# Package 'scam'

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Title Shape Constrained Additive Models
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Description Generalized additive models under shape constraints on the component functions of the linear predictor. Models can include multiple shape-constrained (univariate and bivariate) and unconstrained terms. Routines of the package 'mgcv' are used to set up the model matrix, print, and plot the results. Multiple smoothing parameter estimation by the Generalized Cross Validation or similar. See Pya and Wood (2015) <doi:10.1007 s11222-013-9448-7=""> for an overview. A broad selection of shape-constrained smoothers, linear functionals of smooths with shape constraints, and Gaussian models with AR1 residuals.</doi:10.1007>
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### Description

scam provides functions for generalized additive modelling under shape constraints on the component functions of the linear predictor of the GAM. Models can contain multiple univariate and bivariate shape constrained terms, unconstrained terms and parametric terms. A wide variety of shape constrained smooths covered in shape.constrained.smooth.terms are provided.

The model set-up is similar to that of gam() of the package mgcv, so unconstrained smooths of one or more variables of the mgcv can be included in SCAMs. User-defined smooths can be added as well. SCAM is estimated by penalized log likelihood maximization and provides automatic smoothness selection by minimizing generalized cross validation or similar. A Bayesian approach is used to obtain a covariance matrix of the model coefficients and credible intervals for each smooth. Linear functionals of smooth functions with shape constraints, parametric model terms, simple linear random effects terms, bivariate interaction smooths with increasing/decreasing constraints (smooth ANOVA), and identity link Gaussian models with AR1 residuals are supported.

#### **Details**

scam provides generalized additive modelling under shape constraints functions scam, summary.scam, plot.scam, scam.check, predict.scam, anova.scam, and vis.scam. These are based on the functions of the unconstrained GAM of the package mgcv and are similar in use.

The use of scam() is much like the use of gam(), except that within a scam model formula, shape constrained smooths of one or two predictors can be specified using s terms with a type of shape constraints used specified as a letter character string of the argument bs, e.g. s(x, bs="mpi") for smooth subject to increasing constraint. See shape.constrained.smooth.terms for a complete overview of what is available. scam model estimation is performed by penalized likelihood maximization, with smoothness selection by GCV, UBRE/AIC criteria. See scam, linear.functional.terms for a short discussion of model specification and some examples. See scam arguments optimizer and optim.method, and scam.control for detailed control of scam model fitting. For checking and visualization, see scam.check, plot.scam, qq.scam and vis.scam. For extracting fitting results, see summary.scam and anova.scam.

A Bayesian approach to smooth modelling is used to obtain covariance matrix of the model coefficients and credible intervals for each smooth. Vp element of the fitted object of class scam returns the Bayesian covariance matrix, Ve returns the frequentist estimated covariance matrix for the parameter estimators. The frequentist estimated covariance matrix for the reparametrized parameter estimators (obtained using the delta method) is returned in Ve.t, which is particularly useful for testing individual smooth terms for equality to the zero function (not so useful for CI's as smooths are usually biased). Vp.t returns the Bayesian covariance matrix for the reparametrized parameters. Frequentist approximations can be used for hypothesis testing based on model comparison; see anova.scam and summary.scam for info on hypothesis testing.

For a complete list of functions type library(help=scam).

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#### Author(s)

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Maintainer: Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

Wood S.N. (2017) Generalized Additive Models: An Introduction with R (2nd edition). Chapman and Hall/CRC Press

Wood, S.N. (2008) Fast stable direct fitting and smoothness selection for generalized additive models. Journal of the Royal Statistical Society (B) 70(3):495-518

Wood, S.N. (2011) Fast stable restricted maximum likelihood and marginal likelihood estimation of semiparametric generalized linear models. Journal of the Royal Statistical Society (B) 73(1):3-36

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### **Examples**

## see examples for scam

anova.scam

Approximate hypothesis tests related to SCAM fits

### Description

Performs hypothesis tests relating to one or more fitted scam objects. The function is a clone of anova.gam of the mgcv package.

The documentation below is similar to that of object anova.gam.

#### Usage

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#### **Arguments**

object, ... fitted model objects of class scam as produced by scam().

x an anova.scam object produced by a single model call to anova.scam().

dispersion a value for the dispersion parameter: not normally used.

test what sort of test to perform for a multi-model call. One of "Chisq", "F" or

"Cp".

freq whether to use frequentist or Bayesian approximations for parametric term p-

values. See summary.gam for details.

p. type selects exact test statistic to use for single smooth term p-values. See summary.scam

for details.

digits number of digits to use when printing output.

#### **Details**

see anova. gam for details.

#### Value

In the multi-model case anova. scam produces output identical to anova.glm, which it in fact uses.

In the single model case an object of class anova.scam is produced, which is in fact an object returned from summary.scam.

print.anova.scam simply produces tabulated output.

#### WARNING

If models 'a' and 'b' differ only in terms with no un-penalized components then p values from anova(a,b) are unreliable, and usually much too low.

Default P-values will usually be wrong for parametric terms penalized using 'paraPen': use freq=TRUE to obtain better p-values when the penalties are full rank and represent conventional random effects.

For a single model, interpretation is similar to drop1, not anova.lm.

#### Author(s)

Simon N. Wood <simon.wood@r-project.org>

### References

Scheipl, F., Greven, S. and Kuchenhoff, H. (2008) Size and power of tests for a zero random effect variance or polynomial regression in additive and linear mixed models. Comp. Statist. Data Anal. 52, 3283-3299

Wood, S.N. (2013a) On p-values for smooth components of an extended generalized additive model. Biometrika 100:221-228

Wood, S.N. (2013b) A simple test for random effects in regression models. Biometrika 100:1005-1010

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#### See Also

```
scam, predict.scam, scam.check, summary.scam, anova.gam
```

#### **Examples**

```
library(scam)
set.seed(0)
fac <- rep(1:4,20)
x1 <- runif(80)*5
x2 <- runif(80,-1,2)
x3 <- runif(80, 0, 1)
y <- fac+log(x1)/5
y <- y + exp(-1.3*x2) +rnorm(80)*0.1
fac <- factor(fac)
b <- scam(y ~ fac+s(x1,bs="mpi")+s(x2,bs="mpd")+s(x3))
b1 <- scam(y ~ fac+s(x1,bs="mpi")+s(x2,bs="mpd"))
anova(b,b1,test="F")
## b2 <- scam(y ~ fac +s(x1)+s(x2)+te(x1,x2))</pre>
```

bfgs\_gcv.ubre

Multiple Smoothing Parameter Estimation by GCV/UBRE

#### **Description**

Function to efficiently estimate smoothing parameters of SCAM by GCV/UBRE score optimization. The procedure is outer to the model fitting by the Newton-Raphson method. The function uses the BFGS method where the Hessian matrix is updated iteratively at each step. Backtracking is included to satisfy the sufficient decrease condition.

The function is not normally called directly, but rather service routines for scam.

#### Usage

### Arguments

fn	GCV/UBRE Function which returs the GCV/UBRE value and its derivative wrt log smoothing parameter.
rho	log of the initial values of the smoothing parameters.
ini.fd	If TRUE, a finite difference to the Hessian is used to find the initial inverse Hessian, otherwise the initial inverse Hessian is a diagonal matrix '100*I'.
G	A list of items needed to fit a SCAM.

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env Get the environment for the model coefficients, their derivatives and the smooth-

ing parameter.

n.pen Smoothing parameter dimension.

typx A vector whose component is a positive scalar specifying the typical magnitude

of sp.

typf A positive scalar estimating the magnitude of the gcv near the minimum.

control Control option list as returned by scam. control.

#### Value

A list is returned with the following items:

gcv.ubre The optimal value of GCV/UBRE.

rho The best value of the log smoothing parameter.

dgcv.ubre The gradient of the GCV/UBRE.

iterations The number of iterations taken until convergence.

conv.bfgs Convergence information indicating why the BFGS terminated (given below).

termcode An integer code indicating why the optimization process terminated.

1: relative gradient is close to zero, current iterate probably is a solution.

2: scaled distance between last two steps less than 'steptol', current iterate probably is a local minimizer, but it's possible that the algorithm is making very slow progress, or 'steptol' is too large.

3: last global step failed to locate a point lower than estimate. Either estimate is

an approximate local minimum of the function or steptol is too small.

4: iteration limit exceeded.

5: five consecutive steps of length maxNstep have been taken, it's possible that

'maxstep' is too small.

object A list of elements returned by the fitting procedure scam. fit for an optimal

value of the smoothing parameter.

dgcv.ubre.check

If check.analytical=TRUE this is the finite-difference approximation of the

gradient calculated by gcv.ubre\_grad, otherwise NULL.

check.grad If check.analytical=TRUE this is the relative difference (in and finite differ-

enced derivatives calculated by gcv.ubre\_grad, otherwise NULL.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

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Wood, S.N. (2011) Fast stable restricted maximum likelihood and marginal likelihood estimation of semiparametric generalized linear models. Journal of the Royal Statistical Society: Series B. 73(1): 1–34

#### See Also

scam

check.analytical

Checking the analytical gradient of the GCV/UBRE score

### Description

This function calculates the finite-difference approximation of the GCV/UBRE gradient for the fitted model and compares it with the analytical gradient.

### Usage

```
check.analytical(object, data, del=1e-6,control)
```

### **Arguments**

object A fitted scam object.

data An original data frame or list containing the model response variable and co-

variates.

del A positive scalar (default is 1e-6) giving an increment for finite difference ap-

proximation.

control Control option list as returned by scam. control.

#### Value

A list is returned with the following items:

dgcv.ubre.fd The finite-difference approximation of the gradient.

check.grad The relative difference in percentage between the analytical and finite differ-

enced derivatives.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

### See Also

scam

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derivative.scam

Derivative of the univariate smooth model terms

### Description

Function to get derivatives of the smooth model terms (currently only of the univariate smooths). Analytical derivatives for SCOP-splines (shape constrained P-splines), finite difference approximation is used for all others

### Usage

```
derivative.scam(object,smooth.number=1,deriv=1)
```

### Arguments

object fitted scam object

smooth.number ordered number of the smooth model term (1,2,...), ordered as in the formula,

which derivative is needed to be calculated.

deriv either 1 if the 1st derivative is required, or 2 if the 2nd

#### Value

d values of the derivative of the smooth term.

se.d standard errors of the derivative.

### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

### See Also

scam

### **Examples**

```
set.seed(2) n \leftarrow 200 x1 \leftarrow runif(n)*4-1; f1 \leftarrow exp(4*x1)/(1+exp(4*x1)) # monotone increasing smooth x2 \leftarrow sort(runif(n)*3-1) # decreasing smooth f2 \leftarrow exp(-1.3*x2) f \leftarrow f1+f2 y \leftarrow f+ rnorm(n)*0.2
```

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```
## fit model, results, and plot...
b <- scam(y^ s(x1,k=20,bs="mpi")+s(x2,k=15,bs="mpd"))
d1 <- derivative.scam(b,smooth.number=1,deriv=1)</pre>
par(mfrow=c(1,2))
xx <- sort(x1,index=TRUE)</pre>
plot(xx$x,d1$d[xx$ix],type="l",xlab=expression(x[1]),
     ylab=expression(df[1]/dx[1]))
d2 <- derivative.scam(b,smooth.number=2,deriv=1)</pre>
xx <- sort(x2,index=TRUE)</pre>
plot(xx$x,d2$d[xx$ix],type="1",xlab=expression(x[2]),
     ylab=expression(df[2]/dx[2]))
```

formula.scam

SCAM formula

#### **Description**

Description of scam formula (see gam of the mgcv package for Details), and how to extract it from a fitted scam object.

The function is a clone of formula.gam of the mgcv package.

#### Usage

```
## S3 method for class 'scam'
formula(x,...)
```

### **Arguments**

. . .

fitted model objects of class scam as produced by scam(). Х un-used in this case

```
see formula.gam for details.
```

#### Value

**Details** 

Returns the model formula, x\$formula. Provided so that anova methods print an appropriate description of the model.

#### See Also

scam

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gcv.ubre_grad	The GCV/UBRE score value and its gradient
5 _5	O

#### **Description**

For the estimation of the SCAM smoothing parameters the GCV/UBRE score is optimized outer to the Newton-Raphson procedure of the model fitting. This function returns the value of the GCV/UBRE score and calculates its first derivative with respect to the log smoothing parameter using the method of Wood (2009).

The function is not normally called directly, but rather service routines for bfgs\_gcv.ubre.

### Usage

```
gcv.ubre_grad(rho, G, env, control)
```

#### Arguments

rho log of the initial values of the smoothing parameters.

G a list of items needed to fit a SCAM.

env Get the environment for the model coefficients, their derivatives and the smooth-

ing parameter.

control A list of fit control parameters as returned by scam.control.

#### Value

A list is returned with the following items:

dgcv.ubre The value of GCV/UBRE gradient.

gcv.ubre The GCV/UBRE score value.
scale.est The value of the scale estimate.

object The elements of the fitting procedure monogam. fit for a given value of the

smoothing parameter.

dgcv.ubre.check

If check.analytical=TRUE this returns the finite-difference approximation of

the gradient.

check.grad If check.analytical=TRUE this returns the relative difference (in and finite

differenced derivatives.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

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#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

Wood S.N. (2006) Generalized Additive Models: An Introduction with R. Chapman and Hall/CRC Press.

Wood, S.N. (2011) Fast stable restricted maximum likelihood and marginal likelihood estimation of semiparametric generalized linear models. Journal of the Royal Statistical Society: Series B. 73(1): 1–34

#### See Also

```
scam, scam.fit, bfgs_gcv.ubre
```

linear.functional.terms

Linear functionals of a smooth in GAMs

### **Description**

Since scam uses the model setup of gam of the mgcv package, in the same way as in gam scam allows the response variable to depend on linear functionals of smooth terms in the s with additional shape constraints.

See linear.functional.terms(mgcv).

### **Examples**

```
## Not run:
## similar to a "signal" regression
## example from mgcv() ...
library(scam)
## decreasing smooth...
set.seed(4)
rf <- function(x=seq(-1,3,length=100)) { ## taken from mgcv package</pre>
## generates random functions...
 m <- ceiling(runif(1)*5) ## number of components</pre>
 f <- x*0;
 mu \leftarrow runif(m, min(x), max(x)); sig \leftarrow (runif(m) + .5) * (max(x) - min(x)) / 10
 for (i in 1:m) f \leftarrow f + dnorm(x,mu[i],sig[i])
}
## simulate 200 functions and store in rows of L...
L <- matrix(NA,200,100)</pre>
```

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```
for (i in 1:200) L[i,] <- rf() ## simulate the functional predictors
x \leftarrow seq(-1,3,length=100) ## evaluation points
f2 <- function(x) { ## the coefficient function
      -4*exp(4*x)/(1+exp(4*x))
f \leftarrow f2(x)
plot(x,f ,type="l")
y <- L%%f + rnorm(200)*20 ## simulated response data
X <- matrix(x,200,100,byrow=TRUE)</pre>
b \leftarrow scam(y \sim s(X, by=L, k=20, bs="mpdBy"))
par(mfrow=c(1,2))
plot(b, shade=TRUE); lines(x, f, col=2);
## compare with gam() of mgcv package...
g \leftarrow gam(y\sim s(X,by=L,k=20))
plot(g, shade=TRUE); lines(x, f, col=2)
## increasing smooth....
L <- matrix(NA,200,100)
for (i in 1:200) L[i,] \leftarrow rf() ## simulate the functional predictors
x \leftarrow seq(-1,3,length=100) ## evaluation points
f2 \leftarrow function(x) \{ \# \# \text{ the coefficient function } \}
      4*exp(4*x)/(1+exp(4*x))
f \leftarrow f2(x)
plot(x,f,type="l")
y <- L%*%f + rnorm(200)*20 ## simulated response data
X <- matrix(x,200,100,byrow=TRUE)</pre>
b \leftarrow scam(y\sim s(X,by=L,k=20,bs="mpiBy"))
par(mfrow=c(1,2))
plot(b, shade=TRUE); lines(x, f, col=2);
## compare with unconstrained fit...
g \leftarrow scam(y\sim s(X,by=L,k=20))
plot(g, shade=TRUE); lines(x, f, col=2)
## convex smooth...
 ## simulate 200 functions and store in rows of L...
set.seed(4)
L <- matrix(NA, 200, 100)
for (i in 1:200) L[i,] <- rf(x=sort(2*runif(100)-1)) ## simulate the functional predictors
x \leftarrow sort(runif(100,-1,1)) ## evaluation points
f2 \leftarrow function(x)\{4*x^2\} ## the coefficient function
f \leftarrow f2(x)
plot(x,f ,type="l")
y <- L%*%f + rnorm(200)*30 ## simulated response data
X <- matrix(x,200,100,byrow=TRUE)</pre>
b \leftarrow scam(y\sim s(X,by=L,k=20,bs="cxBy"))
par(mfrow=c(1,2))
```

