n <- 100
    set.seed(123)
    x1 <- runif(n)
    x2 <- runif(n)
    y <- -4 * (x1 + x2 - x1 * x2) + rnorm(n, sd = .2)

# regress y on x1 and x2 under the shape-restriction: "doubly-decreasing"
# using the penalized estimator
    ans <- cgam(y ~ s.decr.decr(x1, x2), pnt = TRUE)

# make a 3D plot of the constrained surface
    plotpersp(ans)

## End(Not run)</pre>
```

s.decr.incr

Specify a Decreasing-Increasing Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that a surface is decreasing in one predictor and increasing in another in a formula argument to cgam.

## Usage

```
s.decr.incr(x1, x2, numknots = c(0, 0), knots = list(k1 = 0, k2 = 0), space = c("E", "E"))
```

# Arguments

k2 = 0).

x1	A numeric predictor which has the same length as the response vector.
x2	A numeric predictor which has the same length as the response vector.
numknots	A vector of the number of knots used to constrain $x_1$ and $x_2$ . It will not be used if the user specifies the <i>knots</i> argument and each predictor is within the range of its knots. The default is numknots = $c(0, 0)$ .
knots	A list of two vectors of knots used to constrain $x_1$ and $x_2$ . User-defined knots will be used if each predictor is within the range of its knots. Otherwise, <i>num-knots</i> and <i>space</i> will be used to create knots. The default is knots = list(k1 = 0,

58 s.decr.incr

space

A vector of the character specifying the method to create knots for  $x_1$  and  $x_2$ . It will not be used if the user specifies the *knots* argument. If "E" is used, then equally spaced knots will be created; if "Q" is used, then a vector of equal quantiles will be created with duplicate elements removed. The number of knots is *numknots* when *numknots* is a positive integer > 4. Otherwise it is of the order  $n^{1/6}$ . The default is space = c("E", "E").

#### **Details**

"s.decr.incr" returns the vectors "x1" and "x2", and imposes on each vector six attributes: name, shape, numknots, knots, space and decreasing.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.decr.incr"; the shape attribute is "wps\_di"(decreasing-increasing); the decreasing values for "x1" and "x2" are TRUE and FALSE. According to the value of the vector itself and its shape, numknots, knots, space and decreasing attributes, the cone edges will be made by warped-plane spline basis functions in Meyer (2016). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.decr.incr" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta\_wps.

See references cited in this section for more details.

#### Value

The vectors  $x_1$  and  $x_2$ . Each of them has six attributes, i.e., name: names of  $x_1$  and  $x_2$ ; shape: "wps\_di"(decreasing-increasing); numknots: the numknots argument in "s.decr.incr"; knots: the knots argument in "s.decr.incr"; space: the space argument in "s.decr.incr"; decreasing: two logical values indicating the monotonicity of the isotonically-constrained surface with respect to  $x_1$  and  $x_2$ , which are TRUE and FALSE.

#### Author(s)

Mary C. Meyer and Xiyue Liao

# References

Meyer, M. C. (2017) Estimation and inference for regression surfaces using shape-constrained splines.

## See Also

```
s.incr.incr, s.incr.decr, s.decr.decr, cgam
```

```
## Not run:
    # generate data
    n <- 100
    set.seed(123)
    x1 <- runif(n)</pre>
```

s.incr 59

```
x2 <- runif(n)
y <- 4 * (x2 - x1) - x1 * x2 + rnorm(n, sd = .2)

# regress y on x1 and x2 under the shape-restriction: "decreasing-increasing"
# using the penalized estimator
ans <- cgam(y ~ s.decr.incr(x1, x2), pnt = TRUE)

# make a 3D plot of the constrained surface
plotpersp(ans)

## End(Not run)</pre>
```

s.incr

Specify a Smooth and Increasing Shape-Restriction in a CGAM Formula

# Description

A symbolic routine to define that the systematic component  $\eta$  is smooth and increasing in a predictor in a formula argument to cgam. This is the smooth version.

# Usage

```
s.incr(x, numknots = 0, knots = 0, var.knots = 0, space = "Q", db.exp = FALSE)
```

# Arguments

x	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to constrain $x$ . It will not be used if the user specifies the <i>knots</i> argument. The default is numknots = $0$ .
knots	The knots used to constrain $x$ . User-defined knots will be used when given. Otherwise, $numknots$ and $space$ will be used to create knots. The default is knots = $0$ .
var.knots	The knots used in variance function estimation. User-defined knots will be used when given. The default is var.knots = $0$ .
space	A character specifying the method to create knots. It will not be used if the user specifies the <i>knots</i> argument. If space == "E", then equally spaced knots will be created; if space == "Q", then a vector of equal $x$ quantiles will be created based on $x$ with duplicate elements removed. The number of knots is $numknots$ when $numknots > 0$ . Otherwise it is of the order $n^{1/7}$ . The default is space = "Q".
db.exp	The parameter will be used in variance function estimation. If db.exp = TRUE, then the errors are assumed to follow a normal distribution; otherwise, the errors are assumed to follow a double-exponential distribution. The default is db.exp = FALSE.

60 s.incr

#### **Details**

"s.incr" returns the vector "x" and imposes on it seven attributes: name, shape, numknots, knots, space, var.knots and db.exp.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.incr"; the shape attribute is 9("smooth and increasing"). According to the value of the vector itself and its shape, numknots, knots and space attributes, the cone edges will be made by I-spline basis functions in Meyer (2008). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.incr" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

var.knots and db.exp will be used for monotonic variance function estimation.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 9("smooth and increasing"); numknots: the numknots argument in "s.incr"; knots: the knots argument in "s.incr"; space: the space argument in "s.incr".

#### Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* **2(3)**, 1013–1033.

## See Also

incr

