Package 'cgam'

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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 Mary C. Meyer (2013) doi:10.1080/10485252.2013.797577 for more details.
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best.fit

best.fit

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Description

best.fit

The is a subroutine which 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.

Extract the Best Fit Returned by the ShapeSelect Routine

Usage

best.fit(x)

Arguments

Χ

x is an object of the ShapeSelect class.

Value

object

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

Author(s)

Xiyue Liao

See Also

```
cgam, ShapeSelect
```

Examples

```
## Not run:
    library(MASS)
    data(Rubber)

# do a variable and shape selection with four possible shapes
# increasing, decreasing, convex and concave
ans <- ShapeSelect(loss ~ shapes(hard, set = c("incr", "decr", "conv", "conc"))
+ shapes(tens, set = c("incr", "decr", "conv", "conc")), data = Rubber, genetic = TRUE)

# check the best fit, which is an object of the cgam class
bf <- best.fit(ans)
class(bf)
plotpersp(bf)

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

cgam

Constrained Generalized Additive Model Fitting

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, nsim = 1e+2, family = gaussian, cpar = 1.2, data = NULL, weights = NULL, sc_x = FALSE, sc_y = FALSE, pnt = TRUE, pen = 0)
```

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 η 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 η and a predictor x in the following way:

Assume that η is the systematic component and x is a predictor:

- incr(x): η is increasing in x. See incr for more details.
- s.incr(x): η is smoothly increasing in x. See s.incr for more details.
- decr(x): η is decreasing in x. See decr for more details.
- s.decr(x): η is smoothly decreasing in x. See s.decr for more details.
- conc(x): η is concave in x. See conc for more details.
- s.conc(x): η is smoothly concave in x. See s.conc for more details.
- conv(x): η is convex in x. See conv for more details.
- s.conv(x): η is smoothly convex in x. See s.conv for more details.
- incr.conc(x): η is increasing and concave in x. See incr.conc for more details.
- s.incr.conc(x): η is smoothly increasing and concave in x. See s.incr.conc for more details.
- decr.conc(x): η is decreasing and concave in x. See decr.conc for more details.
- s.decr.conc(x): η is smoothly decreasing and concave in x. See s.decr.conc for more details.
- incr.conv(x): η is increasing and convex in x. See incr.conv for more details.
- s.incr.conv(x): η is smoothly increasing and convex in x. See s.incr.conv for more details.
- decr.conv(x): η is decreasing and convex in x. See decr.conv for more details.
- s.decr.conv(x): η is smoothly decreasing and convex in x. See s.decr.conv for more details.
- s(x): η is smooth in x. See s for more details.
- tree(x): η has a tree-ordering in x. See tree for more details.
- umbrella(x): η has an umbrella-ordering in x. See umbrella for more details.

nsim

The number of simulations used to get the cic parameter. The default is nsim = 1e+2.

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 cgam: 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.
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 $sc_y = FALSE$.
pen	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 $pen = 0$.
pnt	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.

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 η is the systematic component and describes the relationship with the predictors. The relationship between η and θ 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 , β 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 η 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 ϕ_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 ϕ_l , smooth regression splines or non-smooth ordinal basis functions can be used. The constraints for the component ϕ_l are in C_l . In the first case, $C_l = \{\phi_l \in \mathbb{R}^n : \phi_l = v_l + B_l\beta_l$, 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, $C_l = \{\phi \in \mathbb{R}^n : A_l \phi \geq 0 \text{ and } B_l \phi = 0\}$, 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 \mathcal{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 η .
muhat	The fitted mean value, obtained by transforming the systematic component η 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.

atb 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 predic-

tors.

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 β . A t-distribution is

used as the approximate distribution.

se.beta The standard errors for the estimation of the vector β .

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. See

the official help page (http://stat.ethz.ch/R-manual/R-patched/library/

stats/html/terms.html) of the terms function for more details.

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.
xnms	A vector storing the names of the shape-restricted predictors and the smooth predictors with no shape constraint in xmat.
ynm	The name of the response variable.
znms	A vector storing the names of the parametrically modelled covariate.
is_param	A logical scalar showing if or not a variable is a parametrically modelled covariate, 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, <i>knots</i> 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, $numknots = 0$.
sps	A character vector storing the <i>space</i> parameter to create knots for each shape-restricted predictor.
ms	The centering terms used to make edges for shape-restricted predictors.
cpar	The cpar argument in the cgam formula
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

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. 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.