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```
plot(b, shade=TRUE); lines(x,f,col=2);
g <- scam(y~s(X,by=L,k=20))
plot(g, shade=TRUE); lines(x,f,col=2)
## End(Not run)</pre>
```

logLik.scam

Log likelihood for a fitted SCAM, for AIC

### Description

Function to extract the log-likelihood for a fitted scam model (fitted by penalized likelihood maximization). Used by AIC.

The function is a clone of logLik.gam of the mgcv package.

The documentation below is similar to that of object logLik.gam.

### Usage

```
## S3 method for class 'scam'
logLik(object,...)
```

### Arguments

object fitted model objects of class scam as produced by scam(). ... unused in this case

#### **Details**

```
see logLik.gam for details.
```

#### Value

Standard logLik object: see logLik.

#### References

Hastie and Tibshirani, 1990, Generalized Additive Models.

Wood, S.N. (2008) Fast stable direct fitting and smoothness selection for generalized additive models. J.R.Statist. Soc. B 70(3):495-518

#### See Also

AIC

marginal.matrices.tescv.ps

Constructs marginal model matrices for "tescv" and "tescx" bivariate smooths in case of B-splines basis functions for both unconstrained marginal smooths

### **Description**

This function returns the marginal model matrices and the list of penalty matrices for the tensor product bivariate smooth with the single concavity or convexity restriction along the second covariate. The marginal smooth functions of both covariates are constructed using the B-spline basis functions.

### Usage

```
marginal.matrices.tescv.ps(x, z, xk, zk, m, q1, q2)
```

#### **Arguments**

X	A numeric vector of the values of the first covariate at which to evaluate the B-spline marginal functions. The values in x must be between $xk[m[1]+2]$ and $xk[length(xk) - m[1] - 1]$ .
Z	A numeric vector of the values of the second covariate at which to evaluate the B-spline marginal functions. The values in z must be between $zk[m[2]+2]$ and $zk[length(zk) - m[2] - 1]$ .
xk	A numeric vector of knot positions for the first covariate, x, with non-decreasing values.
zk	A numeric vector of knot positions for the second covariate, z, with non-decreasing values.
m	A pair of two numbers where $m[i]+1$ denotes the order of the basis of the $i^{th}$ marginal smooth (e.g. $m[i] = 2$ for a cubic spline.)
q1	A number denoting the basis dimension of the first marginal smooth.
q2	A number denoting the basis dimension of the second marginal smooth.

## Details

The function is not called directly, but is rather used internally by the constructor smooth.construct.tescv.smooth.spec and smooth.construct.tescx.smooth.spec.

#### Value

X1	Marginal model matrix for the first unconstrained marginal smooth.
X2	Marginal model matrix for the second monotonic marginal smooth.
S	A list of penalty matrices for this tensor product smooth.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

#### See Also

```
smooth.construct.tescv.smooth.spec, smooth.construct.tescx.smooth.spec,
marginal.matrices.tesmi1.ps, smooth.construct.tesmd1.smooth.spec,
smooth.construct.tesmd2.smooth.spec
```

```
marginal.matrices.tesmi1.ps
```

Constructs marginal model matrices for "tesmi1" and "tesmd1" bivariate smooths in case of B-splines basis functions for both unconstrained marginal smooths

### Description

This function returns the marginal model matrices and the list of penalty matrices for the tensor product bivariate smooth with the single monotone increasing or decreasing restriction along the first covariate. The marginal smooth functions of both covariates are constructed using the B-spline basis functions.

### Usage

```
marginal.matrices.tesmi1.ps(x, z, xk, zk, m, q1, q2)
```

### Arguments

X	A numeric vector of the values of the first covariate at which to evaluate the B-spline marginal functions. The values in x must be between $xk[m[1]+2]$ and $xk[length(xk) - m[1] - 1]$ .
Z	A numeric vector of the values of the second covariate at which to evaluate the B-spline marginal functions. The values in z must be between $zk[m[2]+2]$ and $zk[length(zk) - m[2] - 1]$ .
xk	A numeric vector of knot positions for the first covariate, x, with non-decreasing values.
zk	A numeric vector of knot positions for the second covariate, z, with non-decreasing values.
m	A pair of two numbers where $m[i]+1$ denotes the order of the basis of the $i^{th}$ marginal smooth (e.g. $m[i] = 2$ for a cubic spline.)
q1	A number denoting the basis dimension of the first marginal smooth.
q2	A number denoting the basis dimension of the second marginal smooth.

#### **Details**

The function is not called directly, but is rather used internally by the constructor smooth.construct.tesmi1.smooth.spec and smooth.construct.tesmd1.smooth.spec.

#### Value

X1	Marginal model matrix for the first monotonic marginal smooth.
X2	Marginal model matrix for the second unconstrained marginal smooth.
S	A list of penalty matrices for this tensor product smooth.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

Wood S.N. (2006) Generalized Additive Models: An Introduction with R. Chapman and Hall/CRC Press.

### See Also

```
smooth.construct.tesmi1.smooth.spec, smooth.construct.tesmi2.smooth.spec,
marginal.matrices.tesmi2.ps, smooth.construct.tesmd1.smooth.spec,
smooth.construct.tesmd2.smooth.spec
```

```
marginal.matrices.tesmi2.ps
```

Constructs marginal model matrices for "tesmi2" and "tesmd2" bivariate smooths in case of B-splines basis functions for both unconstrained marginal smooths

### Description

This function returns the marginal model matrices and the list of penalty matrices for the tensor product bivariate smooth with the single monotone increasing or decreasing restriction along the second covariate. The marginal smooth functions of both covariates are constructed using the B-spline basis functions.

#### Usage

```
marginal.matrices.tesmi2.ps(x, z, xk, zk, m, q1, q2)
```

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X	A numeric vector of the values of the first covariate at which to evaluate the B-spline marginal functions. The values in x must be between xk[m[1]+2] and xk[length(xk) - m[1] - 1].
Z	A numeric vector of the values of the second covariate at which to evaluate the B-spline marginal functions. The values in z must be between $zk[m[2]+2]$ and $zk[length(zk) - m[2] - 1]$ .
xk	A numeric vector of knot positions for the first covariate, x, with non-decreasing values.
zk	A numeric vector of knot positions for the second covariate, z, with non-decreasing values.
m	A pair of two numbers where m[i]+1 denotes the order of the basis of the $i^{th}$ marginal smooth (e.g. m[i] = 2 for a cubic spline.)
q1	A number denoting the basis dimension of the first marginal smooth.
q2	A number denoting the basis dimension of the second marginal smooth.

#### **Details**

The function is not called directly, but is rather used internally by the constructor smooth.construct.tesmi2.smooth.spec and smooth.construct.tesmd2.smooth.spec.

#### Value

X1	Marginal model matrix for the first unconstrained marginal smooth.
X2	Marginal model matrix for the second monotonic marginal smooth.
S	A list of penalty matrices for this tensor product smooth.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

Wood S.N. (2006) Generalized Additive Models: An Introduction with R. Chapman and Hall/CRC Press.

### See Also

```
smooth.construct.tesmi1.smooth.spec, smooth.construct.tesmi2.smooth.spec,
marginal.matrices.tesmi1.ps, smooth.construct.tesmd1.smooth.spec,
smooth.construct.tesmd2.smooth.spec
```

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plot.scam SCAM plotting

### **Description**

The function is a clone of the plot gam of the mgcv package with the differences in the construction of the Bayesian confidence intervals of the shape constrained smooth terms. The function takes a fitted scam object produced by scam() and plots the component smooth functions that make it up, on the scale of the linear predictor. Optionally produces term plots for parametric model components as well.

Note: The fitted shape constrained smooth functions are centred when plotted, which is done in order to be in line with plots of unconstrained smooths (as in gam()). Although 'zeroed intercept' constraints are applied to deal with identifiability of the scop-splines.

### Usage

```
## S3 method for class 'scam'
plot(x,residuals=FALSE,rug=TRUE,se=TRUE,pages=0,select=NULL,scale=-1,
         n=100, n2=40, pers=FALSE, theta=30, phi=30, jit=FALSE, xlab=NULL,
         ylab=NULL, main=NULL, ylim=NULL, xlim=NULL, too.far=0.1,
         all.terms=FALSE, shade=FALSE, shade.col="gray80",
         shift=0,trans=I,seWithMean=FALSE,unconditional = FALSE,
         by.resids = FALSE,scheme=0,...)
```

#### **Arguments**

The list of the arguments is the same as in plot. gam of the mgcv package.

a fitted gam object as produced by gam().

residuals

If TRUE then partial residuals are added to plots of 1-D smooths. If FALSE then no residuals are added. If this is an array of the correct length then it is used as the array of residuals to be used for producing partial residuals. If TRUE then the residuals are the working residuals from the IRLS iteration weighted by the IRLS weights. Partial residuals for a smooth term are the residuals that would be obtained by dropping the term concerned from the model, while leaving all

other estimates fixed (i.e. the estimates for the term plus the residuals).

when TRUE (default) then the covariate to which the plot applies is displayed as a rug plot at the foot of each plot of a 1-d smooth, and the locations of the covariates are plotted as points on the contour plot representing a 2-d smooth.

when TRUE (default) upper and lower lines are added to the 1-d plots at 2 standard errors above and below the estimate of the smooth being plotted while for 2-d plots, surfaces at +1 and -1 standard errors are contoured and overlayed on the contour plot for the estimate. If a positive number is supplied then this number is multiplied by the standard errors when calculating standard error curves or surfaces. See also shade, below.

rug

se

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(default 0) the number of pages over which to spread the output. For example, pages if pages=1 then all terms will be plotted on one page with the layout performed automatically. Set to 0 to have the routine leave all graphics settings as they are. select Allows the plot for a single model term to be selected for printing. e.g. if you just want the plot for the second smooth term set select=2. scale set to -1 (default) to have the same y-axis scale for each plot, and to 0 for a different y axis for each plot. Ignored if ylim supplied. number of points used for each 1-d plot - for a nice smooth plot this needs to n be several times the estimated degrees of freedom for the smooth. Default value n2 Square root of number of points used to grid estimates of 2-d functions for contouring. Set to TRUE if you want perspective plots for 2-d terms. pers One of the perspective plot angles. theta phi The other perspective plot angle. jit Set to TRUE if you want rug plots for 1-d terms to be jittered. xlab If supplied then this will be used as the x label for all plots. If supplied then this will be used as the y label for all plots. ylab main Used as title (or z axis label) for plots if supplied. vlim If supplied then this pair of numbers are used as the y limits for each plot. xlim If supplied then this pair of numbers are used as the x limits for each plot. too.far If greater than 0 then this is used to determine when a location is too far from data to be plotted when plotting 2-D smooths. This is useful since smooths tend to go wild away from data. The data are scaled into the unit square before deciding what to exclude, and too. far is a distance within the unit square. all.terms if set to TRUE then the partial effects of parametric model components are also plotted, via a call to termplot. Only terms of order 1 can be plotted in this way. shade Set to TRUE to produce shaded regions as confidence bands for smooths (not avaliable for parametric terms, which are plotted using termplot). shade.col define the color used for shading confidence bands. shift constant to add to each smooth (on the scale of the linear predictor) before plotting. Can be useful for some diagnostics, or with trans. function to apply to each smooth (after any shift), before plotting. shift and trans trans are occasionally useful as a means for getting plots on the response scale, when the model consists only of a single smooth. if TRUE the component smooths are shown with confidence intervals that include seWithMean the uncertainty about the overall mean. If FALSE then the uncertainty relates purely to the centred smooth itself. An extension of the argument presented in Nychka (1988) suggests that TRUE results in better coverage performance, and this is also suggested by simulation. unconditional if TRUE then the smoothing parameter uncertainty corrected covariance matrix is used to compute uncertainty bands, if available. Otherwise the bands treat the

smoothing parameters as fixed.

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by resids Should partial residuals be plotted for terms with by variables? Usually the

answer is no, they would be meaningless.

scheme Integer (0,1 or 2) or integer vector selecting a plotting scheme for each plot.

scheme == 0 produces a smooth curve with dashed curves indicating 2 standard error bounds. scheme == 1 illustrates the error bounds using a shaded region. For scheme==0, contour plots are produced for 2-d smooths with the x-axes labelled with the first covariate name and the y axis with the second covariate name. For 2-d smooths scheme==1 produces a perspective plot, while

scheme==2 produces a heatmap, with overlaid contours.

... other graphics parameters to pass on to plotting commands.

#### Value

The function generates plots.

### Author(s)

Natalya Pya <nat.pya@gmail.com> based on the plot.gam of the mgcv by Simon Wood

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

Wood S.N. (2006) Generalized Additive Models: An Introduction with R. Chapman and Hall/CRC Press.

#### See Also

scam

#### **Examples**

```
## simulating data...
require(scam)
n <- 200
set.seed(1)
x0 <- rep(1:4,50)
x1 <- runif(n)*6-3
f1 <- 3*exp(-x1^2) # unconstrained smooth term
x2 <- runif(n)*4-1;
f2 <- exp(4*x2)/(1+exp(4*x2)) # monotone increasing smooth
x3 <- runif(n)*5;
f3 <- -log(x3)/5 # monotone decreasing smooth
f <- f1+f2+f3
y <- 2*x0 + f + rnorm(n)*.3
x0 <- factor(x0)
## fit the model and plot ...</pre>
```

```
b < scam(y^x0+s(x1,k=15,bs="cr")+s(x2,k=30,bs="mpi")+s(x3,k=30,bs="mpd"))
plot(b,pages=1,residuals=TRUE,all.terms=TRUE,shade=TRUE,shade.col=3)
## same with EFS and BFGS methods for smoothing parameter and models coefficients estimations...
b < -scam(y^x0+s(x1,k=15,bs="cr")+s(x2,k=30,bs="mpi")+s(x3,k=30,bs="mpd"),optimizer=c("efs","bfgs"))
plot(b,pages=1,residuals=TRUE,all.terms=TRUE,shade=TRUE,shade.col=3)
## Not run:
 ## example with 2-d plots...
 ## simulating data...
   set.seed(2)
   n <- 30
   x0 < -rep(1:9,100)
   x1 <- sort(runif(n)*4-1)</pre>
   x2 <- sort(runif(n))</pre>
   x3 <- runif(n*n, 0, 1)
   f \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
       \{f[i,j] \leftarrow -\exp(4*x1[i])/(1+\exp(4*x1[i]))+2*\sin(pi*x2[j])\}
   f1 <- as.vector(t(f))</pre>
   f2 <- x3*0
   e <- rnorm(length(f1))*.1
   y < -2*x0 + f1 + f2 + e
   x0 <- factor(x0)</pre>
   x11 <- matrix(0,n,n)</pre>
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x0=x0, x1=x11, x2=x22, x3=x3, y=y)
## fit model and plot ...
  b <- \; scam(y^{x}0 + s(x1, x2, k = c(10, 10), b = c("tesmd1", "ps"), m = 2) + s(x3), \\ data = dat, optimizer = "efs")
   op <- par(mfrow=c(2,2))</pre>
   plot(b,all.terms=TRUE)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data",pch=19,cex=.3)
   par(op)
## and use of schemes...
   op <- par(mfrow=c(2,2))
   plot(b,all.terms=TRUE,scheme=1)
   par(op)
   op <- par(mfrow=c(2,2))</pre>
   plot(b,all.terms=TRUE,scheme=c(2,1))
   par(op)
## End(Not run)
```

Predict.matrix.mpi.smooth

Predict matrix method functions for SCAMs

### **Description**

The various built in smooth classes for use with scam have associate Predict.matrix method functions to enable prediction from the fitted model.

#### Usage

```
## S3 method for class 'mpi.smooth'
Predict.matrix(object, data)
## S3 method for class 'lmpi.smooth'
Predict.matrix(object, data)
## S3 method for class 'miso.smooth'
Predict.matrix(object, data)
## S3 method for class 'mifo.smooth'
Predict.matrix(object, data)
## S3 method for class 'mpd.smooth'
Predict.matrix(object, data)
## S3 method for class 'cv.smooth'
Predict.matrix(object, data)
## S3 method for class 'cx.smooth'
Predict.matrix(object, data)
## S3 method for class 'micx.smooth'
Predict.matrix(object, data)
## S3 method for class 'micv.smooth'
Predict.matrix(object, data)
## S3 method for class 'mdcx.smooth'
Predict.matrix(object, data)
## S3 method for class 'mdcv.smooth'
Predict.matrix(object, data)
## S3 method for class 'po.smooth'
Predict.matrix(object, data)
## S3 method for class 'mpdBy.smooth'
Predict.matrix(object, data)
## S3 method for class 'mpiBy.smooth'
Predict.matrix(object, data)
## S3 method for class 'cxBy.smooth'
Predict.matrix(object, data)
## S3 method for class 'cvBy.smooth'
Predict.matrix(object, data)
## S3 method for class 'mdcxBy.smooth'
Predict.matrix(object, data)
## S3 method for class 'mdcvBy.smooth'
Predict.matrix(object, data)
## S3 method for class 'micxBy.smooth'
Predict.matrix(object, data)
## S3 method for class 'micvBy.smooth'
Predict.matrix(object, data)
## S3 method for class 'tedmd.smooth'
Predict.matrix(object, data)
```