```
data(cubic)
# extract x
x <- cubic$x

# extract y
y <- cubic$y

# regress y on x with the shape restriction: "smooth and increasing"
ans <- cgam(y ~ s.incr(x))
knots <- ans$knots[[1]]</pre>
```

s.incr.conc 61

```
# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "smooth and increasing fit", col = 2, lty = 1)
legend(1.7, 9.2, bty = "o", "knots", pch = "X")
points(knots, 1:length(knots)*0+min(y), pch = "X")
```

s.incr.conc

Specify a Smooth, Increasing and Concave Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that the systematic component  $\eta$  is smooth, increasing and concave in a predictor in a formula argument to cgam. This is the smooth version.

# Usage

```
s.incr.conc(x, numknots = 0, knots = 0, space = "Q")
```

# Arguments

Х	A numeric predictor which has the same length as the response vector.
numknots	The number of knots used to constrain $x$ . It will not be used if the user specifies the <i>knots</i> argument. The default is numknots = $0$ .
knots	The knots used to constrain $x$ . User-defined knots will be used when given. Otherwise, $numknots$ and $space$ will be used to create knots. The default is knots = $0$ .
space	A character specifying the method to create knots. It will not be used if the user specifies the <i>knots</i> argument. If space == "E", then equally spaced knots will be created; if space == "Q", then a vector of equal $x$ quantiles will be created based on $x$ with duplicate elements removed. The number of knots is $numknots$ when $numknots > 0$ . Otherwise it is of the order $n^{1/7}$ . The default is space = "Q".

## **Details**

"s.incr.conc" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.incr.conc"; the shape attribute is 14("smooth, increasing and concave"). According to the value of the vector itself and its shape, numknots, knots and space attributes, the cone edges will be made by C-spline basis functions in Meyer (2008). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.incr.conc" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

s.incr.conv

## Value

The vector x with five attributes, i.e., name: the name of x; shape: 14("smooth, increasing and concave"); numknots: the numknots argument in "s.incr.conc"; knots: the knots argument in "s.incr.conc"; space: the space argument in "s.incr.conc".

#### Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42(5)**, 1126–1139.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* **2(3)**, 1013–1033.

## See Also

incr.conv

```
data(cubic)
# extract x
x <- - cubic$x

# extract y
y <- - cubic$y

# regress y on x with the shape restriction: "smooth, increasing and concave"
ans <- cgam(y ~ s.incr.conc(x))
knots <- ans$knots[[1]]

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "smooth, increasing and concave fit", col = 2, lty = 1)
legend(-.3, 4, bty = "o", "knots", pch = "X")
points(knots, 1:length(knots)*0+min(y), pch = "X")</pre>
```

s.incr.conv 63

### **Description**

A symbolic routine to define that the systematic component  $\eta$  is smooth, increasing and convex in a predictor in a formula argument to cgam. This is the smooth version.

#### Usage

```
s.incr.conv(x, numknots = 0, knots = 0, space = "Q")
```

# **Arguments**

x A numeric predictor which has the same length as the response vector.

numknots The number of knots used to constrain x. It will not be used if the user specifies

the *knots* argument. The default is numknots = 0.

knots The knots used to constrain x. User-defined knots will be used when given.

Otherwise, numknots and space will be used to create knots. The default is

knots = 0.

space A character specifying the method to create knots. It will not be used if the user

specifies the *knots* argument. If space == "E", then equally spaced knots will be created; if space == "Q", then a vector of equal x quantiles will be created based on x with duplicate elements removed. The number of knots is *numknots* when numknots > 0. Otherwise it is of the order  $n^{1/7}$ . The default is space = "Q".

#### **Details**

"s.incr.conv" returns the vector "x" and imposes on it five attributes: name, shape, numknots, knots and space.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.incr.conv"; the shape attribute is 13("smooth, increasing and convex"). According to the value of the vector itself and its shape, numknots, knots and space attributes, the cone edges will be made by C-spline basis functions in Meyer (2008). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.incr.conv" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta in cgam.

See references cited in this section for more details.

#### Value

The vector x with five attributes, i.e., name: the name of x; shape: 13("smooth, increasing and convex"); numknots: the numknots argument in "s.incr.conv"; knots: the knots argument in "s.incr.conv"; space: the space argument in "s.incr.conv".

#### Author(s)

Mary C. Meyer and Xiyue Liao

64 s.incr.decr

## References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* **2(3)**, 1013–1033.

## See Also

```
incr.conv
```

# **Examples**

```
data(cubic)

# extract x
x <- cubic$x

# extract y
y <- cubic$y

# regress y on x with the shape restriction: "smooth, increasing and convex"
ans <- cgam(y ~ s.incr.conv(x))
knots <- ans$knots[[1]]

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$muhat, col = 2)
legend("topleft", bty = "n", "smooth, increasing and convex fit", col = 2, lty = 1)
legend(1.7, 9.2, bty = "o", "knots", pch = "X")
points(knots, 1:length(knots)*0+min(y), pch = "X")</pre>
```

s.incr.decr

Specify an Increasing-Decreasing Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that a surface is decreasing in one predictor and increasing in another in a formula argument to cgam.

## Usage