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.
## Not run:
```

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```
library(gam)
 data(kyphosis)
 # regress Kyphosis on Age, Number, and Start under the restrictions:
 # "concave", "increasing and concave", and "decreasing and concave"
 fit <- cgam(Kyphosis ~ conc(Age) + incr.conc(Number) + decr.conc(Start),</pre>
 family = binomial(), data = kyphosis)
## End(Not run)
# Example 3.
 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)
 # make a 3D plot based on fit.cgam and fit.cgam.s
 plotpersp(fit.cgam, th = 120, main = "3D Plot of a Cgam Fit")
 plotpersp(fit.cgam.s, tens, hard, data = Rubber, th = 120, main = "3D Plot of a Smooth Cgam Fit")
```

conc

Specify a Concave Shape-Restriction in a CGAM Formula

Description

A symbolic routine to define that the systematic component η 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")
```

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".

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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 η 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)

# 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>
```

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conv	Specify a Convex Shape-Restriction in a CGAM Formula

Description

A symbolic routine to define that the systematic component η 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 η 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.

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

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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.

Source

STAT640 HW 14 given by Dr. Meyer.

14 decr

decr	Specify a Decreasing Shape-Restriction in a CGAM Formula

Description

A symbolic routine to define that the systematic component η 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

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" 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 η 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".

Author(s)

Mary C. Meyer and Xiyue Liao

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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 η 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")
```

Arguments

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

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.

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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 η 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

# 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</pre>
```

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```
 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)
```

decr.conv Specify a Decreasing and Convex Shape-Restriction in a CGAM Formula

Description

A symbolic routine to define that the systematic component η 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 "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 η and "x" to be decreasing and convex, will be made. The cone edges are a set of basis employed in the hinge algorithm.

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".

in.or.out

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
```

Examples

```
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>
```

in.or.out

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.

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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
```

Examples

```
## 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
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 η is increasing in a predictor in a formula argument to cgam. This is the unsmoothed version.

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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 η 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.

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
```

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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 η 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")
```

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

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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 η 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

# 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>
```

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incr.conv Specify an Incomula	reasing and Convex Shape-Restriction in a CGAM For-
-------------------------------	---

Description

A symbolic routine to define that the systematic component η 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 η and "x" to be increasing and convex, will be made. The cone edges are a set of basis employed in the hinge algorithm.

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

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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
```

Examples

```
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>
```

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)
```

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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

0rd

Examples

```
# 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>
```

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.

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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

```
## 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"
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)
```

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```
for (i in 1:2) {
abline(h = (ans$zeta)[i], lty = 4, lwd = 1)
lines(sort(x), (5*x^2)[order(x)], lwd = 2)
lines(sort(x), (ans*muhat)[order(x)], col = 2, lty = 2, lwd = 2)
legend("topleft", bty = "n", col = c(1, 2), lty = c(1, 2),
c("true latent variable", "increasing-convex fit"), lwd = c(1, 1))
## End(Not run)
## Not run:
# Example 2. mental impairment data set
# mental impairment is an ordinal response with 4 categories recorded as 1, 2, 3, and 4
# two covariates are life event index and socio-economic status (high = 1, low = 0)
data(mental)
table(mental$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>
# check the estimated probabilities P(mental = k), k = 1, 2, 3, 4
probs.incr <- fitted(fit.incr)</pre>
head(probs.incr)
## End(Not run)
```

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.

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```
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)
```

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, x1 = NULL, x2 = NULL,...)
```

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Arguments

object

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

x1

A non-parametrically modelled predictor in a cgam fit. If the user omits x1 and x2, then the first two non-parametric predictors in a cgam formula will be used.

х2

A non-parametrically modelled predictor in a cgam fit. If the user omits x1 and x2, then the first two non-parametric predictors in a cgam formula will be used.

Arguments to be passed to the S3 method for the cgam class:

- x1nm: Character name of x1.
- x2nm: Character name of x2.
- data: The data frame based on which the user get a cgam fit.
- surface: The type of the surface of a 3D plot. For a cgam fit, if surface == "mu", then the surface of the estimated mean value of the fit will be plotted; if surface == "eta", then the surface of the estimated systematic component value of the fit will be plotted. The default is surface = "mu"; for a warped-plane spline fit, if surface == "C", then the surface of the constrained estimated mean value of the fit will be plotted, while if surface == "U", then the surface of the unconstrained estimated mean value of the fit will be plotted. The default is surface = "C".
- categ: Optional categorical covariate(s) in a cgam fit. 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. The default is categ = NULL.
- col: The color(s) of a 3D plot created by plotpersp. If col == NULL, "white" will be used when there is only one surface in the plot, and a sequence of colors will be used in a fixed order when there are multiple parallel surfaces in the plot. For example, when there are two surfaces, the lower surface will be in the color "peachpuff", and the higher surface will be in the color "lightblue". The default is col = NULL.
- random: A logical scalar. If random == TRUE, color(s) for a 3D plot will be randomly chosen from ten colors, namely, "peachpuff", "lightblue", "limegreen", "grey", "wheat", "yellowgreen", "seagreen1", "palegreen", "azure", "whitesmoke"; otherwise, "white" will be used when there is only one surface in the plot, and a sequence of colors will be used in a fixed order when there are multiple parallel surfaces in the plot.
- ngrid: This is a positive integer specifying how dense the x grid and the y grid will be. The default is ngrid = 12. Note that this argument is only used for a cgam fit.
- xlim: The xlim argument inherited from the persp routine.
- ylim: The ylim argument inherited from the persp routine.
- zlim: The zlim argument inherited from the persp routine.
- xlab: The xlab argument inherited from the persp routine.