```
## S3 method for class 'tedmi.smooth'
Predict.matrix(object, data)
## S3 method for class 'tesmd1.smooth'
Predict.matrix(object, data)
## S3 method for class 'tesmd2.smooth'
Predict.matrix(object, data)
## S3 method for class 'tesmi1.smooth'
Predict.matrix(object, data)
## S3 method for class 'tesmi2.smooth'
Predict.matrix(object, data)
## S3 method for class 'temicx.smooth'
Predict.matrix(object, data)
## S3 method for class 'temicv.smooth'
Predict.matrix(object, data)
## S3 method for class 'tedecx.smooth'
Predict.matrix(object, data)
## S3 method for class 'tedecv.smooth'
Predict.matrix(object, data)
## S3 method for class 'tescx.smooth'
Predict.matrix(object, data)
## S3 method for class 'tescv.smooth'
Predict.matrix(object, data)
## S3 method for class 'tecvcv.smooth'
Predict.matrix(object, data)
## S3 method for class 'tecxcv.smooth'
Predict.matrix(object, data)
## S3 method for class 'tecxcx.smooth'
Predict.matrix(object, data)
## S3 method for class 'tismi.smooth'
Predict.matrix(object, data)
## S3 method for class 'tismd.smooth'
Predict.matrix(object, data)
```

### **Arguments**

object A smooth object, usually generated by a smooth.construct method having

processed a smooth specification object generated by an s term in a scam for-

mula.

data A data frame containing the values of the named covariates at which the smooth

term is to be evaluated.

#### Value

A matrix mapping the coefficients for the smooth term to its values at the supplied data values.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

Wood S.N. (2006) Generalized Additive Models: An Introduction with R. Chapman and Hall/CRC Press.

predict.scam

Prediction from fitted SCAM model

#### **Description**

This function is a clone of the mgcv library code predict.gam with some modifications to adopt shape preserving smooth terms. It takes a fitted scam object produced by scam() and produces predictions given a new set of values for the model covariates or the original values used for the model fit. Predictions can be accompanied by standard errors, based on the posterior distribution of the model coefficients.

It now alows prediction outside the range of knots, and use linear extrapolation in this case.

### Usage

```
## S3 method for class 'scam'
predict(object, newdata, type="link", se.fit=FALSE, terms=NULL, exclude=NULL,
    block.size=NULL, newdata.guaranteed=FALSE, na.action=na.pass,...)
```

#### **Arguments**

object

a fitted scam object as produced by scam().

newdata

A data frame or list containing the values of the model covariates at which predictions are required. If this is not provided then predictions corresponding to the original data are returned. If newdata is provided then it should contain all the variables needed for prediction: a warning is generated if not.

type

When this has the value "link" (default) the linear predictor (possibly with associated standard errors) is returned. When type="terms" each component of the linear predictor is returned seperately (possibly with standard errors): this includes parametric model components, followed by each smooth component, but excludes any offset and any intercept. type="iterms" is the same, except that any standard errors returned for unconstrained smooth components will include the uncertainty about the intercept/overall mean. When type="response" predictions on the scale of the response are returned (possibly with approximate standard errors). When type="lpmatrix" then a matrix is returned which yields the values of the linear predictor (minus any offset) when postmultiplied by the parameter vector (in this case se.fit is ignored). The latter option is

most useful for getting variance estimates for quantities derived from the model: for example integrated quantities, or derivatives of smooths. A linear predictor matrix can also be used to implement approximate prediction outside R (see example code, below).

se.fit when this is TRUE (not default) standard error estimates are returned for each

prediction.

terms if type=="terms" then only results for the terms given in this array will be

returned.

exclude if type=="terms" or type="iterms" then terms (smooth or parametric) named

in this array will not be returned. Otherwise any smooth terms named in this

array will be set to zero. If NULL then no terms are excluded.

block.size maximum number of predictions to process per call to underlying code: larger is

quicker, but more memory intensive. Set to < 1 to use total number of predictions

as this.

newdata.guaranteed

Set to TRUE to turn off all checking of newdata except for sanity of factor levels: this can speed things up for large prediction tasks, but newdata must be

complete, with no NA values for predictors required in the model.

na.action what to do about NA values in newdata. With the default na.pass, any row

of newdata containing NA values for required predictors, gives rise to NA predictions (even if the term concerned has no NA predictors). na.exclude or na.omit result in the dropping of newdata rows, if they contain any NA values for required predictors. If newdata is missing then NA handling is determined from

object\$na.action.

... other arguments.

#### **Details**

See predict.gam for details.

### Value

If type=="1pmatrix" then a matrix is returned which will give a vector of linear predictor values (minus any offest) at the supplied covariate values, when applied to the model coefficient vector. Otherwise, if se.fit is TRUE then a 2 item list is returned with items (both arrays) fit and se.fit containing predictions and associated standard error estimates, otherwise an array of predictions is returned. The dimensions of the returned arrays depends on whether type is "terms" or not: if it is then the array is 2 dimensional with each term in the linear predictor separate, otherwise the array is 1 dimensional and contains the linear predictor/predicted values (or corresponding s.e.s). The linear predictor returned termwise will not include the offset or the intercept.

newdata can be a data frame, list or model.frame: if it's a model frame then all variables must be supplied.

#### Author(s)

Natalya Pya <nat.pya@gmail.com> based partly on mgcv by Simon Wood

#### References

Chambers and Hastie (1993) Statistical Models in S. Chapman & Hall.

Wood S.N. (2006) Generalized Additive Models: An Introduction with R. Chapman and Hall/CRC Press.

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
scam, plot.scam
```

### **Examples**

```
## Not run:
library(scam)
set.seed(2)
n <- 200
x1 <- runif(n)*6-3
f1 <- 3*exp(-x1^2) # unconstrained term
x2 <- runif(n)*4-1;
f2 \leftarrow \exp(4*x2)/(1+\exp(4*x2)) # monotone increasing smooth
f <- f1+f2
y \leftarrow f+rnorm(n)*0.2
dat <- data.frame(x1=x1,x2=x2,y=y)</pre>
b < -scam(y \sim s(x1, k=15, bs="cr") + s(x2, k=30, bs="mpi"), data=dat)
newd <- data.frame(x1=seq(-3,3,length.out=20),x2=seq(-1,3,length.out=20))
pred <- predict(b,newd)</pre>
pred
predict(b,newd,type="terms",se=TRUE)
## prediction on the original data...
pr <- predict(b,type="terms")</pre>
x<-sort(x1,index=TRUE)
old.par <- par(mfrow=c(2,2))
plot(x$x,(pr[,1])[x$ix],type="l",col=3,xlab="x1")
z<-sort(x2,index=TRUE)</pre>
plot(z$x,(pr[,2])[z$ix],type="l",col=3,xlab="x2")
plot(b, select=1, scale=0, se=FALSE)
plot(b, select=2, scale=0, se=FALSE)
par(old.par)
## linear extrapolation with predict.scam()...
set.seed(3)
n <- 100
x <- sort(runif(n)*3-1)</pre>
f <- exp(-1.3*x)
y <- rpois(n,exp(f))</pre>
```

```
dat <- data.frame(x=x,y=y)</pre>
b \leftarrow scam(y \sim s(x,k=15,b="mpd"),family=poisson(link="log"),data=dat)
newd <- data.frame(x=c(2.3,2.7,3.2))
fe <- predict(b,newd,type="link",se=TRUE)</pre>
ylim<- c(min(y,exp(fe$fit)),max(y,exp(fe$fit)))</pre>
plot(c(x,newd[[1]]),c(y,NA,NA),ylim=ylim,ylab="y",xlab="x")
lines(c(x,newd[[1]]),c(b$fitted,exp(fe$fit)),col=3)
## prediction on the original data...
pr <- predict(b)</pre>
plot(x,y)
lines(x,exp(pr),col=3)
## Gaussian model ....
## simulating data...
 set.seed(2)
 n <- 200
 x <- sort(runif(n)*4-1)</pre>
 f <- \exp(4*x)/(1+\exp(4*x)) # monotone increasing smooth
 y \leftarrow f+rnorm(n)*0.1
 dat <- data.frame(x=x,y=y)</pre>
 b \leftarrow scam(y \sim s(x,k=25,bs="mpi"),data=dat)
 newd <- data.frame(x=c(3.2,3.3,3.6))
 fe <- predict(b,newd)</pre>
 plot(c(x,newd[[1]]),c(y,NA,NA,NA),ylab="y",xlab="x")
 lines(c(x,newd[[1]]),c(b$fitted,fe),col=3)
### passing observed data + new data...
 newd <- data.frame(x=c(x,3.2,3.3,3.6))
 fe <- predict(b,newd,se=TRUE)</pre>
 plot(newd[[1]],c(y,NA,NA),ylab="y",xlab="x")
 lines(newd[[1]],fe$fit,col=2)
 lines(newd[[1]],fe$fit+2*fe$se.fit,col=3)
 lines(newd[[1]],fe$fit-2*fe$se.fit,col=4)
## prediction with CI...
 newd <- data.frame(x=seq(-1.2,3.5,length.out=100))</pre>
 fe <- predict(b,newd,se=TRUE)</pre>
 ylim<- c(min(y,fe$se.fit),max(y,fe$se.fit))</pre>
 plot(newd[[1]],fe$fit,type="1",ylim=ylim,ylab="y",xlab="x")
 lines(newd[[1]],fe$fit+2*fe$se.fit,lty=2)
 lines(newd[[1]],fe$fit-2*fe$se.fit,lty=2)
## prediction on the original data...
pr <- predict(b)</pre>
plot(x,y)
lines(x,pr,col=3)
## bivariate example...
   set.seed(2)
   n <- 30
   x1 <- sort(runif(n)); x2 <- sort(runif(n)*4-1)</pre>
```

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```
f \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
         f[i,j] \leftarrow 2*sin(pi*x1[i]) +exp(4*x2[j])/(1+exp(4*x2[j]))
   f <- as.vector(t(f));</pre>
   y <- f+rnorm(length(f))*0.1
   x11 \leftarrow matrix(0,n,n); x11[,1:n] \leftarrow x1; x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
   b \leftarrow scam(y\sim s(x1,x2,k=c(10,10),b="tesmi2"),data=dat,optimizer="efs")
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b,se=TRUE); plot(b,pers=TRUE,theta = 80, phi = 40)
   n.out <- 20
   xp <- seq(0,1.4,length.out=n.out)</pre>
   zp <- seq(-1,3.4,length.out=n.out)</pre>
   xp1 \leftarrow matrix(0, n.out, n.out);  xp1[,1:n.out] \leftarrow xp
   xp1 \leftarrow as.vector(t(xp1)); xp2 \leftarrow rep(zp,n.out)
   newd <- data.frame(x1=xp1,x2=xp2)</pre>
   fe <- predict(b,newd)</pre>
   fc <- t(matrix(fe,n.out,n.out))</pre>
   persp(xp,zp,fc,expand= 0.85,ticktype = "simple",xlab="x1",
     ylab="x2",zlab="f^",main="", theta = 80, phi = 40)
## obtaining a 'prediction matrix'...
newd <- data.frame(x1=c(-2,-1),x2=c(0,1))
Xp <- predict(b,newdata=newd,type="lpmatrix")</pre>
fv <- Xp%*% b$beta.t
## End(Not run)
```

print.scam

Print a SCAM object

#### **Description**

The default print method for a scam object. The code is a clone of print.gam of the mgcv package with a slight simplification since only two methods of smoothing parameter selection (by GCV or UBRE) was implemented for scam.

#### Usage

```
## S3 method for class 'scam' print(x,...)
```

### **Arguments**

x fitted model objects of class scam as produced by scam().

... other arguments.

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#### **Details**

As for mgcv(gam) prints out the family, model formula, effective degrees of freedom for each smooth term, and optimized value of the smoothness selection criterion used.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Wood S.N. (2006) Generalized Additive Models: An Introduction with R. Chapman and Hall/CRC Press.

#### See Also

```
scam, summary.scam
```

qq.scam

QQ plots for scam model residuals

### **Description**

Takes a fitted scam object produced by scam() and produces QQ plots of its residuals (conditional on the fitted model coefficients and scale parameter). This is an adapted short version of qq.gam() of mgcv package of Simon N Wood.

### Usage

#### **Arguments**

object	a fitted scam object as produced by scam() (or a glm object).
rep	How many replicate datasets to generate to simulate quantiles of the residual distribution. 0 results in an efficient simulation free method for direct calculation, if this is possible for the object family.
level	If simulation is used for the quantiles, then reference intervals can be provided for the QQ-plot, this specifies the level. 0 or less for no intervals, 1 or more to simply plot the QQ plot for each replicate generated.
s.rep	how many times to randomize uniform quantiles to data under direct computation.
type	what sort of residuals should be plotted? See residuals.scam.
pch	plot character to use. 19 is good.

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r1.col color for the reference line on the plot.
rep.col color for reference bands or replicate reference plots.
... extra graphics parameters to pass to plotting functions.

#### **Details**

QQ-plots of the the model residuals can be produced in one of two ways. The cheapest method generates reference quantiles by associating a quantile of the uniform distribution with each datum, and feeding these uniform quantiles into the quantile function associated with each datum. The resulting quantiles are then used in place of each datum to generate approximate quantiles of residuals. The residual quantiles are averaged over s.rep randomizations of the uniform quantiles to data.

The second method is to use direct simulatation. For each replicate, data are simulated from the fitted model, and the corresponding residuals computed. This is repeated rep times. Quantiles are readily obtained from the empirical distribution of residuals so obtained. From this method reference bands are also computable.

Even if rep is set to zero, the routine will attempt to simulate quantiles if no quantile function is available for the family. If no random deviate generating function family is available (e.g. for the quasi families), then a normal QQ-plot is produced. The routine conditions on the fitted model coefficients and the scale parameter estimate.

The plots are very similar to those proposed in Ben and Yohai (2004), but are substantially cheaper to produce (the interpretation of residuals for binary data in Ben and Yohai is not recommended).

#### Author(s)

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Natalya Pya <nat.pya@gmail.com> adapted for usage with scam

#### References

N.H. Augustin, E-A Sauleaub, S.N. Wood (2012) On quantile quantile plots for generalized linear models Computational Statistics & Data Analysis. 56(8), 2404-2409.

M.G. Ben and V.J. Yohai (2004) JCGS 13(1), 36-47.

#### See Also

scam

residuals.scam SCAM residuals

#### **Description**

This function is a clone of the mgcv library code residuals.gam. It returns residuals for a fitted scam model object. Pearson, deviance, working and response residuals are available.

### Usage

#### **Arguments**

object a scam fitted model object. type the type of residuals wanted.

... other arguments.

#### **Details**

See residuals. gam for details.

#### Value

An array of residuals.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

### See Also

scam

scam	Shape constrained additive models (SCAM) and integrated smooth-
	ness selection

### Description

This function fits a SCAM to data. Various shape constrained smooths (SCOP-splines), including univariate smooths subject to monotonicity, convexity, or monotonicity plus convexity, bivariate smooths with double or single monotonicity are available as model terms. See <a href="mailto:shape.constrained.smooth.terms">shape.constrained.smooth.terms</a> for a complete overview of what is available. Smoothness selection is estimated as part of the fitting. Confidence/credible intervals are available for each smooth term.

The shaped constrained smooths have been added to the gam() in package mgcv setup using the smooth.construct function. The routine calls a gam() function for the model set up, but there are separate functions for the model fitting, scam.fit, and smoothing parameter selection, bfgs\_gcv.ubre. Any smooth available in the mgcv can be taken as a model term for SCAM. User-defined smooths can be included as well.

#### Usage