```
s.incr.decr(x1, x2, numknots = c(0, 0), knots = list(k1 = 0, k2 = 0), space = c("E", "E"))
```

s.incr.decr 65

## **Arguments**

A numeric predictor which has the same length as the response vector.

A numeric predictor which has the same length as the response vector.

numknots A vector of the number of knots used to constrain  $x_1$  and  $x_2$ . It will not be used

if the user specifies the knots argument and each predictor is within the range of

its knots. The default is numknots = c(0, 0).

knots A list of two vectors of knots used to constrain  $x_1$  and  $x_2$ . User-defined knots

will be used if each predictor is within the range of its knots. Otherwise, num-knots and space will be used to create knots. The default is knots = list(k1 = 0,

k2 = 0).

space A vector of the character specifying the method to create knots for  $x_1$  and  $x_2$ .

It will not be used if the user specifies the *knots* argument. If "E" is used, then equally spaced knots will be created; if "Q" is used, then a vector of equal quantiles will be created with duplicate elements removed. The number of knots is numknots when numknots is a positive integer > 4. Otherwise it is of the order

 $n^{1/6}$ . The default is space = c("E", "E").

#### **Details**

"s.incr.decr" returns the vectors "x1" and "x2", and imposes on each vector six attributes: name, shape, numknots, knots, space and decreasing.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.incr.decr"; the shape attribute is "wps\_id"(increasing-decreasing); the decreasing values for "x1" and "x2" are TRUE and FALSE. According to the value of the vector itself and its shape, numknots, knots, space and decreasing attributes, the cone edges will be made by warped-plane spline basis functions in Meyer (2016). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.incr.decr" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta\_wps.

See references cited in this section for more details.

#### Value

The vectors  $x_1$  and  $x_2$ . Each of them has six attributes, i.e., name: names of  $x_1$  and  $x_2$ ; shape: "wps\_id"(increasing-decreasing); numknots: the numknots argument in "s.incr.decr"; knots: the knots argument in "s.incr.decr"; space: the space argument in "s.incr.decr"; decreasing: two logical values indicating the monotonicity of the isotonically-constrained surface with respect to  $x_1$  and  $x_2$ , which are FALSE and TRUE.

### Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2017) Estimation and inference for regression surfaces using shape-constrained splines.

66 s.incr.incr

## See Also

```
s.incr.incr, s.decr.decr, s.decr.incr, cgam
```

# **Examples**

```
## Not run:
  # generate data
  n <- 100
  set.seed(123)
  x1 <- runif(n)</pre>
  x2 <- runif(n)</pre>
  y < -4 * (x1 - x2) - x1 * x2 + rnorm(n, sd = .2)
  # regress y on x1 and x2 under the shape-restriction: "increasing-decreasing"
  # using the penalized estimator
  ans <- cgam(y \sim s.incr.decr(x1, x2), pnt = TRUE)
  # make a 3D plot of the constrained surface
  plotpersp(ans)
## End(Not run)
```

s.incr.incr

Specify a Doubly-Increasing Shape-Restriction in a CGAM Formula

# **Description**

A symbolic routine to define that a surface is increasing in two predictors in a formula argument to cgam.

#### Usage

```
s.incr.incr(x1, x2, numknots = c(0, 0), knots = list(k1 = 0, k2 = 0), space = c("E", "E"))
```

# **Arguments**

x1	A numeric predictor which has the same length as the response vector.
x2	A numeric predictor which has the same length as the response vector.
numknots	A vector of the number of knots used to constrain $x_1$ and $x_2$ . It will not be used if the user specifies the <i>knots</i> argument and each predictor is within the range of its knots. The default is numknots = $c(0, 0)$ .
knots	A list of two vectors of knots used to constrain $x_1$ and $x_2$ . User-defined knots will be used if each predictor is within the range of its knots. Otherwise, $num$ -

*knots* and *space* will be used to create knots. The default is knots = list(k1 = 0,

k2 = 0).

s.incr.incr 67

space

A vector of the character specifying the method to create knots for  $x_1$  and  $x_2$ . It will not be used if the user specifies the *knots* argument. If "E" is used, then equally spaced knots will be created; if "Q" is used, then a vector of equal quantiles will be created with duplicate elements removed. The number of knots is *numknots* when *numknots* is a positive integer > 4. Otherwise it is of the order  $n^{1/6}$ . The default is space = c("E", "E").

#### **Details**

"s.incr.incr" returns the vectors "x1" and "x2", and imposes on each vector six attributes: name, shape, numknots, knots, space and decreasing.

The name attribute is used in the subroutine plotpersp; the numknots, knots and space attributes are the same as the numknots, knots and space arguments in "s.incr.incr"; the shape attribute is "wps\_ii"(doubly-increasing); the decreasing values for both vectors are FALSE. According to the value of the vector itself and its shape, numknots, knots, space and decreasing attributes, the cone edges will be made by warped-plane spline basis functions in Meyer (2016). The cone edges are a set of basis employed in the hinge algorithm.

Note that "s.incr.incr" does not make the corresponding cone edges itself. It sets things up to a subroutine called makedelta\_wps.

See references cited in this section for more details.

#### Value

The vectors  $x_1$  and  $x_2$ . Each of them has six attributes, i.e., name: names of  $x_1$  and  $x_2$ ; shape: "wps\_ii"(doubly-increasing); numknots: the numknots argument in "s.incr.incr"; knots: the knots argument in "s.incr.incr"; space: the space argument in "s.incr.incr"; decreasing: two logical values indicating the monotonicity of the isotonically-constrained surface with respect to  $x_1$  and  $x_2$ , which are both FALSE.

#### Author(s)

Mary C. Meyer and Xiyue Liao

# References

Meyer, M. C. (2017) Estimation and inference for regression surfaces using shape-constrained splines.

## See Also

```
s.decr.decr, s.decr.incr, cgam
```

```
## Not run:
    # generate data
    n <- 100
    set.seed(123)
    x1 <- runif(n)</pre>
```

68 shapes

```
x2 <- runif(n)
y <- 4 * (x1 + x2 - x1 * x2) + rnorm(n, sd = .2)

# regress y on x1 and x2 under the shape-restriction: "doubly-increasing"
# using the penalized estimator
ans <- cgam(y ~ s.incr.incr(x1, x2), pnt = TRUE)