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- ylab: The ylab argument inherited from the persp routine.
- zlab: The zlab argument inherited from the persp routine.
- main: The main argument inherited from the persp routine.
- th: The theta argument inherited from the persp routine.
- Itheta: The Itheta argument inherited from the persp routine.
- main: The main argument inherited from the persp routine.
- ticktype: The ticktype argument inherited from the persp routine.

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.

Author(s)

Mary C. Meyer and Xiyue Liao

References

The official documentation for the generic R routine persp: http://stat.ethz.ch/R-manual/R-patched/library/graphics/html/persp.html

```
# Example 1.
 data(FEV)
 # extract the variables
 y <- FEV$FEV
 age <- FEV$age
 height <- FEV$height
 sex <- FEV$sex
 smoke <- FEV$smoke</pre>
 fit <- cgam(y ~ incr(age) + incr(height) + factor(sex) + factor(smoke), nsim = 0)</pre>
 fit.s <- cgam(y ~ s.incr(age) + s.incr(height) + factor(sex) + factor(smoke), nsim = 0)</pre>
 plotpersp(fit, age, height, ngrid = 10, main = "Cgam Increasing Fit",
 sub = "Categorical Variable: Sex", categ = "factor(sex)")
 plotpersp(fit.s, age, height, ngrid = 10, main = "Cgam Smooth Increasing Fit",
 sub = "Categorical Variable: Smoke", categ = "factor(smoke)")
# Example 2.
 data(plasma)
 # extract the variables
 y <- plasma$logplasma
 bmi <- plasma$bmi
 logdietfat <- plasma$logdietfat</pre>
 cholest <- plasma$cholest</pre>
```

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```
fiber <- plasma$fiber</pre>
  betacaro <- plasma$betacaro</pre>
  retinol <- plasma$retinol</pre>
  smoke <- plasma$smoke</pre>
  vituse <- plasma$vituse</pre>
  fit <- cgam(y ~ s.decr(bmi) + s.decr(logdietfat) + s.decr(cholest) + s.incr(fiber)</pre>
+ s.incr(betacaro) + s.incr(retinol) + factor(smoke) + factor(vituse))
  plotpersp(fit, bmi, logdietfat, 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)")
# Example 3.
  data(plasma)
  addl <- 1:314*0 + 1
  addl[runif(314) < .3] < -2
  addl[runif(314) > .8] <- 4
  addl[runif(314) > .8] <- 3
  ans <- cgam(logplasma ~ s.incr(betacaro, 5) + s.decr(bmi) + s.decr(logdietfat)</pre>
+ as.factor(addl), data = plasma)
  plotpersp(ans, betacaro, logdietfat, th = 240, random = TRUE,
categ = "as.factor(addl)", data = plasma)
# Example 4.
  n <- 100
  set.seed(123)
  x1 <- sort(runif(n))</pre>
  x2 <- sort(runif(n))</pre>
  y \leftarrow 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 \sim s.decr.incr(x1, x2), pen = .1)
# plot the constrained surface
  plotpersp(ans)
```

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"), level = 0.95,...)
```

32 predict.cgam

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. level Tolerance/confidence level.

... 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".

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

Author(s)

Mary C. Meyer and Xiyue Liao

References

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

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

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

```
# 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>
```

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```
# make a data frame
x0 < - seq(min(x), max(x), by = 0.05)
new.Data <- data.frame(x = x0)
# predict values in new.Data based on the cgam fit without a confidence interval
pfit <- predict(fit, new.Data)</pre>
# or
pfit <- predict(fit, new.Data, interval = "none")</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, pfit$fit, col = 2, pch = 20)
# predict values in new.Data based on the cgam fit with a confidence interval
pfit <- predict(fit, new.Data, interval = "confidence")</pre>
# make a plot to check the prediction
plot(x, y, main = "Predict Method for CGAM with Confidence Bands")
lines(sort(x), (fitted(fit)[order(x)]))
lines(sort(x0), (pfitslower)[order(x0)], col = 2, lty = 2)
lines(sort(x0), (pfitper)[order(x0)], col = 2, lty = 2)
points(x0, pfitfit, col = 2, pch = 20)
```

Specify a Smooth Shape-Restriction in a CGAM Formula

Description

s

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

Usage

```
s(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 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, <i>numknots</i> and <i>space</i> will be used to create knots. The default is knots = 0 .