```
scam(formula, family = gaussian(), data = list(), gamma = 1,
     sp = NULL, weights = NULL, offset = NULL, optimizer=c("bfgs", "newton"),
     optim.method=c("Nelder-Mead","fd"),scale = 0, knots=NULL,
     not.exp=FALSE, start= NULL, etastart=NULL, mustart= NULL,
     control=list(),AR1.rho=0, AR.start=NULL,drop.unused.levels=TRUE)
```

#### **Arguments**

formula A SCAM formula. This is exactly like the formula for a GAM (see formula, gam

of the mgcv library) except that shape constrained smooth terms, can be added in the expression of the form, e.g., s(x1,k=12,bs="mpi",by=z), where bs indicates the basis to use for the constrained smooth (increasing in this case): the built in options for the shape constrained smooths are described in

shape.constrained.smooth.terms,

family A family object specifying the distribution and link to use in fitting etc. See glm

and family for more details.

A data frame or list containing the model response variable and covariates re-

quired by the formula. By default the variables are taken from environment (formula):

typically the environment from which gam is called.

A constant multiplier to inflate the model degrees of freedom in the GCV or gamma

UBRE/AIC score.

A vector of smoothing parameters can be provided here. Smoothing paramesp

> ters must be supplied in the order that the smooth terms appear in the model formula. The default sp=NULL indicates that smoothing parameters should be estimated. If length(sp) does not correspond to the number of underlying smoothing parameters or negative values supplied then the vector is ignored and

all the smoothing parameters will be estimated.

weights Prior weights on the data.

Used to supply a model offset for use in fitting. Note that this offset will always

be completely ignored when predicting, unlike an offset included in formula.

This conforms to the behaviour of lm, glm and gam.

optimizer An array specifying the numerical optimization methods to optimize the smooth-

ing parameter estimation criterion (specified in the first element of optimizer) and to use to estimate the model coefficients (specified in the second element of optimizer). For the model coefficients estimation there are two alternatives: "newton" (default) and "bfgs" methods. For the smoothing parameter selection the available methods are "bfgs" (default) for the built in to scam package routine bfgs\_gcv.ubre, "optim", "nlm", "nlm.fd" (based on finite-difference approximation of the derivatives), "efs". "efs" for the extended Fellner Schall method of Wood and Fasiolo (2017) (rather than minimizing REML as in gam(mgcv) this minimizes the GCV/UBRE criterion) Note that 'bfgs' method for the coefficient

estimation works only with 'efs'.

In case of optimizer="optim" this specifies the numerical method to be used in optim in the first element, the second element of optim.method indicates

whether the finite difference approximation should be used ("fd") or analytical gradient ("grad"). The default is optim.method=c("Nelder-Mead", "fd").

data

offset

optim.method

scale	If this is positive then it is taken as the known scale parameter of the exponential family distribution. Negative value indicates that the scale paraemter is unknown. 0 indicates that the scale parameter is 1 for Poisson and binomial and unknown otherwise. This conforms to the behaviour of gam.	
knots	An optional list containing user specified knot values to be used for basis construction. Different terms can use different numbers of knots.	
not.exp	if TRUE then notExp(x,b,threshold) re-parameterization function will be used in place of exp() (default value) to ensure positivity in the model coefficients (scop-splines coefficients). notExp() is a softplus function, $1/b*log(1+exp(b*x),$ as implemented in PyTorch, it reverts to the linear function when $x*b >$ threshold, for numerical stability.	
start	Initial values for the model coefficients.	
etastart	Initial values for the linear predictor.	
mustart	Initial values for the expected values.	
control	A list of fit control parameters to replace defaults returned by scam.control. Values not set assume default values.	
AR1.rho	The AR1 correlation parameter. An AR1 error model can be used for the residuals of Gaussian-identity link models. Standardized residuals (approximately uncorrelated under correct model) returned in std.rsd if non-zero.	
AR.start	logical variable of same length as data, TRUE at first observation of an independent section of AR1 correlation. Very first observation in data frame does not need this. If NULL (default) then there are no breaks in AR1 correlation.	
drop.unused.levels		

drop.unused.levels

as with gam by default unused levels are dropped from factors before fitting.

#### **Details**

A shape constrained additive model (SCAM) is a generalized linear model (GLM) in which the linear predictor is given by strictly parametric components plus a sum of smooth functions of the covariates where some of the functions are assumed to be shape constrained. For example,

$$\log(E(Y_i)) = X_i^* b + f_1(x_{1i}) + m_2(x_{2i}) + f_3(x_{3i})$$

where the independent response variables  $Y_i$  follow Poisson distribution with log link function,  $f_1$ ,  $m_2$ , and  $f_3$  are smooth functions of the corresponding covariates, and  $m_2$  is subject to monotone increasing constraint.

Available shape constrained smooths are decsribed in shape.constrained.smooth.terms.

Residual auto-correlation with a simple AR1 correlation structure can be dealt with, for Gaussian models with identity link. Currently, the AR1 correlation parameter should be supplied (rather than estimated) in AR1.rho. AR.start input argument (logical) allows to set independent sections of AR1 correlation. Standardized residuals (approximately uncorrelated under correct model) are returned in std.rsd if AR1.rho is non zero. Use acf(model\$std.rsd) for computing and plotting estimates of the autocorrelation function to check correlation.

#### Value

The function returns an object of class "scam" with the following elements (this agrees with gamObject):

aic AIC of the fitted model: the degrees of freedom used to calculate this are the

effective degrees of freedom of the model, and the likelihood is evaluated at the

maximum of the penalized likelihood, not at the MLE.

assign Array whose elements indicate which model term (listed in pterms) each pa-

rameter relates to: applies only to non-smooth terms.

bfgs.info If optimizer[1]="bfgs", a list of convergence diagnostics relating to the BFGS

method of smoothing parameter selection. The items are: conv, indicates why the BFGS algorithm of the smoothness selection terminated; iter, number of iterations of the BFGS taken to get convergence; grad, the gradient of the GCV/UBRE score at convergence; score.hist, the succesive values of the

score up until convergence.

call the matched call.

coefficients the coefficients of the fitted model. Parametric coefficients are first, followed by

coefficients for each spline term in turn.

coefficients.t the parametrized coefficients of the fitted model (exponentiated for the mono-

tonic smooths).

conv indicates whether or not the iterative fitting method converged.

CPU. time indicates the real and CPU time (in seconds) taken by the fitting process in case

of unknown smoothing parameters

data the original supplied data argument. Only included if the scam argument keepData

is set to TRUE (default is FALSE).

deviance model deviance (not penalized deviance).

df.null null degrees of freedom.

df.residual effective residual degrees of freedom of the model.

edf estimated degrees of freedom for each model parameter. Penalization means

that many of these are less than 1.

edf1 alternative estimate of edf.

efs.info If optimizer[1]="efs", a list of convergence diagnostics relating to the ex-

tended Fellner Schall method fot smoothing parameter selection. The items are: conv, indicates why the efs algorithm of the smoothness selection terminated; iter, number of iterations of the efs taken to get convergence; score.hist, the

succesive values of the score up until convergence.

family family object specifying distribution and link used.

fitted.values fitted model predictions of expected value for each datum.

formula the model formula.

gcv.ubre the minimized GCV or UBRE score.

dgcv.ubre the gradient of the GCV or UBRE score.

iter number of iterations of the Newton-Raphson method taken to get convergence.

linear.predictors

fitted model prediction of link function of expected value for each datum.

method "GCV" or "UBRE", depending on the fitting criterion used.
min.edf Minimum possible degrees of freedom for whole model.

model model frame containing all variables needed in original model fit.

nlm.info If optimizer[1]="nlm" or optimizer[1]="nlm.fd", a list of convergence di-

agnostics relating to the BFGS method of smoothing parameter selection. The items are: conv, indicates why the BFGS algorithm of the smoothness selection terminated; iter, number of iterations of BFGS taken to get convergence; grad,

the gradient of the GCV/UBRE score at convergence.

not.exp if TRUE then notExp() function will be used in place of exp (default value) in

positivity ensuring model parameters re-parameterization.

nsdf number of parametric, non-smooth, model terms including the intercept.

null.deviance deviance for single parameter model.

offset model offset.

optim.info If optimizer[1]="optim", a list of convergence diagnostics relating to the

BFGS method of smoothing parameter selection. The items are: conv, indicates why the BFGS algorithm of the smoothness selection terminated; iter, number of iterations of BFGS taken to get convergence; optim.method, the numerical

optimization method used.

prior.weights prior weights on observations.

pterms terms object for strictly parametric part of model.

R Factor R from QR decomposition of weighted model matrix, unpivoted to be in

same column order as model matrix.

residuals the working residuals for the fitted model.

scale.estimated

TRUE if the scale parameter was estimated, FALSE otherwise.

sig2 estimated or supplied variance/scale parameter.

smooth list of smooth objects, containing the basis information for each term in the

model formula in the order in which they appear. These smooth objects are

returned by the smooth. construct objects.

sp estimated smoothing parameters for the model. These are the underlying smooth-

ing parameters, subject to optimization.

std.rsd Standardized residuals (approximately uncorrelated under correct model) if AR1.rho

non zero

termcode an integer indicating why the optimization process of the smoothness selection

terminated (see bfgs\_gcv.ubre).

terms object of model model frame.

trA trace of the influence matrix, total number of the estimated degrees of freedom

(sum(edf)).

var.summary A named list of summary information on the predictor variables. See gamObject.

Ve frequentist estimated covariance matrix for the parameter estimators.

Vp	estimated covariance matrix for the parameters. This is a Bayesian posterior covariance matrix that results from adopting a particular Bayesian model of the smoothing process.
Ve.t	frequentist estimated covariance matrix for the reparametrized parameter estimators obtained using the delta method. Particularly useful for testing whether terms are zero. Not so useful for CI's as smooths are usually biased.
Vp.t	estimated covariance matrix for the reparametrized parameters obtained using the delta method. Paricularly useful for creating credible/confidence intervals.
weights	final weights used in the Newton-Raphson iteration.
cmX	column means of the model matrix (with elements corresponding to smooths set to zero).
contrasts	contrasts associated with a factor.
xlevels	levels of a factor variable used in the model.
у	response data.

# Author(s)

Natalya Pya <nat.pya@gmail.com> based partly on mgcv by Simon Wood

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

Wood, S.N. (2011) Fast stable restricted maximum likelihood and marginal likelihood estimation of semiparametric generalized linear models. Journal of the Royal Statistical Society (B) 73(1):3-36

Wood S.N. (2017) Generalized Additive Models: An Introduction with R (2nd edition). Chapman and Hall/CRC Press

Wood, S.N. (2006) On confidence intervals for generalized additive models based on penalized regression splines. Australian and New Zealand Journal of Statistics. 48(4): 445-464.

Wood, S.N. and M. Fasiolo (2017) A generalized Fellner-Schall method for smoothing parameter optimization with application to Tweedie location, scale and shape models. Biometrics 73 (4), 1071-1081

### See Also

 $\verb|scam-package, shape.constrained.smooth.terms, gam, s, plot.scam, summary.scam, scam.check, predict.scam|$ 

# Examples

```
set.seed(4)
n <- 200
x1 <- runif(n)*6-3
f1 <- 3*exp(-x1^2) # unconstrained term
x2 <- runif(n)*4-1;
f2 \leftarrow \exp(4*x2)/(1+\exp(4*x2)) # monotone increasing smooth
y < -f1+f2 + rnorm(n)*.5
dat <- data.frame(x1=x1,x2=x2,y=y)</pre>
## fit model, get results, and plot...
b <- scam(y \sim s(x1, bs="cr")+s(x2, bs="mpi"), data=dat)
summary(b)
plot(b,pages=1,shade=TRUE)
## Gaussian model, two smooth terms: increasing and mixed (decreasing and convex)...
 ## simulating data...
set.seed(4)
n <- 200
x1 <- runif(n)*4-1;</pre>
f1 <- exp(4*x1)/(1+exp(4*x1)) # increasing smooth
x2 <- runif(n)*3-1;</pre>
f2 \leftarrow \exp(-3*x2)/15 # decreasing and convex smooth
y <- f1+f2 + rnorm(n)*.4
dat <- data.frame(x1=x1,x2=x2,y=y)</pre>
  ## fit model, results, and plot...
b \leftarrow scam(y \sim s(x1,bs="mpi")+s(x2,bs="mdcx"),data=dat)
summary(b)
plot(b,pages=1,scale=0,shade=TRUE)
##-----
## Not run:
## using the extended Fellner-Schall method for smoothing parameter selection...
b0 <- scam(y~ s(x1,bs="mpi")+s(x2,bs="mdcx"),data=dat,optimizer="efs")
summary(b0)
## using the extended Fellner-Schall method for smoothing parameter selection,
## and BFGS for model coefficient estimation...
b0 <- scam(y~ s(x1,bs="mpi")+s(x2,bs="mdcx"),data=dat,optimizer=c("efs","bfgs"))
summary(b0)
## using optim() for smoothing parameter selection...
b1 <- scam(y^{s(x1,bs="mpi")+s(x2,bs="mdcx"),data=dat,optimizer="optim")}
summary(b1)
b2 <- scam(y~ s(x1,bs="mpi")+s(x2,bs="mdcx"),data=dat,optimizer="optim",
           optim.method=c("BFGS","fd"))
summary(b2)
## using nlm()...
b3 <- scam(y~ s(x1,bs="mpi")+s(x2,bs="mdcx"),data=dat,optimizer="nlm")
summary(b3)
```

```
## End(Not run)
## Poisson model ....
 ## simulating data...
set.seed(2)
n <- 200
x1 <- runif(n)*6-3
f1 <- 3*exp(-x1^2) # unconstrained term
x2 <- runif(n)*4-1;</pre>
f2 \leftarrow \exp(4*x2)/(1+\exp(4*x2)) # monotone increasing smooth
f <- f1+f2
y <- rpois(n,exp(f))</pre>
dat <- data.frame(x1=x1,x2=x2,y=y)</pre>
  ## fit model, get results, and plot...
b <- scam(y < s(x1,bs = "cr") + s(x2,bs = "mpi"),
      family=poisson(link="log"),data=dat,optimizer=c("efs","bfgs"))
summary(b)
plot(b,pages=1,shade=TRUE)
scam.check(b)
## Gamma model...
   ## simulating data...
set.seed(6)
n <- 300
x1 <- runif(n)*6-3
f1 <- 1.5*sin(1.5*x1) # unconstrained term
x2 <- runif(n)*4-1;</pre>
f2 <- 1.5/(1+exp(-10*(x2+.75)))+1.5/(1+exp(-5*(x2-.75))) # increasing smooth
x3 <- runif(n)*6-3;
f3 <- 3*exp(-x3^2) # unconstrained term
f <- f1+f2+f3
y <- rgamma(n,shape=1,scale=exp(f))</pre>
dat <- data.frame(x1=x1,x2=x2,x3=x3,y=y)</pre>
   ## fit model, get results, and plot...
b \leftarrow scam(y^s(x1,bs="ps")+s(x2,k=15,bs="mpi")+s(x3,bs="ps"),
          family=Gamma(link="log"),data=dat,optimizer=c("efs","bfgs"))
summary(b)
par(mfrow=c(2,2))
plot(b, shade=TRUE)
## Not run:
## bivariate example...
 ## simulating data...
   set.seed(2)
   n <- 30
   x1 <- sort(runif(n)*4-1)</pre>
   x2 <- sort(runif(n))</pre>
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
       { f1[i,j] <- -exp(4*x1[i])/(1+exp(4*x1[i]))+2*sin(pi*x2[j])}
```

```
f <- as.vector(t(f1))</pre>
   y <- f+rnorm(length(f))*.2
   x11 <- matrix(0,n,n)</pre>
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
## fit model and plot ...
   b \leftarrow scam(y\sim s(x1,x2,k=c(10,10),b=c("tesmd1","ps")),data=dat,optimizer="efs")
   summary(b)
   old.par <- par(mfrow=c(2,2),mar=c(4,4,2,2))
   plot(b,se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data",pch=".",cex=3)
   par(old.par)
## example with random effect smoother...
   set.seed(2)
   n <- 200
   x1 <- runif(n)*6-3
   f1 <- 3*exp(-x1^2) # unconstrained term
   x2 <- runif(n)*4-1;</pre>
   f2 \leftarrow \exp(4*x2)/(1+\exp(4*x2)) # increasing smooth
   f <- f1+f2
   a <- factor(sample(1:10,200,replace=TRUE))</pre>
   Xa <- model.matrix(~a-1) # random main effects</pre>
   y \leftarrow f + Xa\% * rnorm(length(levels(a))) * .5 + rnorm(n) * .4
   dat <- data.frame(x1=x1,x2=x2,y=y,a=a)</pre>
   ## fit model and plot...
   b < -scam(y \sim s(x1, bs = "cr") + s(x2, bs = "mpi") + s(a, bs = "re"), data=dat)
   summary(b)
   scam.check(b)
   plot(b,pages=1,shade=TRUE)
## example with AR1 errors...
set.seed(8)
n <- 500
x1 <- runif(n)*6-3
f1 <- 3*exp(-x1^2) # unconstrained term
x2 <- runif(n)*4-1;</pre>
f2 \leftarrow \exp(4*x2)/(1+\exp(4*x2)) # increasing smooth
f <- f1+f2
e <- rnorm(n,0,sd=2)
for (i in 2:n) e[i] \leftarrow .6*e[i-1] + e[i]
y \leftarrow f + e
dat <- data.frame(x1=x1,x2=x2,y=y)
b \leftarrow scam(y \sim s(x1, bs = "cr") + s(x2, k = 25, bs = "mpi"),
             data=dat, AR1.rho=.6, optimizer="efs")
## Raw residuals still show correlation...
acf(residuals(b))
## But standardized are now fine...
x11()
```

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```
acf(b$std.rsd)
## End(Not run)
```

scam.check

Some diagnostics for a fitted scam object

# **Description**

Takes a fitted scam object produced by scam() and produces some diagnostic information about the fitting procedure and results. This function is almost the same as gam.check of the mgcv library. The default is to produce four residual plots and some information about the convergence of the smoothness selection optimization.

# Usage

## Arguments

```
b a fitted scam object as produced by scam().

old.style produces qq-norm plots as it was in scam versions < 1.2-15 when set to TRUE.

type type of residuals, see residuals.scam, used in all plots.

rep, level, rep.col arguments passed to qq.scam() when old.style is FALSE (default).

rl.col color for the reference line on the quantile-quantile plot.

pch plot character to use for the quantile-quantile plot.

extra graphics parameters to pass to plotting functions.
```

#### **Details**

As for mgcv(gam) plots 4 standard diagnostic plots, and some other convergence diagnostics. The printed information relates to the optimization process used to select smoothing parameters.