# make a 3D plot of the constrained surface
plotpersp(ans)

## End(Not run)</pre>
```

shapes

To Include a Non-Parametrically Modelled Predictor in a SHAPESE-LECT Formula

# **Description**

A symbolic routine to indicate that a predictor is included as a non-parametrically modelled predictor in a formula argument to ShapeSelect.

#### Usage

```
shapes(x, set = "s.9")
```

## **Arguments**

Χ

A numeric predictor which has the same length as the response vector.

set

A character or a numeric vector indicating all possible shapes defined for x. For example, we are not only interested in modeling the relationship between the growth of an organism (dependent variable y) and time (independent variable x), but we are also interested in the shape of the growth curve. Suppose we know  $a\ priori$  that the shape could be flat, increasing, increasing concave, or increasing convex, and we further know that the curve is smooth, we can write  $y \sim \text{shapes}(x, \text{set} = c(\text{"flat"}, \text{"s.incr.}, \text{"s.incr.conc"}, \text{"s.incr.conv"}))$  in a formula to impose the four possible shape constraints on the growth curve and model it with splines.

To be more specific, the user can choose to specify this argument as following

1. It could be written as "s.5", "s.9", "ord.5", "ord.9", and "tree", where "s.5" ("ord.5") means that the relationship between the response and a predictor x is modelled with regression splines (ordinal regression basis functions) with five possible shapes, i.e., flat, increasing, decreasing, convex, and concave; "s.9" ("ord.9") includes four more possible shapes, which are the combination of monotonicity and convexity; "tree" specifies that x is included as an ordinal predictor with three possibilities: no effect, tree-ordering, and unordered effect.

shapes 69

2. Or the user can choose any subset of the possible shapes, i.e., flat, increasing, decreasing, convex, concave, and combination of monotonicity and convexity. The symbols are "flat", "incr", "decr", "conv", "conc", "incr.conv", "decr.conv", "incr.conc", and "decr.conc". To specify a spline-based regression, the user needs write something like "s.incr", "s.decr", etc.

3. It can also be a subset of integers between 0 and 16, where 0 is the flat shape, 1 ~ 8 indicate increasing, decreasing, convex, concave, increasing-convex, decreasing-convex, increasing-concave, and decreasing-concave, while 9 ~ 16 indicate the same shapes with a smooth assumption.

The default is set = "s.9".

#### Value

The vector x with three attributes, i.e., nm: the name of x; shape: a numeric vector ranging from 0 to 16 to indicate possible shapes imposed on the relationship between the response and x; type: "nparam", i.e., x is non-parametrically modelled.

### Author(s)

Xiyue Liao

#### See Also

```
in.or.out, ShapeSelect
```

```
## Not run:
# Example 1.
 n <- 100
 # generate predictors, x is non-parametrically modelled
 # and z is parametrically modelled
 x <- runif(n)</pre>
 z \leftarrow rep(0:1, 50)
 \# E(y) is generated as correlated to both x and z
 \# the relationship between E(y) and x is smoothly increasing-convex
 y <- x^2 + 2 * I(z == 1) + rnorm(n, sd = 1)
 # call ShapeSelect to find the best model by the genetic algorithm
 fit <- ShapeSelect(y ~ shapes(x) + in.or.out(factor(z)), genetic = TRUE)</pre>
# Example 2.
 n <- 100
 z <- rep(c("A", "B"), n / 2)
 x <- runif(n)</pre>
 # y0 is generated as correlated to z with a tree-ordering in it
 # y0 is smoothly increasing-convex in x
 y0 <- x^2 + I(z == "B") * 1.5
```

70 ShapeSelect

```
y <- y0 + rnorm(n, 1)

fit <- ShapeSelect(y ~ s.incr(x) + shapes(z, set = "tree"), genetic = FALSE)

# check the best fit in terms of z
fit$top

## End(Not run)</pre>
```

ShapeSelect

Variable and Shape Selection via Genetic Algorithm

# **Description**

The partial linear generalized additive model is considered, where the goal is to choose a subset of predictor variables and describe the component relationships with the response, in the case where there is very little *a priori* information. For each predictor, the user need only specify a set of possible shape or order restrictions. A model selection method chooses the shapes and orderings of the relationships as well as the variables. For each possible combination of shapes and orders for the predictors, the maximum likelihood estimator for the constrained generalized additive model is found using iteratively re-weighted cone projections. The cone information criterion is used to select the best combination of variables and shapes.

## Usage