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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 = "E".

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".

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
```

```
# 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]]</pre>
```

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```
# 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")
```

s.conc

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

Description

A symbolic routine to define that the systematic component η 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 = "E")
```

Arguments

space

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.

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 = "E".

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.

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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

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(\emptyset, \emptyset), knots = list(k1 = \emptyset, k2 = \emptyset), space = c("E", "E"))
```

s.conc.conc 37

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

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

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.

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See Also

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

Examples

```
# generate data
n <- 200
set.seed(123)
x1 <- runif(n); x2 <- runif(n)</pre>
y < -(x1 - 1)^2 - (x2 - 3)^2 + rnorm(n)
    # regress y on x1 and x2 under the shape-restriction: "doubly-concave"
    ans \leftarrow cgam(y \sim s.conc.conc(x1, x2), nsim = 0)
    # make a 3D plot of the constrained surface
    plotpersp(ans)
```

s.conv

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

Description

A symbolic routine to define that the systematic component η 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 = "E")
```

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.

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

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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".

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

```
# 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")</pre>
```

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```
points(knots, 1:length(knots)*0+min(y), pch = "X")
```

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"))
```

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, 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").

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.

s.decr 41

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.

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 η 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, space = "E")
```

42 s.decr

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 = "E".

Details

"s.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 "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.

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

s.decr.conc 43

Examples

```
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]]

# 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")</pre>
```

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 η 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 = "E")
```

Arguments

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 = "E".

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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.

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))</pre>
```

s.decr.conv 45

```
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")
```

s.decr.conv

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

Description

A symbolic routine to define that the systematic component η 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 = "E")
```

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 = "E".

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.

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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

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.

s.decr.decr 47

Usage

```
s.decr.decr(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 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

 $n^{1/6}$. 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

48 s.decr.incr

References

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

See Also

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

Examples

```
# 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)</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

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, k2 = 0).

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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
```

```
# generate data
n <- 100
set.seed(123)
x1 <- runif(n)
x2 <- runif(n)</pre>
```

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```
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)</pre>
```

s.incr

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

Description

A symbolic routine to define that the systematic component η 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, space = "E")
```

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 <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 <i>numknots</i> when

Details

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

numknots > 0. Otherwise it is of the order $n^{1/7}$. The default is space = "E".

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.

See references cited in this section for more details.

s.incr.conc 51

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

Examples

```
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]]

# 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")</pre>
```

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

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Description

A symbolic routine to define that the systematic component η 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 = "E")
```

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 = "E".

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.

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

s.incr.conv 53

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 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

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

Description

A symbolic routine to define that the systematic component η 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 = "E")
```

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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 = "E".

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

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

55 s.incr.decr

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 \sim s.incr.conv(x))
knots <- ans$knots[[1]]</pre>
# make a plot
par(mar = c(4, 4, 1, 1))
plot(x, y, cex = .7, xlab = "x", ylab = "y")
lines(x, ans$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")
```

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"))
```

Arguments

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

х2 A numeric predictor which has the same length as the response vector.

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

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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.

See Also

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

```
# generate data
n <- 100
set.seed(123)
x1 <- runif(n)
x2 <- runif(n)</pre>
```

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```
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 ~ s.incr.decr(x1, x2), pnt = TRUE)
# make a 3D plot of the constrained surface
plotpersp(ans)</pre>
```

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 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.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

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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
```

```
# 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-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)</pre>
```

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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.
- 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".

shapes

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
 \mbox{\tt\#} 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
 y <- y0 + rnorm(n, 1)
 fit <- ShapeSelect(y ~ s.incr(x) + shapes(z, set = "tree"), genetic = FALSE)</pre>
 \# check the best fit in terms of z
 fit$top
## End(Not run)
```

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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 = 1.2, data = NULL, weights = NULL,
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 η 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 η 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.

cpar

A multiplier to estimate the model variance, which is defined as $\sigma^2 = SSR/(n-d_0-cpar*edf)$. 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 = 1.2. 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.

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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.

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

top 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.

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.

ShapeSelect 63

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

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. 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"),</pre>
 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"),</pre>
 data = Rubber, genetic = TRUE)
 # check the best model
 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
 n <- 100
 x1 <- runif(n)</pre>
 x2 <- runif(n)</pre>
 y0 < -x1^2 + x2 + x2^3
 z \leftarrow rep(0:1, 50)
```

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```
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)))
 \# include z as a linear term in the formula and determine if z should be in the model
 fit <- 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)
```

tree

Specify a Tree-Ordering in a CGAM Formula

Description

A symbolic routine to define that the systematic component η 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.

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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 η 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)
```

66 umbrella

umbrella

Specify an Umbrella-Ordering in a CGAM Formula

Description

A symbolic routine to define that the systematic component η 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 η 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 67

```
# 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>
```

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