## Author(s)

Natalya Pya <nat.pya@gmail.com> based partly on mgcv by Simon N Wood

#### References

Wood S.N. (2006) Generalized Additive Models: An Introduction with R. Chapman and Hall/CRC Press.

## See Also

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## **Examples**

```
## Not run:
library(scam)
set.seed(2)
n <- 200
x1 <- runif(n)*4-1;</pre>
f1 <- exp(4*x1)/(1+exp(4*x1)) # monotone increasing smooth
x2 <- runif(n)*3-1;</pre>
f2 \leftarrow \exp(-3*x^2)/15 # monotone decreasing and convex smooth
f <- f1+f2
y \leftarrow f + rnorm(n) * 0.2
dat <- data.frame(x1=x1,x2=x2,y=y)
b \leftarrow scam(y \sim s(x1,k=25,bs="mpi",m=2)+s(x2,k=25,bs="mdcx",m=2),
    family=gaussian(link="identity"),data=dat)
plot(b,pages=1)
scam.check(b)
## End(Not run)
```

scam.control

Setting SCAM fitting defaults

## **Description**

This is an internal function of package scam which allows control of the numerical options for fitting a SCAM.

# Usage

# **Arguments**

maxit	Maximum number of IRLS iterations to perform used in scam. fit.
maxHalf	If a step of the BFGS optimization method leads to a worse penalized deviance, then the step length of the model coefficients is halved. This is the number of halvings to try before giving up used in bfgs_gcv.ubre.
devtol.fit	A positive scalar giving the convergence control for the model fitting algorithm in scam.fit.
steptol.fit	A positive scalar giving the tolerance at which the scaled distance between two successive iterates is considered close enough to zero to terminate the model fitting algorithm in scam. fit.
keepData	Should a copy of the original data argument be kept in the scam object?
efs.lspmax	maximum log smoothing parameters to allow under extended Fellner Schall smoothing parameter optimization.

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efs.tol change in GCV to count as negligible when testing for EFS convergence. If the step is small and the last 3 steps led to a GCV change smaller than this, then stop. n1m list of control parameters to pass to nlm if this is used for outer estimation of smoothing parameters (not default). list of control parameters to pass to optim if this is used for outer estimation of optim smoothing parameters (not default). bfgs list of control parameters to pass to default BFGS optimizer used for outer estimation of log smoothing parameters. trace turns on or off some de-bugging information. when set to FALSE turns off printing warning messages for step halving under print.warn non-finite exponentiated coefficients, non-finite deviance and/or if mu or eta are out of bounds. b.notexp

parameter b of the model coefficients re-parameterization softPlus() function

used as the notExp() function in place of exp() to ensure positivity.

threshold.notexp

parameter threshold of the softPlus() function used as the notExp() function. The implementation reverts to the linear function when coef\*b > threshold.

#### **Details**

Outer iteration is used to estimate smoothing parameters of SCAM by GCV/UBRE score optimization. The default procedure is the built-in BFGS method which is controlled by the list bfgs with the following elements: steptol.bfgs (default 1e-7) is the relative convergence tolerance; gradtol.bfgs (default 6.0554\*1e-6) is a tolerance at which the gradient is considered to be close enougth to 0 to terminate the BFGS algorithm; maxNstep is a positive scalar which gives the maximum allowable step length (default 5); maxHalf gives the maximum number of step halving in "backtracking" to permit before giving up(default 30); check.analytical is logical whether the analytical gradient of GCV/UBRE should be checked numerically (default FALSE); del is an increment for finite differences when checking analytical gradients (default 1e-4).

If outer iteration using nlm is used for fitting, then the control list nlm stores control arguments for calls to routine nlm. As in gam.control the list has the following named elements: ndigit is the number of significant digits in the GCV/UBRE score; gradtol is the tolerance used to judge convergence of the gradient of the GCV/UBRE score to zero (default 1e-6); stepmax is the maximum allowable log smoothing parameter step (default 2); steptol is the minimum allowable step length (default 1e-4); iterlim is the maximum number of optimization steps allowed (default 200); check.analyticals indicates whether the built in exact derivative calculations should be checked numerically (default FALSE). Any of these which are not supplied and named in the list are set to their default values.

Outer iteration using optim is controlled using list optim, which currently has one element: factr which takes default value 1e7.

### Author(s)

Natalya Pya Arnqvist <nat.pya@gmail.com> based partly on gam.control by Simon Wood

44 scam.fit

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

Wood, S.N. (2011) Fast stable restricted maximum likelihood and marginal likelihood estimation of semiparametric generalized linear models. Journal of the Royal Statistical Society (B) 73(1):3-36

### See Also

```
scam, scam.fit, gam.control
```

scam.fit

Newton-Raphson method to fit SCAM

# **Description**

This routine estimates SCAM coefficients given log smoothing parameters using the Newton-Raphson method. The estimation of the smoothing parameters by the GCV/UBRE score optimization is outer to the model fitting. Routine gcv.ubre\_grad evaluates the first derivatives of the smoothness selection scores with respect to the log smoothing parameters. Routine bfgs\_gcv.ubre estimates the smoothing parameters using the BFGS method.

The function is not normally called directly, but rather service routines for scam.

# Usage

## **Arguments**

G	A list of items needed to fit a SCAM.
sp	The vector of smoothing parameters.
etastart	Initial values for the linear predictor.
mustart	Initial values for the expected values.
env	Get the environment for the model coefficients, their derivatives and the smoothing parameter.
null.coef	coefficients for a null model, needed for an ability to check for immediate divergence.
control	A list of fit control parameters returned by scam.control. It includes: maxit, a positive scalar which gives the maximum number of iterations for Newton's method; devtol.fit, a scalar giving the tolerance at which the relative penalized deviance is considered to be close enough to 0 to terminate the algorithm; steptol.fit, a scalar giving the tolerance at which the scaled distance between

two successive iterates is considered close enough to zero to terminate the algorithm; trace turns on or off some de-bugging information; print.warn, when set to FALSE turns off printing warning messages for step halving under non-finite exponentiated coefficients, non-finite deviance and/or if mu or eta are out of bounds.

#### **Details**

The routine applies step halving to any step that increases the penalized deviance substantially.

### Author(s)

Natalya Pya <nat.pya@gmail.com>

### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

Wood, S.N. (2008) Fast stable direct fitting and smoothness selection for generalized additive models. Journal of the Royal Statistical Society (B) 70(3):495-518

Wood, S.N. (2011) Fast stable restricted maximum likelihood and marginal likelihood estimation of semiparametric generalized linear models. Journal of the Royal Statistical Society (B) 73(1):3-36

### See Also

scam

shape.constrained.smooth.terms

Shape preserving smooth terms in SCAM

## **Description**

As in mgcv(gam), shape preserving smooth terms are specified in a scam formula using s terms. All the shape constrained smooth terms (SCOP-splines) are constructed using the B-splines basis proposed by Eilers and Marx (1996) with a discrete penalty on the basis coefficients.

The univariate single penalty built-in shape constrained smooth classes are summarized as follows.

- Monotone increasing SCOP-splines: bs="mpi". To achieve monotone increasing smooths this reparameterizes the coefficients so that they form an increasing sequence.

  For details see smooth.construct.mpi.smooth.spec.
- Monotone decreasing SCOP-splines: bs="mpd". To achieve monotone decreasing smooths
  this reparameterizes the coefficients so that they form a decreasing sequence. A first order
  difference penalty applied to the basis coefficients starting with the second is used for the
  monotone increasing and decreasing cases.

- Convex SCOP-splines: bs="cx". This reparameterizes the coefficients so that the second order differences of the basis coefficients are greater than zero.
  - For details see smooth.construct.cx.smooth.spec.
- Concave SCOP-splines: bs="cv". This reparameterizes the coefficients so that the second order differences of the basis coefficients are less than zero.
  - For details see smooth.construct.cv.smooth.spec.
- Increasing and convex SCOP-splines: bs="micx". This reparameterizes the coefficients so that the first and the second order differences of the basis coefficients are greater than zero. For details see smooth.construct.micx.smooth.spec.
- Increasing and concave SCOP-splines: bs="micv". This reparameterizes the coefficients so that the first order differences of the basis coefficients are greater than zero while the second order difference are less than zero.
- Decreasing and convex SCOP-splines: bs="mdcx". This reparameterizes the coefficients so that the first order differences of the basis coefficients are less than zero while the second order difference are greater. For details see smooth.construct.mdcx.smooth.spec.
- Decreasing and concave SCOP-splines: bs="mdcv". This reparameterizes the coefficients so that the first and the second order differences of the basis coefficients are less than zero.
- Increasing with an additional 'finish-at-zero' constraint SCOP-splines: bs="mifo". This sets the last (m+1) spline coefficients to zero. According to the B-spline basis functions properties, the value of the spline, f(x), is determined by m+2 non-zero basis functions, and only m+1 B-splines are non-zero at knots. Only m+2 B-splines are non-zero on any (k\_i, k\_{i+1}), and the sum of these m+2 basis functions is 1.
  - For details see smooth.construct.mifo.smooth.spec.
- Increasing with an additional 'start-at-zero' constraint SCOP-spline: bs="miso". This sets the first (m+1) spline coefficients to zero. According to the B-spline basis functions properties, the value of the spline, f(x), is determined by m+2 non-zero basis functions, and only m+1 B-splines are non-zero at knots. Only m+2 B-splines are non-zero on any (k\_i, k\_{i+1}), and the sum of these m+2 basis functions is 1.
  - For details see smooth.construct.miso.smooth.spec.
- SCOP-spline with positivity constraint: bs="po". This reparameterizes the coefficients so that there are positive. For details see smooth.construct.po.smooth.spec.
- Decreasing/increasing SCOP-splines used with numeric 'by' variable: bs="mpdBy", bs="mpiBy". These work similar to mpd. smooth. spec, mpi. smooth. spec, but without applying an identifiability constraint ('zero intercept' constraint). Use when the smooth term has a numeric by variable that takes more than one value. For details see smooth.construct.mpd.smooth.spec, smooth.construct.mpi.smooth.spec.
- Convex/concave SCOP-splines used with numeric 'by' variable: bs="cxdBy", bs="cvBy". These work similar to cx.smooth.spec, cv.smooth.spec, but without applying an identifiability constraint ('zero intercept' constraint). Use when the smooth term has a numeric by variable that takes more than one value.

```
For details see smooth.construct.cx.smooth.spec, smooth.construct.cv.smooth.spec.
```

• Decreasing/increasing and convex/concave SCOP-splines used with numeric 'by' variable: bs="mdcxBy", bs="mdcvBy", bs="micxBy", bs="micxBy".

These work similar to mdcx.smooth.spec, mdcv.smooth.spec, micx.smooth.spec, micv.smooth.spec, but without applying an identifiability constraint ('zero intercept' constraint). Use when the smooth term has a numeric by variable that takes more than one value. For details see smooth.construct.mdcx.smooth.spec,

```
smooth.construct.mdcv.smooth.spec,
smooth.construct.micx.smooth.spec,
smooth.construct.micv.smooth.spec.
```

• Locally shape-constrained P-splines (LSCOP-splines): bs="lmpi". Locally increasing splines that are monotone increasing up to a specified change point and become unconstrained beyond that point. For details see smooth.construct.lmpi.smooth.spec.

For all types of the mixed constrained smoothing a first order difference penalty applied to the basis coefficients starting with the third one is used. Centring ('sum-to-zero') constraint has been applied to univariate SCOP-splines subject to monotonicity (convexity) constraints after implementing the 'zero intercept' identifiability constraint. This is achieved by dropping the first (constant) column of the spline model matrix and subtracting the corresponding column means from the elements of the remaining columns afterwards. 'Sum-to-zero' constraint orthogonalized the smooth to the model intercept term, thus avoiding confounding with the intercept. The standard errors of the estimated intercept become lower with the centring constraint.

Using the concept of the tensor product spline bases bivariate smooths under monotonicity constraint where monotonicity may be assumed on only one of the covariates (single monotonicity) or both of them (double monotonicity) are added as the smooth terms of the SCAM. Bivariate B-spline is constructed by expressing the coefficients of one of the marginal univariate B-spline bases as the B-spline of the other covariate. Double or single monotonicity is achieved by the corresponding re-parametrization of the bivariate basis coefficients to satisfy the sufficient conditions formulated in terms of the first order differences of the coefficients. The following explains the built in bivariate shape constrained smooth classes.

- Double monotone increasing SCOP-splines: bs="tedmi". See smooth.construct.tedmi.smooth.spec for details.
- Double monotone decreasing SCOP-splines: bs="tedmd".
- Single monotone increasing SCOP-splines along the first covariate direction: bs="tesmi1".
- Single monotone increasing SCOP-splines along the second covariate direction: bs="tesmi2".
- Single monotone decreasing SCOP-splines along the first covariate direction: bs="tesmd1".
- Single monotone decreasing SCOP-splines along the second covariate direction: bs="tesmd2".
- SCOP-splines with double concavity constraint: bs="tecvcv". See smooth.construct.tecvcv.smooth.spec for details.
- SCOP-splines with double convexity constraint: bs="tecxcx".
   See smooth.construct.tecxcx.smooth.spec for details.
- SCOP-splines with convexity wrt the first covariate and concavity wrt the second covariate: bs="tecxcv". See smooth.construct.tecxcv.smooth.spec for details.
- Decreasing along the first covariate and concave along the second covariate SCOP-splines: bs="tedecv". See smooth.construct.tedecv.smooth.spec for details.
- Decreasing along the first covariate and convex along the second covariate SCOP-splines: bs="tedecx". See smooth.construct.tedecx.smooth.spec for details.

- Increasing along the first covariate and concave along the second covariate SCOP-splines: bs="temicv". See smooth.construct.temicv.smooth.spec for details.
- Increasing along the first covariate and convex along the second covariate SCOP-splines: bs="temicx". See smooth.construct.temicx.smooth.spec for details.
- Convex along the second covariate SCOP-splines: bs="tescx".

See smooth.construct.tescx.smooth.spec for details.

Concave along the second covariate SCOP-splines: bs="tescv".
 See smooth.construct.tescv.smooth.spec for details.

• Tensor product interaction with increasing constraint along the first covariate and unconstrained along the second covariate: bs="tismi".

See smooth.construct.tismi.smooth.spec for details.

• Tensor product interaction with decreasing constraint along the first covariate and unconstrained along the second covariate: bs="tismd".

See smooth.construct.tismd.smooth.spec for details.

Double penalties for the shape constrained tensor product smooths are obtained from the penalties of the marginal smooths. For the bivariate SCOP-splines with monotonicity (convexity) constraints along one covariate, the 'sum-to-zero' constraints are applied after dropping the first columns of the model matrix of the constrained marginal smooth. The basis for the unconstrained marginal must be non-negative over the region where the marginal monotonicity (convexity) is to hold. For the bivariate interaction smooths "tismi" and "tismd" the following identifiability steps are implemented: i) dropped the first column of the "mpi" ("mpd") marginals, ii) applied 'sum-to-zero' constraints to the marginals and to the unconstrained B-spline basis, iii) tensor product constructed. The 'sum-to-zero' constraint is applied to the final tensor product model matrix afters removing its first column when constructing bivariate SCOP-splines with double monotonicity (convexity). These result in faster convergence of the optimization routines and more stable intercept estimates.

Also linear functionals of smooths with shape constraints (increasing/decreasing and convex/concave) are supported. See linear.functional.terms.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

Eilers, P.H.C. and B.D. Marx (1996) Flexible Smoothing with B-splines and Penalties. Statistical Science, 11(2):89-121

Wood S.N. (2017) Generalized Additive Models: An Introduction with R (2nd edition). Chapman and Hall/CRC Press

Wood, S.N. (2006) Low rank scale invariant tensor product smooths for generalized additive mixed models. Biometrics 62(4):1025-1036

#### See Also

```
s, smooth.construct.mpi.smooth.spec, smooth.construct.mpd.smooth.spec, smooth.construct.cx.smooth.spec, smooth.construct.cv.smooth.spec, smooth.construct.micx.smooth.spec, smooth.construct.micv.smooth.spec, smooth.construct.mdcv.smooth.spec, smooth.construct.mdcv.smooth.spec, smooth.construct.tedmi.smooth.spec, smooth.construct.tedmi.smooth.spec, smooth.construct.tesmi1.smooth.spec, smooth.construct.tesmi2.smooth.spec, smooth.construct.tesmd2.smooth.spec, smooth.construct.tesmd1.smooth.spec, smooth.construct.tesmd2.smooth.spec, smooth.construct.tismi.smooth.spec, smooth.construct.tismd.smooth.spec
```

## **Examples**

## see examples for scam

```
smooth.construct.cv.smooth.spec
```

Constructor for concave P-splines in SCAMs

# Description

This is a special method function for creating smooths subject to concavity constraint which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed using concave P-splines. This smooth is specified via model terms such as s(x,k,bs="cv",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

cvBy.smooth.spec works similar to cv.smooth.spec but without applying an identifiability constraint ('zero intercept' constraint). cvBy.smooth.spec should be used when the smooth term has a numeric by variable that takes more than one value. In such cases, the smooth terms are fully identifiable without a 'zero intercept' constraint, so they are left unconstrained. This smooth is specified as s(x,by=z,bs="cvBy"). See an example below.