```
ShapeSelect(formula, family = gaussian, cpar = 2, data = NULL, weights = NULL, npop = 200, per.mutate = 0.05, genetic = FALSE)
```

# Arguments

formula

A formula object which includes a set of predictors to be selected. It has the form "response ~ predictor". The response is a vector of length n. The specification of the model can be one of the three exponential families: gaussian, binomial and poisson. The systematic component  $\eta$  is E(y), the log odds of y=1, and the logarithm of E(y) respectively. The user is supposed to define at least one predictor in the formula, which could be a non-parametrically modelled variable or a parametrically modelled covariate (categorical or linear). Assume that  $\eta$  is the systematic component and x is a predictor, two symbolic routines shapes and in.or.out are used to include x in the formula.

**shapes(x):** x is included as a non-parametrically modelled predictor in the formula. See shapes for more details.

**in.or.out(x):** x is included as a categorical or linear predictor in the formula. See in.or.out for more details.

family

A parameter indicating the error distribution and link function to be used in the model. It can be a character string naming a family function or the result of a call to a family function. This is borrowed from the glm routine in the stats package. There are three families used in ShapeSelect: gaussian, binomial and poisson.

ShapeSelect 71

cpar A multiplier to estimate the model variance, which is defined as  $\sigma^2 = SSR/(n-1)$ 

 $d_0 - cpar * edf$ ). SSR is the sum of squared residuals for the full model,  $d_0$  is the dimension of the linear space in the cone, and edf is the effective degrees of freedom. The default is cpar = 2. See Meyer, M. C. and M. Woodroofe (2000)

for more details.

data An optional data frame, list or environment containing the variables in the model.

The default is data = NULL.

weights An optional non-negative vector of "replicate weights" which has the same

length as the response vector. If weights are not given, all weights are taken

to equal 1. The default is weights = NULL.

npop The population size used for the genetic algorithm. The default is npop = 200.

per.mutate The percentage of mutation used for the genetic algorithm. The default is per.mutate

= 0.05

genetic A logical scalar showing if or not the genetic algorithm is defined by the user to

select the best model. The default is genetic = FALSE.

#### **Details**

Note that when the argument genetic is set to be FALSE, the routine will check to see if using the genetic algorithm is better than going through all models to find the best fit. The primary concern is running time. An interactive dialogue window may pop out to ask the user if they prefer to the genetic algorithm when it may take too long to do a brutal search, and if there are too many possible models to go through, like more than one million, the routine will implement the genetic algorithm anyway.

See references cited in this section for more details.

# Value

The best model of the final population, which shows the variables chosen along

with their best shapes.

pop The final population ordered by its fitness values. It is a data frame, and each

row of this data frame shows the shapes chosen for predictors in an individual model. Besides, the fitness value for each individual model is included in the last column of the data frame. For example, we have two continuous predictors  $x_1$ ,  $x_2$ , and a categorical predictor z, then a row of this data frame may look like: "flat", "s.incr", "in", -12.3806, which means that  $x_1$  is not chosen,  $x_2$  is chosen with the shape constraint to be smoothly increasing, z is included in the

model, and the fitness value for the model is -12.3806.

fitness The sorted fitness values for the final population.

tm Total cpu running time.

xnms A vector storing the name of the nonparametrically-modelled predictor in a

ShapeSelect formula.

znms A vector storing the name of the parametrically-modelled predictor in a Shape-

Select formula, which is a categorical predictor or a linear term.

trnms A vector storing the name of the treatment predictor in a ShapeSelect formula,

which has three possible levels: no effect, tree ordering, unordered.

72 ShapeSelect

zfacs	A logical vector keeping track of if the parametrically-modelled predictor in a ShapeSelect formula is a categorical predictor or a linear term.
mxf	A vector keeping track of the largest fitness value in each generation.
mnf	A vector keeping track of the mean fitness value in each generation.
GA	A logical scalar showing if or not the genetic algorithm is actually implemented to select the best model.
best.fit	The best model fitted by the cgam routine, given the best variables with their shape constraints chosen by the ShapeSelect routine.
call	The matched call.

# Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013a) Semi-parametric additive constrained regression. *Journal of Nonparametric Statistics* **25**(3), 715

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Meyer, M. C. and M. Woodroofe (2000) On the degrees of freedom in shape-restricted regression. *Annals of Statistics* **28**, 1083–1104.

Meyer, M. C. (2008) Inference using shape-restricted regression splines. *Annals of Applied Statistics* **2**(3), 1013–1033.

Meyer, M. C. and Liao, X. (2016) Variable and shape selection for the generalized additive model. *under preparation* 

# See Also

cgam

```
## Not run:
# Example 1.
    library(MASS)
    data(Rubber)

# ShapeSelect can be used to go through all models to find the best model
    fit <- ShapeSelect(loss ~ shapes(hard, set = "s.9") + shapes(tens, set = "s.9"),
    data = Rubber, genetic = FALSE)

# the user can also choose to find the best model by the genetic algorithm
# given any total number of possible models
    fit <- ShapeSelect(loss ~ shapes(hard, set = "s.9") + shapes(tens, set = "s.9"),
    data = Rubber, genetic = TRUE)

# check the best model</pre>
```

testpar 73

```
fit$top
 # check the running time
 fit$tm
# Example 2.
 # simulate a data set such that the mean is smoothly increasing-convex in x1 and x2
 x1 <- runif(n)</pre>
 x2 <- runif(n)</pre>
 y0 < -x1^2 + x2 + x2^3
 z \leftarrow rep(0:1, 50)
 for (i in 1:n) {
   if (z[i] == 1)
      y0[i] = y0[i] * 1.5
 }
 # add some random errors and call the routine
 y <- y0 + rnorm(n)
 # include factor(z) in the formula and determine if factor(z) should be in the model
 fit \leftarrow ShapeSelect(y \sim shapes(x1, set = "s.9") + shapes(x2, set = "s.9") + in.or.out(factor(z)))
 # use the genetic algorithm
 fit <- ShapeSelect(y \sim shapes(x1, set = "s.9") + shapes(x2, set = "s.9") + in.or.out(factor(z)),
  npop = 300, per.mutate=0.02)
 \# include z as a linear term in the formula and determine if z should be in the model
 fit \leftarrow ShapeSelect(y \sim shapes(x1, set = "s.9") + shapes(x2, set = "s.9") + in.or.out(z))
 \# include z as a linear term in the model
 fit <- ShapeSelect(y \sim shapes(x1, set = "s.9") + shapes(x2, set = "s.9") + z)
 # include factor(z) in the model
 fit <- ShapeSelect(y \sim shapes(x1, set = "s.9") + shapes(x2, set = "s.9") + factor(z))
 # check the best model
 bf <- fit$best.fit</pre>
 # make a 3D plot of the best fit
 plotpersp(bf, categ = "z")
## End(Not run)
```

74 testpar

# Description

Performs a hypothesis test comparing a parametric model (e.g., linear, quadratic, warped plane) to a constrained smooth alternative under shape restrictions.

# Usage