However a factor by variable requires identifiability constraints, so s(x,by=fac,bs="cv") is used in this case.

#### **Usage**

```
## $3 method for class 'cv.smooth.spec'
smooth.construct(object, data, knots)
## $3 method for class 'cvBy.smooth.spec'
smooth.construct(object, data, knots)
```

#### **Arguments**

object	A smooth specification object, generated by an s term in a GAM formula.
data	A data frame or list containing the data required by this term, with names given
	by object\$term. The by variable is the last element.
knots	An optional list containing the knots supplied for basis setup. If it is NULL then
	the knot locations are generated automatically.

#### Value

An object of class "cv. smooth", "cvBy. smooth".

## Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.cx.smooth.spec, smooth.construct.mpi.smooth.spec,
smooth.construct.mdcv.smooth.spec, smooth.construct.mdcx.smooth.spec,
smooth.construct.micx.smooth.spec, smooth.construct.mpd.smooth.spec
```

# **Examples**

```
## Not run:
## Concave P-splines example
 ## simulating data...
  require(scam)
  set.seed(1)
  n <- 100
  x \leftarrow sort(2*runif(n)-1)
  f < -4*x^2
  y < -f + rnorm(n)*0.45
  dat <- data.frame(x=x,y=y)</pre>
  b <- scam(y~s(x,k=15,bs="cv"),family=gaussian,data=dat,not.exp=FALSE)
  ## fit unconstrained model...
  b1 <- scam(y~s(x,k=15,bs="cr"),family=gaussian, data=dat,not.exp=FALSE)
  ## plot results ...
  plot(x,y,xlab="x",ylab="y",cex=.5)
  lines(x,f)
                  ## the true function
  lines(x,b$fitted,col=2) ## constrained fit
  lines(x,b1$fitted,col=3) ## unconstrained fit
## Poisson version...
  y \leftarrow rpois(n, 15*exp(f))
  dat <- data.frame(x=x,y=y)</pre>
  ## fit model ...
  b <- scam(y~s(x,k=15,bs="cv"),family=poisson(link="log"),data=dat,not.exp=FALSE)
  ## fit unconstrained model...
  b1<-scam(y~s(x,k=15,bs="cr"),family=poisson(link="log"), data=dat,not.exp=FALSE)
  ## plot results ...
```

```
plot(x,y,xlab="x",ylab="y",cex=.5)
   lines(x,15*exp(f)) ## the true function
   lines(x,b$fitted,col=2) ## constrained fit
   lines(x,b1$fitted,col=3) ## unconstrained fit
## plotting on log scale...
   plot(x, log(15*exp(f)), type="l", cex=.5)
                                                  ## the true function
   lines(x,log(b$fitted),col=2) ## constrained fit
   lines(x,log(b1\$fitted),col=3) ## unconstrained fit
## 'by' factor example...
 set.seed(9)
 n <- 400
 x <- sort(runif(n,-.5,.5))</pre>
 f1 < -.7*x + cos(x) - 3
 f2 <- -20*x^2
 par(mfrow=c(1,2))
 plot(x,f1,type="l");plot(x,f2,type="l")
 e <- rnorm(n, 0, 1.5)
 fac <- as.factor(sample(1:2,n,replace=TRUE))</pre>
 fac.1 <- as.numeric(fac==1)</pre>
 fac.2 <- as.numeric(fac==2)</pre>
 y <- f1*fac.1 + f2*fac.2 + e
 dat <- data.frame(y=y,x=x,fac=fac,f1=f1,f2=f2)</pre>
 b2 <- scam(y ~ fac+s(x,by=fac,bs="cv"),data=dat,optimizer="efs")</pre>
 plot(b2,pages=1,scale=0,shade=TRUE)
 summary(b2)
 x11()
 vis.scam(b2,theta=50,color="terrain")
 ## numeric 'by' variable example...
 set.seed(6)
 n <- 100
x <- sort(2*runif(n)-1)</pre>
z <- runif(n,-2,3)
f < -4*x^2
y \leftarrow f*z + rnorm(n)*0.6
dat <- data.frame(x=x,z=z,y=y)</pre>
b <- scam(y\sim s(x,k=15,by=z,bs="cvBy"),data=dat)
 summary(b)
 par(mfrow=c(1,2))
plot(b, shade=TRUE)
 ## unconstrained fit...
b1 <- scam(y \sim s(x,k=15,by=z),data=dat)
plot(b1, shade=TRUE)
 summary(b1)
## End(Not run)
```

```
smooth.construct.cx.smooth.spec

**Constructor for convex P-splines in SCAMs**
```

# **Description**

This is a special method function for creating smooths subject to convexity constraint which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed using convex P-splines. This smooth is specified via model terms such as s(x,k,bs="cx",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

cxBy.smooth.spec works similar to cx.smooth.spec but without applying an identifiability constraint ('zero intercept' constraint). cxBy.smooth.spec should be used when the smooth term has a numeric by variable that takes more than one value. In such cases, the smooth terms are fully identifiable without a 'zero intercept' constraint, so they are left unconstrained. This smooth is specified as s(x,by=z,bs="cxBy"). See an example below.

However a factor by variable requires identifiability constraints, so s(x,by=fac,bs="cx") is used in this case.

# Usage

```
## S3 method for class 'cx.smooth.spec'
smooth.construct(object, data, knots)
## S3 method for class 'cxBy.smooth.spec'
smooth.construct(object, data, knots)
```

## **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the data required by this term, with names given

by object\$term. The by variable is the last element.

knots An optional list containing the knots supplied for basis setup. If it is NULL then

the knot locations are generated automatically.

## Value

```
An object of class "cx.smooth", "cxBy.smooth".
```

## Author(s)

Natalya Pya <nat.pya@gmail.com>

### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.cv.smooth.spec, smooth.construct.mpi.smooth.spec,
smooth.construct.mdcv.smooth.spec, smooth.construct.mdcx.smooth.spec,
smooth.construct.micv.smooth.spec, smooth.construct.mpd.smooth.spec
```

### **Examples**

```
## Not run:
## Convex SCOP-splines example...
 ## simulating data...
 require(scam)
 set.seed(16)
 n <- 100
 x <- sort(2*runif(n)-1)</pre>
 f < -4*x^2
 y < -f + rnorm(n)*0.4
 dat <- data.frame(x=x,y=y)</pre>
 b <- scam(y~s(x,k=15,bs="cx"),family=gaussian,data=dat)</pre>
 ## unconstrained fit...
 b1 <- scam(y \sim s(x, k=15), family=gaussian, data=dat)
 ## plot results ...
 plot(x,y,xlab="x",ylab="y")
 lines(x,f) ## the true function
 lines(x,b$fitted,col=2) ## constrained fit
 lines(x,b1$fitted,col=3) ## unconstrained fit
## Poisson version...
 set.seed(18)
 y <- rpois(n,exp(f))</pre>
 dat <- data.frame(x=x,y=y)
 ## fit shape constrained model ...
 b <- scam(y~s(x,k=15,bs="cx"),family=poisson(link="log"),data=dat,optimizer="efs")
 ## unconstrained fit...
 b1 <- scam(y \sim s(x,k=15),family=poisson(link="log"), data=dat,optimizer="efs")
 ## plot results ...
 plot(x,y,xlab="x",ylab="y")
 lines(x,exp(f))
                      ## the true function
 lines(x,b$fitted,col=2) ## constrained fit
 lines(x,b1$fitted,col=3) ## unconstrained fit
## 'by' factor example...
 set.seed(9)
 n <- 400
 x \leftarrow sort(runif(n, -.5, .5))
 f1 < -.7*x - cos(x) + 3
 f2 <- 20*x^2
 par(mfrow=c(1,2))
 plot(x,f1,type="l");plot(x,f2,type="l")
 e < - rnorm(n, 0, 1.5)
 fac <- as.factor(sample(1:2,n,replace=TRUE))</pre>
```

```
fac.1 <- as.numeric(fac==1)</pre>
 fac.2 <- as.numeric(fac==2)</pre>
 y <- f1*fac.1 + f2*fac.2 + e
 dat <- data.frame(y=y,x=x,fac=fac,f1=f1,f2=f2)</pre>
 b2 <- scam(y ~ fac+s(x,by=fac,bs="cx"),data=dat,optimizer="efs")
 plot(b2,pages=1,scale=0)
 summary(b2)
 x11()
 vis.scam(b2,theta=50,color="terrain")
## numeric 'by' variable example...
set.seed(6)
n <- 100
x <- sort(2*runif(n)-1)</pre>
z \leftarrow runif(n,-2,3)
f < -4*x^2
y \leftarrow f*z + rnorm(n)*.6
dat <- data.frame(x=x,z=z,y=y)</pre>
b \leftarrow scam(y\sim s(x,k=15,by=z,bs="cxBy"),data=dat)
summary(b)
par(mfrow=c(1,2))
plot(b, shade=TRUE)
## unconstrained fit...
b1 <- scam(y \sim s(x,k=15,by=z),data=dat)
plot(b1, shade=TRUE)
summary(b1)
## End(Not run)
```

```
smooth.construct.lmpi.smooth.spec
```

Locally shape-constrained P-spline based constructor (LSCOP-spline): locally increasing splines up to a change point.

# Description

scam can use locally shape-constrained smooths that are monotone increasing up to a specified change point and become unconstrained beyond that point. This smooth is specified via model terms like s(x,bs="lmpi",xt=list(xc=xc)), where xc sets a change point. The construction of the smooths uses B-spline bases with mildly non-linear re-parametrization of the basis coefficients over the shape-constrained interval. The 'wiggliness' of the smooths is controlled by discrete penalties applied directly to the basis coefficients, in particular, by penalizing the squared differences between adjacent spline coefficients.

The method is build by the mgcv constructor function for smooth terms, smooth.construct.

### Usage

```
## S3 method for class 'lmpi.smooth.spec'
smooth.construct(object, data, knots)
```

#### **Arguments**

object A smooth specification object, generated by an s term in a SCAM formula.

data A data frame or list containing the data required by this term, with names given

by object\$term. The by variable is the last element.

knots An optional list containing the knots supplied for basis setup. If it is NULL then

the knot locations are generated automatically.

#### **Details**

A smooth term of the form s(x,k,bs="lmpi",xt=list(xc=xc),m=2), where xc specifies a change point. k denotes the basis dimension and m+1 is the order of the B-spline basis. The default is a cubic spline m=2. The smooth uses a first order difference penalty on the coefficients starting from the second coefficient over the constrained part, and a second order difference penalty (a second order P-spline penalty) over the unconstrained part. The first order difference penalty over the constrained part shares with a second order P-spline penalty the feature of 'smoothing towards a straight line'.

The default basis dimension is k=10. The basis dimensions for constrained and unconstrained parts are set proportionally to the share of each part from the total range of the covariate value, but with a minimum of 5 basis functions on each side.

The smooth currently does not support user-supplied knots. The knots are placed evenly throughout the constrained and unconstrained ranges of the covariate values (inner knots) and outside the covariate values range (outer knots). The change point xc is set as an inner knot m times. Having multiple knots at the change point guarantees the correct imposing of the shape constraints up to the change point, avoiding 'leakage' of the transformed basis functions of the constrained part into the unconstrained part.

Sum-to-zero ('centering') constraint is applied to the LSCOP-splines after imposing the shape-constrained model matrix transformation. Linear extrapolation is (only) used for prediction that requires extrapolation, i.e. prediction outside the range of the interior knots.

### Value

An object of class "lmpi.smooth".

#### Author(s)

Natalya Pya <nat.pya@gmail.com> with contributions from Jens Lichter

## References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

## See Also

```
smooth.construct.mpd.smooth.spec, smooth.construct.cv.smooth.spec,
smooth.construct.cx.smooth.spec, smooth.construct.mdcv.smooth.spec,
smooth.construct.mdcx.smooth.spec, smooth.construct.micv.smooth.spec,
smooth.construct.micx.smooth.spec
```

## **Examples**

```
## Local monotone increasing LSCOP-spline example...
## simulating data...
require(scam)
set.seed(4)
n <- 200
x <- sort(runif(n)*6)</pre>
f <- 4*tanh(2*x-5)-5*exp(-(x-4)^2) ## increasing up untill xt=2.978
xc <- 2.978
y \leftarrow f + rnorm(n) * .7
old.par <- par(mfrow=c(1,2))</pre>
plot(x,y,cex=.5)
lines(x,f,lty=2); abline(v=xc,lty=2,col="red")
## fit model ...
b \leftarrow scam(y\sim s(x,bs="lmpi",xt=list(xc=xc),k=15))
summary(b)
lines(x,fitted(b),col=2,lwd=2)
plot(b, shade=TRUE)
par(old.par)
## unconstrained model to compare with...
g \leftarrow scam(y\sim s(x))
plot(x,y,cex=.5)
lines(x,f,lty=2); abline(v=xc,lty=2,col=2)
lines(x,fitted(g),col=4,lwd=2)
lines(x,fitted(b),col=2,lwd=1)
```

```
smooth.construct.mdcv.smooth.spec
```

Constructor for monotone decreasing and concave P-splines in SCAMs

# **Description**

This is a special method function for creating smooths subject to both monotone decreasing and concavity constraints which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed using mixed constrained P-splines. This smooth is specified via model terms such as s(x,k,bs="mdcv",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

mdcvBy.smooth.spec works similar to mdcv.smooth.spec but without applying an identifiability constraint ('zero intercept' constraint). mdcvBy.smooth.spec should be used when the smooth term has a numeric by variable that takes more than one value. In such cases, the smooth terms are fully identifiable without a 'zero intercept' constraint, so they are left unconstrained. This smooth is specified as s(x,by=z,bs="mdcvBy"). See an example below.

However a factor by variable requires identifiability constraints, so s(x,by=fac,bs="mdcv") is used in this case.

# Usage

```
## $3 method for class 'mdcv.smooth.spec'
smooth.construct(object, data, knots)
## $3 method for class 'mdcvBy.smooth.spec'
smooth.construct(object, data, knots)
```

## **Arguments**

object	A smooth specification objec	t, generated by an s terr	n in a GAM formula.

data A data frame or list containing the data required by this term, with names given

by object\$term. The by variable is the last element.

knots An optional list containing the knots supplied for basis setup. If it is NULL then

the knot locations are generated automatically.

## Value

An object of class "mdcv.smooth", "mdcvBy.smooth".

# Author(s)

Natalya Pya <nat.pya@gmail.com>

### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

# See Also

```
smooth.construct.mpi.smooth.spec, smooth.construct.mpd.smooth.spec,
smooth.construct.cx.smooth.spec, smooth.construct.cv.smooth.spec,
smooth.construct.mdcx.smooth.spec, smooth.construct.micx.smooth.spec,
smooth.construct.micv.smooth.spec
```

## **Examples**

```
## Not run:
## Monotone decreasing and concave SCOP-splines example
  ## simulating data...
  require(scam)
   set.seed(2)
  n <- 100
   x <- sort(runif(n))</pre>
   f < - -x^4
   y \leftarrow f + rnorm(n) * .2
   dat <- data.frame(x=x,y=y)
 ## fit model ...
   b \leftarrow scam(y\sim s(x,bs="mdcv"),family=gaussian(),data=dat)
 ## fit unconstrained model ...
  b1 <- scam(y~s(x,bs="ps"),family=gaussian(),data=dat)
 ## plot results ...
   plot(x,y,xlab="x",ylab="y",cex=.5)
                         ## the true function
   lines(x,f)
   lines(x,b\$fitted.values,col=2) \ \textit{## mixed constrained fit}
   lines(x,b1$fitted.values,col=3) ## unconstrained fit
 ## numeric 'by' variable example...
 set.seed(6)
n <- 100
x <- sort(runif(n))</pre>
z \leftarrow runif(n,-2,3)
 f < -x^4
y \leftarrow f*z + rnorm(n)*0.4
dat <- data.frame(x=x,z=z,y=y)</pre>
b <- scam(y\sim s(x,k=15,by=z,bs="mdcvBy"),data=dat)
summary(b)
par(mfrow=c(1,2))
plot(b, shade=TRUE)
 ## unconstrained fit...
b1 <- scam(y \sim s(x,k=15,by=z),data=dat)
 plot(b1, shade=TRUE)
summary(b1)
## End(Not run)
```

smooth.construct.mdcx.smooth.spec

Constructor for monotone decreasing and convex P-splines in SCAMs

## **Description**

This is a special method function for creating smooths subject to both monotone decreasing and convexity constraints which is built by the mgcv constructor function for smooth terms, smooth.construct.