```
testpar(
  formula0,
  formula,
  data,
  family = gaussian(link = "identity"),
  ps = NULL,
  edfu = NULL,
  nsim = 1000,
  multicore = getOption("cgam.parallel"),
  method = "testpar.fit",
  arp = FALSE,
  p = NULL,
  space = "E",
  ...
)
```

# Arguments

formula0	A model formula representing the null hypothesis (e.g., linear or quadratic).
formula	A model formula under the alternative hypothesis, possibly with shape constraints.
data	A data frame or environment containing the variables in the model.
family	A description of the error distribution and link function to be used in the model (e.g., gaussian()). Gaussian and binomial are now included.
ps	User-defined penalty term. If NULL, optimal values are estimated.
edfu	User-defined unconstrained effective degrees of freedom.
nsim	Number of simulations to perform to get the mixture distribution of the test statistic. (default is 1000).
multicore	Logical. Whether to enable parallel computation (default uses global option cgam.parallel).
method	A character string (default is "testpar.fit"), currently unused.
arp	Logical. If TRUE, uses autoregressive structure estimation.
p	Integer vector or value specifying $AR(p)$ order. Ignored if arp = FALSE.
space	Character. Either "Q" for quantile-based knots or "E" for evenly spaced knots. Default is "E".
	Additional arguments passed to internal functions.

# Value

A list containing test statistics, fitted values, coefficients, and other relevant objects.

testpar 75

```
# Example 1: Linear vs. monotone alternative
set.seed(123)
n <- 100
x <- sort(runif(n))</pre>
y \leftarrow 2 * x + rnorm(n)
dat \leftarrow data.frame(y = y, x = x)
ans <- testpar(formula0 = y ~ x, formula = y ~ s.incr(x), multicore = FALSE, nsim = 10)
ans$pval
summary(ans)
## Not run:
# Example 2: Binary response: linear vs. monotone alternative
set.seed(123)
n <- 100
x <- runif(n)</pre>
eta <- 8 * x - 4
mu \leftarrow exp(eta) / (1 + exp(eta))
y <- rbinom(n, size = 1, prob = mu)
ans <- testpar(formula0 = y \sim x, formula = y \sim s.incr(x),
family = binomial(link = "logit"), nsim = 10)
summary(ans)
xs = sort(x)
ord = order(x)
 par(mfrow = c(1,1))
 plot(x, y, cex = .2)
 lines(xs, binomial(link="logit")$linkinv(ans$etahat0)[ord], col=4, lty=4)
 lines(xs, binomial(link="logit")$linkinv(ans$etahat)[ord], col=2, lty=2)
 lines(xs, mu[ord])
 legend("topleft", legend = c("H0 fit (etahat0)", "H1 fit (etahat)", "True mean"),
 col = c(4, 2, 1), lty = c(4, 2, 1), bty = "n", cex = 0.8)
## End(Not run)
# Example 3: Bivariate warped-plane surface test
set.seed(1)
n <- 100
x1 <- runif(n)</pre>
x2 <- runif(n)</pre>
mu < -4 * (x1 + x2 - x1 * x2)
eps <- rnorm(n)</pre>
y <- mu + eps
# options(cgam.parallel = TRUE) #allow parallel computation
ans <- testpar(formula0 = y \sim x1 * x2, formula = y \sim s.incr.incr(x1, x2), nsim = 10)
summary(ans)
par(mfrow = c(1, 2))
persp(ans$k1, ans$k2, ans$etahat0_surf, th=-50, main = 'H0 fit')
persp(ans$k1, ans$k2, ans$etahat_surf, th=-50, main = 'H1 fit')
```

76 tree

```
## Not run:
# Example 4: AR(1) error, quadratic vs smooth convex
set.seed(123)
n = 100
x = runif(n)
mu = 1+x+2*x^2
eps = arima.sim(n = n, list(ar = c(.4)), sd = 1)
y = mu + eps
ans = testpar(y^x^2, y^s.conv(x), arp=TRUE, p=1, nsim=10)
ans$pval
ans$phi #autoregressive coefficient estimate
## End(Not run)
## Not run:
# Example 5: Three additive components with shape constraints
n <- 100
x1 <- runif(n)</pre>
x2 <- runif(n)</pre>
x3 <- runif(n)
z <- rnorm(n)</pre>
mu1 < -3 * x1 + 1
mu2 <- x2 + 3 * x2^2
mu3 <- -x3^2
mu \leftarrow mu1 + mu2 + mu3
y \leftarrow mu + rnorm(n)
ans <- testpar(formula0 = y \sim x1 + x2^2 + x3^2 + z,
formula = y \sim s.incr(x1) + s.incr.conv(x2) + s.decr.conc(x3)
+ z, family = "gaussian", nsim = 10)
ans$pval
summary(ans)
## End(Not run)
```

tree

Specify a Tree-Ordering in a CGAM Formula

# Description

A symbolic routine to define that the systematic component  $\eta$  has a tree-ordering in a predictor in a formula argument to cgam.

# Usage

```
tree(x, pl = NULL)
```

# **Arguments**

x A numeric vector which has the same length as the response vector. Note that the placebo level of x must be 0.

pl The placebo level.

tree 77

#### **Details**

"tree" returns the vector "x" and imposes on it two attributes: name and shape.

The name attribute is used in the subroutine plotpersp; the shape attribute is "tree", and according to the value of the vector itself and its shape attribute, the cone edges of the cone generated by the constraint matrix, which constrains that  $\eta$  has a tree-ordering in "x" will be made. The cone edges are a set of basis employed in the hinge algorithm.

Note that "tree" does not make the corresponding cone edges itself. It sets things up to a sub-routine called tree.fun in cgam which will make the cone edges. A tree-ordering is a partial ordering: For a categorical variable x, if there are treatment levels  $x_1, \ldots, x_k$ , where  $x_1$  is a placebo, we compare  $x_i, i = 2, \ldots, k$  with  $x_1$ , and not have any other comparable pairs.

See references cited in this section for more details.

#### Value

The vector x with two attributes, i.e., name: the name of x; shape: "tree".

#### Author(s)

Mary C. Meyer and Xiyue Liao

#### References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

# See Also

umbrella