It is constructed using mixed constrained P-splines. This smooth is specified via model terms such as s(x,k,bs="mdcx",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

mdcxBy.smooth.spec works similar to mdcx.smooth.spec but without applying an identifiability constraint ('zero intercept' constraint). mdcxBy.smooth.spec should be used when the smooth term has a numeric by variable that takes more than one value. In such cases, the smooth terms are fully identifiable without a 'zero intercept' constraint, so they are left unconstrained. This smooth is specified as s(x,by=z,bs="mdcxBy"). See an example below.

However a factor by variable requires identifiability constraints, so s(x,by=fac,bs="mdcx") is used in this case.

#### **Usage**

```
## S3 method for class 'mdcx.smooth.spec'
smooth.construct(object, data, knots)
## S3 method for class 'mdcxBy.smooth.spec'
smooth.construct(object, data, knots)
```

## **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the data required by this term, with names given

by object\$term. The by variable is the last element.

knots An optional list containing the knots supplied for basis setup. If it is NULL then

the knot locations are generated automatically.

## Value

An object of class "mdcx.smooth", "mdcxBy.smooth".

### Author(s)

Natalya Pya <nat.pya@gmail.com>

### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

### See Also

```
smooth.construct.mpi.smooth.spec, smooth.construct.mpd.smooth.spec,
smooth.construct.cx.smooth.spec, smooth.construct.cv.smooth.spec,
smooth.construct.mdcv.smooth.spec, smooth.construct.micx.smooth.spec,
smooth.construct.micv.smooth.spec
```

## **Examples**

```
## Not run:
 ## Monotone decreasing and convex SCOP-splines example
   ## simulating data...
    require(scam)
    set.seed(2)
    n <- 100
    x \leftarrow sort(runif(n)*3-1)
    f <- (x-3)^6/1000 \# monotone decreasing and convex smooth
    y \leftarrow f+rnorm(n)*.4
    dat <- data.frame(x=x,y=y)</pre>
    ## fit model ...
    b < -scam(y^s(x,k=15,bs="mdcx"),family=gaussian(link="identity"),data=dat)
    ## fit unconstrained model ...
    b1 <- scam(y~s(x,k=15,bs="ps"),family=gaussian(link="identity"),data=dat)
    ## plot results ...
    plot(x,y,xlab="x",ylab="y")
    lines(x,f)
                           ## the true function
    lines(x,b$fitted.values,col=2) ## mixed constrained fit
    lines(x,b1$fitted.values,col=3) ## unconstrained fit
  ## numeric 'by' variable example...
  set.seed(6)
  n <- 100
  x <- sort(runif(n)*3-1)</pre>
  z \leftarrow runif(n,-2,3)
  f <- (x-3)^6/1000
  y \leftarrow f*z + rnorm(n)*.4
  dat <- data.frame(x=x,z=z,y=y)</pre>
  b <- scam(y \sim s(x,k=15,by=z,bs="mdcxBy"),data=dat)
  summary(b)
  par(mfrow=c(1,2))
  plot(b, shade=TRUE)
  ## unconstrained fit...
  b1 <- scam(y \sim s(x, k=15, by=z), data=dat)
  plot(b1, shade=TRUE)
  summary(b1)
 ## End(Not run)
smooth.construct.micv.smooth.spec
```

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Constructor for monotone increasing and concave P-splines in SCAMs

# **Description**

This is a special method function for creating smooths subject to both monotone increasing and concavity constraints which is built by the mgcv constructor function for smooth terms, smooth.construct.

It is constructed using mixed constrained P-splines. This smooth is specified via model terms such as s(x,k,bs="micv",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

micvBy.smooth.spec works similar to micv.smooth.spec but without applying an identifiability constraint ('zero intercept' constraint). micvBy.smooth.spec should be used when the smooth term has a numeric by variable that takes more than one value. In such cases, the smooth terms are fully identifiable without a 'zero intercept' constraint, so they are left unconstrained. This smooth is specified as s(x,by=z,bs="micvBy"). See an example below.

However a factor by variable requires identifiability constraints, so s(x,by=fac,bs="micv") is used in this case.

#### **Usage**

```
## S3 method for class 'micv.smooth.spec'
smooth.construct(object, data, knots)
## S3 method for class 'micvBy.smooth.spec'
smooth.construct(object, data, knots)
```

## **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the data required by this term, with names given

by object\$term. The by variable is the last element.

knots An optional list containing the knots supplied for basis setup. If it is NULL then

the knot locations are generated automatically.

## Value

An object of class "micv.smooth", "micvBy.smooth".

### Author(s)

Natalya Pya <nat.pya@gmail.com>

### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

### See Also

```
smooth.construct.mpi.smooth.spec, smooth.construct.cx.smooth.spec,
smooth.construct.cv.smooth.spec, smooth.construct.mdcv.smooth.spec,
smooth.construct.mdcx.smooth.spec, smooth.construct.micx.smooth.spec,
smooth.construct.mpd.smooth.spec
```

# **Examples**

```
## Not run:
## Monotone increasing and concave SCOP-splines example
  ## simulating data...
  set.seed(3)
  n <- 100
  x \leftarrow sort(runif(n)*99+1)
   f < -\log(x)/2
   y \leftarrow f + rnorm(n) * .3
   dat <- data.frame(x=x,y=y)</pre>
   ## fit model ...
   b \leftarrow scam(y\sim s(x,k=15,bs="micv"), data=dat)
   summary(b)
   # fit unconstrained model ...
   b1 \leftarrow scam(y\sim s(x,k=15,bs="ps"),data=dat)
   ## plot results ...
   plot(x,y,xlab="x",ylab="y",cex=.5)
   lines(x,f)
                          ## the true function
   lines(x,b$fitted.values,col=2) ## mixed constrained fit
   lines(x,b1$fitted.values,col=3) ## unconstrained fit
 ## numeric 'by' variable example...
 set.seed(3)
n <- 100
x \leftarrow sort(runif(n)*99+1)
f < -\log(x)/2
z \leftarrow runif(n,-2,3)
y < -f*z + rnorm(n)*0.3
 dat <- data.frame(x=x,z=z,y=y)</pre>
 b <- scam(y \sim s(x, k=15, by=z, bs="micvBy")-1, data=dat)
 summary(b)
par(mfrow=c(1,2))
plot(b, shade=TRUE)
 ## unconstrained fit...
b1 <- scam(y\sim s(x,k=15,by=z)-1,data=dat)
 plot(b1, shade=TRUE)
 summary(b1)
## End(Not run)
```

smooth.construct.micx.smooth.spec

Constructor for monotone increasing and convex P-splines in SCAMs

# Description

This is a special method function for creating smooths subject to both monotone increasing and convexity constraints which is built by the mgcv constructor function for smooth terms, smooth construct. It is constructed using the mixed constrained P-splines. This smooth is specified via model terms

such as s(x,k,bs="micx",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

micxBy.smooth.spec works similar to micx.smooth.spec but without applying an identifiability constraint ('zero intercept' constraint). micxBy.smooth.spec should be used when the smooth term has a numeric by variable that takes more than one value. In such cases, the smooth terms are fully identifiable without a 'zero intercept' constraint, so they are left unconstrained. This smooth is specified as s(x,by=z,bs="micvBy"). See an example below.

However a factor by variable requires identifiability constraints, so s(x,by=fac,bs="micx") is used in this case.

## Usage

```
## $3 method for class 'micx.smooth.spec'
smooth.construct(object, data, knots)
## $3 method for class 'micxBy.smooth.spec'
smooth.construct(object, data, knots)
```

### **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the data required by this term, with names given

by object\$term. The by variable is the last element.

knots An optional list containing the knots supplied for basis setup. If it is NULL then

the knot locations are generated automatically.

#### Value

An object of class "micx.smooth", "micxBy.smooth".

# Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

## See Also

```
smooth.construct.mpi.smooth.spec, smooth.construct.cx.smooth.spec,
smooth.construct.cv.smooth.spec, smooth.construct.mdcv.smooth.spec,
smooth.construct.mdcx.smooth.spec, smooth.construct.micv.smooth.spec,
smooth.construct.mpd.smooth.spec
```

## **Examples**

```
## Not run:
## Monotone increasing and convex SCOP-splines example
  ## simulating data...
  set.seed(1)
  n <- 100
   x \leftarrow runif(n)*2
   f < -5*x^2/8
   y <- rpois(n,exp(f))</pre>
   dat <- data.frame(x=x,y=y)</pre>
   ## fit model ...
   b <- scam(y~s(x,bs="micx"),family=poisson,data=dat)</pre>
   ## fit unconstrained model ...
   b1 <- scam(y^s(x,bs="cr"),family=poisson,data=dat)
   ## plot results ...
   plot(x,y,xlab="x",ylab="y",cex=.5)
   x1 <- sort(x,index=TRUE)</pre>
   lines(x1$x,exp(f)[x1$ix])
                                     ## the true function
   lines(x1$x,b$fitted.values[x1$ix],col=2) ## mixed constrained fit
   lines(x1\$x,b1\$fitted.values[x1\$ix],col=3) \ \textit{## unconstrained fit}
## numeric 'by' variable example...
 set.seed(10)
n <- 100
x \leftarrow runif(n)*2
f \leftarrow x^2
z \leftarrow runif(n,-2,3)
y <- f*z + rnorm(n)*0.4
 dat <- data.frame(x=x,z=z,y=y)</pre>
 b <- scam(y~s(x,by=z,bs="micxBy"),data=dat)</pre>
 summary(b)
par(mfrow=c(1,2))
plot(b, shade=TRUE)
 ## unconstrained fit...
b1 <- scam(y \sim s(x, by=z), data=dat)
 plot(b1, shade=TRUE)
 summary(b1)
## End(Not run)
```

```
smooth.construct.mifo.smooth.spec
```

Constructor for monotone increasing SCOP-splines with an additional 'finish at zero' constraint

## **Description**

This is a special method function for creating smooths subject to a monotone increasing constraint plus the smooths should pass through zero at the right-end point of the covariate range. This is

similar to the pc argument to s in mgcv(gam) when pc=max(x), where x is a covariate. The smooth is built by the mgcv constructor function for smooth terms, smooth.construct. 'Zero intercept' identifiability constraints used for univariate SCOP-splines are substituted with a 'finish at zero' constraint here. This smooth is specified via model terms such as s(x,k,bs="mifo",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

### **Usage**

```
## S3 method for class 'mifo.smooth.spec'
smooth.construct(object, data, knots)
```

### **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the data required by this term, with names given

by object\$term. The by variable is the last element.

knots An optional list containing the knots supplied for basis setup. If it is NULL then

the knot locations are generated automatically.

#### **Details**

The constructor is not called directly, but as with gam(mgcv) is used internally.

A 'finish at zero' constraint is achieved by setting the last (m+1) spline coefficients to zero. According to the B-spline basis functions properties, the value of the spline, f(x), is determined by m+2 non-zero basis functions, and only m+1 B-splines are non-zero at knots. Only m+2 B-splines are non-zero on any  $[k_i, k_{i+1})$ , and the sum of these m+2 basis functions is 1.

If the knots of the spline are not supplied, then they are placed evenly throughout the covariate values with an exception of the minner knots preceding the last inner knot that are joined with that last knot. This is done in order to avoid an otherwise plateau fit at the right-end region. If the knots are supplied, then the number of supplied knots should be k+m+2, and the range of the middle k-m knots must include all the covariate values.

Note: when a plateau region is expected at the righ-end covariate region, the smooth might result in some decrease when approaching to zero.

### Value

An object of class "mifo.smooth".

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.mpi.smooth.spec, smooth.construct.miso.smooth.spec,
smooth.construct.mpd.smooth.spec, smooth.construct.mdcv.smooth.spec,
smooth.construct.mdcx.smooth.spec, smooth.construct.micv.smooth.spec,
smooth.construct.micx.smooth.spec
```

### **Examples**

```
## Monotone increasing SCOP-spline examples with a finish at zero constraint... set.seed(53)  n <- 100; x <- runif(n); z <- runif(n) \\ pc <- max(x) \\ y <- exp(3*x)/10-exp(3*pc)/10 + z*(1-z)*5 + rnorm(100)*.4 \\ m1 <- scam(y^s(x,bs='mifo')+s(z)) #,knots=knots) \\ plot(m1,pages=1,scale=0) \\ summary(m1) \\ newd<- data.frame(x=pc,z=0) \\ predict(m1,newd, type='terms')
```

```
smooth.construct.miso.smooth.spec
```

Constructor for monotone increasing SCOP-splines with an additional 'start at zero' constraint

## Description

This is a special method function for creating smooths subject to a monotone increasing constraint plus the smooths should pass through zero at the left-end point of the covariate range. This is similar to the pc argument to s in mgcv(gam) when pc=min(x), where x is a covariate. The smooth is built by the mgcv constructor function for smooth terms, smooth.construct. 'Zero intercept' identifiability constraints used for univariate SCOP-splines are substituted with a 'start at zero' constraint here. This smooth is specified via model terms such as s(x,k,bs="miso",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

## Usage

```
## S3 method for class 'miso.smooth.spec'
smooth.construct(object, data, knots)
```

# **Arguments**

object	A smooth specification object, generated by an s term in a GAM formula.
data	A data frame or list containing the data required by this term, with names given by object\$term. The by variable is the last element.
knots	An optional list containing the knots supplied for basis setup. If it is NULL then the knot locations are generated automatically.

#### **Details**

The constructor is not called directly, but as with gam(mgcv) is used internally.

A 'start at zero' constraint is achieved by setting the first (m+1) spline coefficients to zero. According to the B-spline basis functions properties, the value of the spline, f(x), is determined by m+2 non-zero basis functions, and only m+1 B-splines are non-zero at knots. Only m+2 B-splines are non-zero on any  $[k_i, k_{i+1})$ , and the sum of these m+2 basis functions is 1.

If the knots of the spline are not supplied, then they are placed evenly throughout the covariate values with an exception of the minner knots following the first inner knot that are joined with that first knot. This is done in order to avoid an otherwise plateau fit at the left-end region. If the knots are supplied, then the number of supplied knots should be k+m+2, and the range of the middle k-m knots must include all the covariate values.

#### Value

An object of class "miso.smooth".

## Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

### See Also

```
smooth.construct.mpi.smooth.spec, smooth.construct.mifo.smooth.spec,
smooth.construct.mpd.smooth.spec, smooth.construct.mdcv.smooth.spec,
smooth.construct.mdcx.smooth.spec, smooth.construct.micv.smooth.spec,
smooth.construct.micx.smooth.spec
```

## **Examples**

```
## Monotone increasing SCOP-spline examples with a start at zero constraint...

## passing through 0 at -1...

require(scam)

set.seed(7)

n <-100;

x <-c(-1,runif(n-1)*4-1); ## starting at -1 for a function to be zero at a start z <- runif(n)

y <-exp(4*x)/(1+exp(4*x)) -0.01798621+ z*(1-z)*5 + rnorm(100)*.4

m1 <-scam(y^xs(x,bs='miso')+s(z))

plot(m1,pages=1)

newd<- data.frame(x=-1,z=0)

predict(m1,newd, type='terms')
```

```
## Not run:
    ## passing through 0 at 0...
    set.seed(53)
    n <- 100;
    x <- c(0,runif(n-1)); ## starting at 0 for a function to be zero at a start
    z <- runif(n)
    y <- exp(3*x)/10-.1 + z*(1-z)*5 + rnorm(100)*.4
    m2 <- scam(y~s(x,bs='miso')+s(z))
    plot(m2,pages=1)
    newd<- data.frame(x=0,z=0)
    predict(m2,newd, type='terms')

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

smooth.construct.mpd.smooth.spec

Constructor for monotone decreasing P-splines in SCAMs

# Description

This is a special method function for creating smooths subject to monotone decreasing constraints which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed using monotonic P-splines. This smooth is specified via model terms such as s(x,k,bs="mpd",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

mpdBy.smooth.spec works similar to mpd.smooth.spec but without applying an identifiability constraint ('zero intercept' constraint). mpdBy.smooth.spec should be used when the smooth term has a numeric by variable that takes more than one value. In such cases, the smooth terms are fully identifiable without a 'zero intercept' constraint, so they are left unconstrained. This smooth is specified as s(x,by=z,bs="mpdBy"). See an example below.

However a factor by variable requires identifiability constraints, so s(x,by=fac,bs="mpd") is used in this case.

## Usage

```
## S3 method for class 'mpd.smooth.spec'
smooth.construct(object, data, knots)
## S3 method for class 'mpdBy.smooth.spec'
smooth.construct(object, data, knots)
```

### **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

A data frame or list containing the data required by this term, with names given by object\$term. The by variable is the last element.

Knots An optional list containing the knots supplied for basis setup. If it is NULL then the knot locations are generated automatically.

#### Value

An object of class "mpd. smooth", "mpdBy. smooth".