```
# generate y
set.seed(123)
n <- 100
x < - rep(0:4, each = 20)
z <- rep(c("a", "b"), 50)
y <- x + I(z == "a") + rnorm(n, 1)
xu <- unique(x)</pre>
# regress y on x under the tree-ordering restriction
fit.tree <- cgam(y \sim tree(x) + factor(z))
# make a plot
plot(x, y, cex = .7)
mua = unique(fit.tree$muhat)[unique(z) == "a"]
points(xu, unique(fit.tree$muhat)[unique(z) == "a"], pch = '+', col = 4, cex = 3)
legend(0,7.5, bty = "n", "tree-ordering fit: z = 'a'", col = 4, pch = '+', cex = 1.3)
mub = unique(fit.tree$muhat)[unique(z) == "b"]
points(xu, unique(fit.tree$muhat)[unique(z) == "b"], pch = '+', col = 2, cex = 3)
legend(0,8.5, bty = "n", "tree-ordering fit: z = b'", col = 2, pch = '+', cex = 1.3)
```

78 umbrella

umbrella

Specify an Umbrella-Ordering in a CGAM Formula

# **Description**

A symbolic routine to define that the systematic component  $\eta$  has an umbrella-ordering in a predictor in a formula argument to cgam.

## Usage

umbrella(x)

## **Arguments**

Х

A numeric vector which has the same length as the response vector.

#### **Details**

"umbrella" returns the vector "x" and imposes on it two attributes: name and shape.

The name attribute is used in the subroutine plotpersp; the shape attribute is "umbrella", and to the value of the vector itself and its shape attribute, the cone edges of the cone generated by the constraint matrix, which constrains that  $\eta$  has an umbrella-ordering in "x" will be made. The cone edges are a set of basis employed in the hinge algorithm.

Note that "umbrella" does not make the corresponding cone edges itself. It sets things up to a subroutine called umbrella.fun in cgam which will make the cone edges. An umbrella-ordering is a partial ordering: Suppose we have a  $x_0$  that is known to be a "mode" so that for  $x, y >= x_0$ , we have a binary relation between x and y if x <= y and for  $x, y <= x_0$  we have the opposite binary relation if x <= y, but if  $x < x_0$  and  $y > x_0$ , there is no such binary relation.

See references cited in this section for more details.

# Value

The vector x with two attributes, i.e., name: the name of x; shape: "umbrella".

# Author(s)

Mary C. Meyer and Xiyue Liao

# References

Meyer, M. C. (2013b) A simple new algorithm for quadratic programming with applications in statistics. *Communications in Statistics* **42**(5), 1126–1139.

#### See Also

tree

umbrella 79

```
# generate y
set.seed(123)
n <- 20
x <- seq(-2, 2, length = n)
y <- - x^2 + rnorm(n)

# regress y on x under the umbrella-ordering restriction
fit <- cgam(y ~ umbrella(x))

# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, ylab = "y")
lines(x, fit$muhat, col = 2)
legend("topleft", bty = "n", "umbrella-ordering fit", col = 2, lty = 1)</pre>
```

# **Index**

an 1	
* 3D plot routine	incr.conc, 28
plotpersp, 36	incr.conv, 30
* 3D	s, 42
plotpersp_control, 38	s.conc, 43
* ShapeSelect	s.conc.conc, 45
best.fit, 3	s.conv, 47
* best	s.conv.conv, 48
best.fit,3	s.decr, 50
* cgam routine	s.decr.conc, 52
cgam, 4	s.decr.conv, 53
* cgamm routine	s.decr.decr, 55
cgamm, 11	s.decr.incr, 57
* data set	s.incr, 59
cubic, 20	s.incr.conc, 61
* datasets	s.incr.conv, 62
COforest, 14	s.incr.decr, 64
mental, 32	s.incr.incr, 66
plasma, 35	tree, 76
* fit	umbrella, 78
hart Cit 2	* the
best.fit,3	h+ C:+ 2
* genetic algorithm	best.fit, 3
	* variable and shape selection
* genetic algorithm	* variable and shape selection ShapeSelect, 70
* genetic algorithm ShapeSelect, 70	<ul> <li>* variable and shape selection</li> <li>ShapeSelect, 70</li> <li>* variable selection routine</li> </ul>
* genetic algorithm ShapeSelect, 70 * graphics	* variable and shape selection ShapeSelect, 70 * variable selection routine in.or.out, 26
* genetic algorithm ShapeSelect, 70 * graphics plotpersp_control, 38	<ul> <li>* variable and shape selection</li> <li>ShapeSelect, 70</li> <li>* variable selection routine</li> </ul>
<pre>* genetic algorithm</pre>	* variable and shape selection ShapeSelect, 70 * variable selection routine in.or.out, 26
<pre>* genetic algorithm     ShapeSelect, 70 * graphics     plotpersp_control, 38 * of     best.fit, 3</pre>	<pre>* variable and shape selection     ShapeSelect, 70 * variable selection routine     in.or.out, 26     shapes, 68 best.fit, 3</pre>
<pre>* genetic algorithm     ShapeSelect, 70 * graphics     plotpersp_control, 38 * of     best.fit, 3 * ordered categorical family</pre>	* variable and shape selection ShapeSelect, 70  * variable selection routine in.or.out, 26 shapes, 68
<pre>* genetic algorithm</pre>	<pre>* variable and shape selection     ShapeSelect, 70 * variable selection routine     in.or.out, 26     shapes, 68 best.fit, 3</pre>
<pre>* genetic algorithm     ShapeSelect, 70 * graphics     plotpersp_control, 38 * of     best.fit, 3 * ordered categorical family     Ord, 33</pre>	<pre>* variable and shape selection     ShapeSelect, 70 * variable selection routine     in.or.out, 26     shapes, 68  best.fit, 3 cgam, 3, 4, 12, 46, 50, 57, 58, 66, 67, 72</pre>
<pre>* genetic algorithm     ShapeSelect, 70 * graphics     plotpersp_control, 38 * of     best.fit, 3 * ordered categorical family     Ord, 33 * prediction routine     predict.cgam, 39</pre>	* variable and shape selection ShapeSelect, 70  * variable selection routine in.or.out, 26 shapes, 68  best.fit, 3  cgam, 3, 4, 12, 46, 50, 57, 58, 66, 67, 72 cgamm, 11
<pre>* genetic algorithm</pre>	* variable and shape selection ShapeSelect, 70  * variable selection routine in.or.out, 26 shapes, 68  best.fit, 3  cgam, 3, 4, 12, 46, 50, 57, 58, 66, 67, 72 cgamm, 11 COforest, 14
<pre>* genetic algorithm     ShapeSelect, 70 * graphics     plotpersp_control, 38 * of     best.fit, 3 * ordered categorical family     Ord, 33 * prediction routine     predict.cgam, 39 * routine     best.fit, 3 * shape routine</pre>	* variable and shape selection ShapeSelect, 70  * variable selection routine in.or.out, 26 shapes, 68  best.fit, 3  cgam, 3, 4, 12, 46, 50, 57, 58, 66, 67, 72 cgamm, 11 COforest, 14 conc, 4, 17, 20, 44
<pre>* genetic algorithm</pre>	* variable and shape selection     ShapeSelect, 70  * variable selection routine     in.or.out, 26     shapes, 68  best.fit, 3  cgam, 3, 4, 12, 46, 50, 57, 58, 66, 67, 72 cgamm, 11 COforest, 14 conc, 4, 17, 20, 44 conv, 4, 18, 19, 48 cubic, 20
<pre>* genetic algorithm</pre>	* variable and shape selection     ShapeSelect, 70  * variable selection routine     in.or.out, 26     shapes, 68  best.fit, 3  cgam, 3, 4, 12, 46, 50, 57, 58, 66, 67, 72 cgamm, 11 COforest, 14 conc, 4, 17, 20, 44 conv, 4, 18, 19, 48 cubic, 20  decr, 4, 21, 23, 25, 51, 53
<pre>* genetic algorithm     ShapeSelect, 70 * graphics     plotpersp_control, 38 * of     best.fit, 3 * ordered categorical family     Ord, 33 * prediction routine     predict.cgam, 39 * routine     best.fit, 3 * shape routine     conc, 17     conv, 19     decr, 21</pre>	* variable and shape selection     ShapeSelect, 70  * variable selection routine     in.or.out, 26     shapes, 68  best.fit, 3  cgam, 3, 4, 12, 46, 50, 57, 58, 66, 67, 72 cgamm, 11 COforest, 14 conc, 4, 17, 20, 44 conv, 4, 18, 19, 48 cubic, 20  decr, 4, 21, 23, 25, 51, 53 decr.conc, 4, 22, 22, 25
<pre>* genetic algorithm     ShapeSelect, 70 * graphics     plotpersp_control, 38 * of     best.fit, 3 * ordered categorical family     Ord, 33 * prediction routine     predict.cgam, 39 * routine     best.fit, 3 * shape routine     conc, 17     conv, 19     decr, 21     decr.conc, 22</pre>	* variable and shape selection     ShapeSelect, 70  * variable selection routine     in.or.out, 26     shapes, 68  best.fit, 3  cgam, 3, 4, 12, 46, 50, 57, 58, 66, 67, 72 cgamm, 11 COforest, 14 conc, 4, 17, 20, 44 conv, 4, 18, 19, 48 cubic, 20  decr, 4, 21, 23, 25, 51, 53
<pre>* genetic algorithm     ShapeSelect, 70 * graphics     plotpersp_control, 38 * of     best.fit, 3 * ordered categorical family     Ord, 33 * prediction routine     predict.cgam, 39 * routine     best.fit, 3 * shape routine     conc, 17     conv, 19     decr, 21</pre>	* variable and shape selection     ShapeSelect, 70  * variable selection routine     in.or.out, 26     shapes, 68  best.fit, 3  cgam, 3, 4, 12, 46, 50, 57, 58, 66, 67, 72 cgamm, 11 COforest, 14 conc, 4, 17, 20, 44 conv, 4, 18, 19, 48 cubic, 20  decr, 4, 21, 23, 25, 51, 53 decr.conc, 4, 22, 22, 25

INDEX 81

```
incr, 4, 27, 31, 60
incr.conc, 4, 28, 28, 31
incr.conv, 5, 28, 29, 30, 62, 64
mental, 32, 33
Ord, 32, 33
persp, 39
plasma, 35
plotpersp, 36, 39
plotpersp_control, 36, 38
predict.cgam, 39
s, 5, 42
s.conc, 4, 43, 43
s.conc.conc, 45
s.conv, 4, 43, 47
s.conv.conv, 46, 48, 50
s.decr, 4, 5, 43, 50
s.decr.conc, 4, 43, 52
s.decr.conv, 5, 43, 53
s.decr.decr, 55, 58, 66, 67
s.decr.incr, 57, 57, 66, 67
s.incr, 4, 5, 43, 59
s.incr.conc, 4, 43, 61
s.incr.conv, 5, 43, 62
s.incr.decr, 57, 58, 64
s.incr.incr, 57, 58, 66, 66
shapes, 26, 68, 70
ShapeSelect, 3, 26, 69, 70
testpar, 73
tree, 5, 76, 78
umbrella, 5, 77, 78
```