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.mpi.smooth.spec, smooth.construct.cx.smooth.spec,
smooth.construct.cv.smooth.spec, smooth.construct.mdcv.smooth.spec,
smooth.construct.mdcx.smooth.spec, smooth.construct.micv.smooth.spec,
smooth.construct.micx.smooth.spec
```

# **Examples**

```
## Not run:
## Monotone decreasing SCOP-splines example...
 ## simulating data...
  require(scam)
  set.seed(3)
  n <- 100
  x \leftarrow runif(n)*3-1
  f <- exp(-1.3*x)
  y <- rpois(n,exp(f))</pre>
  dat <- data.frame(x=x,y=y)</pre>
## fit model ...
  b <- scam(y~s(x,k=15,bs="mpd"),family=poisson(link="log"),</pre>
       data=dat)
## unconstrained model fit for comparison...
  b1 <- scam(y \sim s(x, k=15, bs="ps"), family=poisson(link="log"),
         data=dat)
## plot results ...
  plot(x,y,xlab="x",ylab="y",cex=.5)
  x1 <- sort(x,index=TRUE)</pre>
  lines(x1$x,exp(f)[x1$ix])
                                  ## the true function
  lines(x1$x,b$fitted.values[x1$ix],col=2) ## decreasing fit
  lines(x1$x,b1$fitted.values[x1$ix],col=3) ## unconstrained fit
## 'by' factor example...
set.seed(3)
n <- 400
x <- runif(n, 0, 1)
```

```
## all three smooths are decreasing...
 f1 < -\log(x *5)
 f2 < -exp(2 * x) + 4
 f3 < -5* \sin(x)
 e \leftarrow rnorm(n, 0, 2)
 fac <- as.factor(sample(1:3,n,replace=TRUE))</pre>
 fac.1 <- as.numeric(fac==1)</pre>
 fac.2 <- as.numeric(fac==2)</pre>
 fac.3 <- as.numeric(fac==3)</pre>
 y <- f1*fac.1 + f2*fac.2 + f3*fac.3 + e
 \texttt{dat} \leftarrow \texttt{data.frame}(\texttt{y=y}, \texttt{x=x}, \texttt{fac=fac}, \texttt{f1=f1}, \texttt{f2=f2}, \texttt{f3=f3})
 b2 <- scam(y ~ fac+s(x,by=fac,bs="mpd"),data=dat)</pre>
 plot(b2,pages=1,scale=0,shade=TRUE)
 summary(b2)
 vis.scam(b2,theta=120,color="terrain")
 ## comparing with unconstrained fit...
 b3 <- scam(y \sim fac+s(x,by=fac),data=dat)
 x11()
 plot(b3,pages=1,scale=0,shade=TRUE)
 summary(b3)
## Note that since in scam() as in mgcv::gam() when using factor 'by' variables, 'centering'
 ## constraints are applied to the smooths, which usually means that the 'by'
 ## factor variable should be included as a parametric term, as well.
## numeric 'by' variable example...
set.seed(3)
n <- 100
x \leftarrow sort(runif(n,-1,2))
z \leftarrow runif(n,-2,3)
f <- exp(-1.3*x)
y < - f*z + rnorm(n)*0.4
dat <- data.frame(x=x,y=y,z=z)</pre>
b <- scam(y~s(x,k=15,by=z,bs="mpdBy"),data=dat,optimizer="efs")</pre>
plot(b, shade=TRUE)
summary(b)
## unconstrained fit...
b1 <- scam(y\sim s(x,k=15,by=z),data=dat)
plot(b1, shade=TRUE)
summary(b1)
## End(Not run)
```

## **Description**

This is a special method function for creating smooths subject to a monotone increasing constraint which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed using monotonic P-splines. This smooth is specified via model terms such as s(x,k,bs="mpi",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

mpiBy.smooth.spec works similar to mpi.smooth.spec but without applying an identifiability constraint ('zero intercept' constraint). mpiBy.smooth.spec should be used when the smooth term has a numeric by variable that takes more than one value. In such cases, the smooth terms are fully identifiable without a 'zero intercept' constraint, so they are left unconstrained. This smooth is specified as s(x,by=z,bs="mpiBy"). See an example below.

However a factor by variable requires identifiability constraints, so s(x,by=fac,bs="mpi") is used in this case.

## Usage

```
## $3 method for class 'mpi.smooth.spec'
smooth.construct(object, data, knots)
## $3 method for class 'mpiBy.smooth.spec'
smooth.construct(object, data, knots)
```

### **Arguments**

object	smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the data required by this term, with names given

by object\$term. The by variable is the last element.

knots An optional list containing the knots supplied for basis setup. If it is NULL then

the knot locations are generated automatically.

## **Details**

The constructor is not called directly, but as with gam(mgcv) is used internally.

If the knots of the spline are not supplied, then they are placed evenly throughout the covariate values. If the knots are supplied, then the number of supplied knots should be k+m+2, and the range of the middle k-m knots must include all the covariate values.

### Value

```
An object of class "mpi.smooth", "mpiBy.smooth".
```

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.mpd.smooth.spec, smooth.construct.cv.smooth.spec,
smooth.construct.cx.smooth.spec, smooth.construct.mdcv.smooth.spec,
smooth.construct.mdcx.smooth.spec, smooth.construct.micv.smooth.spec,
smooth.construct.micx.smooth.spec
```

## **Examples**

```
## Monotone increasing P-splines example
 ## simulating data...
   require(scam)
   set.seed(12)
   n <- 100
   x \leftarrow runif(n)*4-1
   f <- 4*exp(4*x)/(1+exp(4*x))
   y <- rpois(n,exp(f))</pre>
   dat <- data.frame(x=x,y=y)</pre>
   b <- scam(y~s(x,k=15,bs="mpi"),family=poisson(link="log"),
       data=dat)
 ## fit unconstrained model...
   b1 <- scam(y~s(x,k=15,bs="ps"),family=poisson(link="log"),
         data=dat)
 ## plot results ...
   plot(x,y,xlab="x",ylab="y")
   x1 <- sort(x,index=TRUE)</pre>
   lines(x1$x,exp(f)[x1$ix])
                                   ## the true function
   lines(x1$x,b$fitted.values[x1$ix],col=2) ## monotone fit
   lines(x1$x,b1$fitted.values[x1$ix],col=3) ## unconstrained fit
## example with supplied knots...
   knots \leftarrow list(x=c (-1.5, -1.2, -.99, -.97, -.7, -.5, -.3, 0, 0.7,
           0.9, 1.1, 1.22, 1.5, 2.2, 2.77, 2.93, 2.99, 3.2, 3.6)
   b2 < -scam(y \sim s(x, k=15, bs="mpi"), knots=knots,
          family=poisson(link="log"), data=dat)
   summary(b2)
   plot(b2, shade=TRUE)
## Not run:
## example with two terms...
   set.seed(0)
   n <- 200
   x1 <- runif(n)*6-3
```

```
f1 <- 3*exp(-x1^2) # unconstrained term
   x2 <- runif(n)*4-1;
   f2 \leftarrow \exp(4*x2)/(1+\exp(4*x2)) # monotone increasing smooth
   f <- f1+f2
   y \leftarrow f+rnorm(n)*.7
   dat \leftarrow data.frame(x1=x1,x2=x2,y=y)
   knots \leftarrow list(x1=c(-4,-3.5,-2.99,-2.7,-2.5,-1.9,-1.1,-.9,-.3,0.3,.8,1.2,1.9,2.3,
2.7, 2.99, 3.5, 4.1, 4.5), x2=c(-1.5, -1.2, -1.1, -.89, -.69, -.5, -.3, 0, 0.7,
0.9, 1.1, 1.22, 1.5, 2.2, 2.77, 2.99, 3.1, 3.2, 3.6)
   b3 < -scam(y \sim s(x1, k=15) + s(x2, bs="mpi", k=15),
         knots=knots,data=dat)
   summary(b3)
   plot(b3,pages=1,shade=TRUE)
## setting knots for f(x2) only...
   knots <- list(x2=c(-1.5,-1.2,-1.1, -.89,-.69,-.5,-.3,
   0, 0.7, 0.9, 1.1, 1.22, 1.5, 2.2, 2.77, 2.99, 3.1, 3.2, 3.6)
   b4 \leftarrow scam(y^s(x1,k=15,bs="bs")+s(x2,bs="mpi",k=15),
       knots=knots,data=dat)
   summary(b4)
   plot(b4,pages=1,shade=TRUE)
## 'by' factor example...
set.seed(10)
n <- 400
x <- runif(n, 0, 1)
## all three smooths are increasing...
 f1 < -\log(x *5)
 f2 \leftarrow exp(2*x) - 4
 f3 \leftarrow 5* \sin(x)
 e <- rnorm(n, 0, 2)
 fac <- as.factor(sample(1:3,n,replace=TRUE))</pre>
 fac.1 <- as.numeric(fac==1)</pre>
 fac.2 <- as.numeric(fac==2)</pre>
 fac.3 <- as.numeric(fac==3)</pre>
 y <- f1*fac.1 + f2*fac.2 + f3*fac.3 + e
 dat <- data.frame(y=y,x=x,fac=fac,f1=f1,f2=f2,f3=f3)</pre>
 b5 <- scam(y ~ fac+s(x,by=fac,bs="mpi"),data=dat)</pre>
 plot(b5,pages=1,scale=0,shade=TRUE)
 summary(b5)
 vis.scam(b5,theta=50,color="terrain")
 ## comparing with unconstrained fit...
 b6 <- scam(y \sim fac+s(x,by=fac),data=dat)
 x11()
 plot(b6,pages=1,scale=0,shade=TRUE)
 summary(b6)
 vis.scam(b6,theta=50,color="terrain")
## Note that since in scam() as in mgcv::gam() when using factor 'by' variables, 'centering'
 ## constraints are applied to the smooths, which usually means that the 'by'
 ## factor variable should be included as a parametric term, as well.
```

```
## numeric 'by' variable example...
set.seed(3)
n <- 200
x \leftarrow sort(runif(n,-1,2))
z \leftarrow runif(n,-2,3)
f \leftarrow exp(1.3*x)-5
y \leftarrow f*z + rnorm(n)*2
dat <- data.frame(x=x,y=y,z=z)</pre>
b <- scam(y~s(x,by=z,bs="mpiBy"),data=dat)</pre>
plot(b, shade=TRUE)
summary(b)
## unconstrained fit...
b1 <- scam(y \sim s(x,k=15,by=z),data=dat)
plot(b1, shade=TRUE)
summary(b1)
## End(Not run)
```

smooth.construct.po.smooth.spec

Constructor for SCOP-splines with positivity constraint

# Description

This is a special method function for creating univariate smooths subject to a positivity constraint which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed using monotonic P-splines. This smooth is specified via model terms suach as s(x,k,bs="po",m=2), where k denotes the basis dimension and m+1 is the order of the B-spline basis.

Note: Models that include this smooth should not have an intercept. See examples below.

#### Usage

```
## S3 method for class 'po.smooth.spec'
smooth.construct(object, data, knots)
```

# **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the data required by this term, with names given

by object\$term. The by variable is the last element.

knots An optional list containing the knots supplied for basis setup. If it is NULL then

the knot locations are generated automatically.

#### Value

An object of class "po.smooth".

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.mpd.smooth.spec, smooth.construct.cv.smooth.spec,
smooth.construct.cx.smooth.spec, smooth.construct.mdcv.smooth.spec,
smooth.construct.mdcx.smooth.spec, smooth.construct.micv.smooth.spec,
smooth.construct.micx.smooth.spec
```

```
## SCOP-splines example with positivity constraint...
  ## simulating data...
## Not run:
  require(scam)
   set.seed(3)
  n <- 100
   x \leftarrow seq(-3,3,length.out=100)
   f \leftarrow dnorm(x)
   y < -f + rnorm(n)*0.1
   b <- scam(y^s(x,bs="po")-1)
   b1 <- scam(y \sim s(x)) ## unconstrained model
   plot(x,y)
   lines(x,f)
   lines(x,fitted(b),col=2)
   lines(x,fitted(b1),col=3)
  ## two-term example...
  set.seed(3)
  n <- 200
  x1 <- seq(-3,3,length.out=n)
  f1 <- 3*exp(-x1^2) ## positively constrained smooth
  x2 <- runif(n)*3-1;</pre>
  f2 \leftarrow \exp(4*x2)/(1+\exp(4*x2)) ## increasing smooth
  f <- f1+f2
  y \leftarrow f+rnorm(n)*0.3
  dat <- data.frame(x1=x1,x2=x2,y=y)</pre>
  ## fit model, results, and plot...
  b2 <- scam(y < (x1, bs = "po") + s(x2, bs = "mpi") - 1, data = dat)
  summary(b2)
  plot(b2,pages=1)
```

```
b3 <- scam(y~s(x1,bs="ps")+s(x2,bs="ps"),data=dat) ## unconstrained model
summary(b3)
plot(b3,pages=1)
## End(Not run)</pre>
```

smooth.construct.tecvcv.smooth.spec

Tensor product smoothing constructor for bivariate function subject to double concavity constraint

## **Description**

This is a special method function for creating tensor product bivariate smooths subject to double concavity constraint, i.e. concavity constraint wrt both the first and the second covariates. This is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths which are represented using the B-spline basis functions. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),b="tecvcv",m=c(2,2)), where q1 and q2 denote the basis dimensions for the marginal smooths.

#### **Usage**

```
## S3 method for class 'tecvcv.smooth.spec'
smooth.construct(object, data, knots)
```

## Arguments

data

object A smooth specification object, generated by an s term in a GAM formula.

A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### Value

An object of class "tecvcv.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p.ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

## Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

#### See Also

```
smooth.construct.tedmd.smooth.spec smooth.construct.temicx.smooth.spec
smooth.construct.tedecx.smooth.spec smooth.construct.tecxcx.smooth.spec
smooth.construct.tecxcv.smooth.spec
```

```
## Not run:
## tensor product `tecvcv' example
  ## simulating data...
   set.seed(3)
   n <- 30
   x1 <- sort(2*runif(n)-1)</pre>
   x2 \leftarrow sort(2*runif(n)-1)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
         f1[i,j] < -4*(x1[i]^2+x2[j]^2)
   f <- as.vector(t(f1))</pre>
   y \leftarrow f+rnorm(length(f))*.05
   x11 <- matrix(0,n,n)</pre>
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)</pre>
## fit model ...
   b <- scam(y \sim s(x1, x2, k = c(10, 10), b = "tecvcv"), data=dat)
## plot results ...
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b, se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   vis.scam(b, theta=30,phi=40)
   ## plotting the truth...
   x1 \leftarrow seq(min(x1), max(x1), length.out=30)
   x2 \leftarrow seq(min(x2), max(x2), length.out=30)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n) f1[i,j] \leftarrow -4*(x1[i]^2+x2[j]^2)
   persp(x1, x2, f1, theta = 30, phi = 40)
## End(Not run)
```

smooth.construct.tecxcv.smooth.spec

Tensor product smoothing constructor for bivariate function subject to mixed constraints: convexity constraint wrt the first covariate and concavity wrt the second one

# **Description**

This is a special method function for creating tensor product bivariate smooths subject to mixed constraints, convexity constraint wrt the first covariate and concavity wrt the second one. This is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths which are represented using the B-spline basis functions. This tensor product is specified by model terms such as  $s(x_1,x_2,k=c(q_1,q_2),b="tecxcv",m=c(2,2))$ , where  $q_1$  and  $q_2$  denote the basis dimensions for the marginal smooths.

# Usage

```
## S3 method for class 'tecxcv.smooth.spec'
smooth.construct(object, data, knots)
```

## **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### Value

An object of class "tecxcv.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p.ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

#### See Also

```
smooth.construct.tedmd.smooth.spec smooth.construct.tedecv.smooth.spec
smooth.construct.tedecx.smooth.spec smooth.construct.tecvcv.smooth.spec
smooth.construct.tecxcx.smooth.spec
```

# **Examples**

```
## Not run:
## tensor product `tecxcv' example
  ## simulating data...
   set.seed(5)
   n <- 30
   x1 <- sort(2*runif(n)-1)</pre>
   x2 \leftarrow sort(2*runif(n)-1)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
        f1[i,j] \leftarrow 2*x1[i]^2 - 4*x2[j]^2
   f <- as.vector(t(f1))</pre>
   y \leftarrow f+rnorm(length(f))*.05
   x11 <- matrix(0,n,n)</pre>
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 < - rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
## fit model ...
   b < -scam(y \sim s(x1, x2, k = c(10, 10), b = "tecxcv"), data=dat)
## plot results ...
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b,se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   x11()
   vis.scam(b,theta=30,phi=40)
   ## plotting the truth...
   x1 \leftarrow seq(min(x1), max(x1), length.out=30)
   x2 <- seq(min(x2),max(x2),length.out=30)</pre>
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n) f1[i,j] \leftarrow 2*x1[i]^2 - 4*x2[j]^2
   persp(x1, x2, f1, theta = 30, phi = 40)
## End(Not run)
```

smooth.construct.tecxcx.smooth.spec

Tensor product smoothing constructor for bivariate function subject to double convexity constraint

## **Description**

This is a special method function for creating tensor product bivariate smooths subject to double convexity constraint, convexity constraint wrt both the first and the second covariates. This is built by the mgcv constructor function for smooth terms, smooth. construct. It is constructed from a pair of single penalty marginal smooths which are represented using the B-spline basis functions. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),bs="tecxcx",m=c(2,2)), where q1 and q2 denote the basis dimensions for the marginal smooths.

# Usage

```
## S3 method for class 'tecxcx.smooth.spec'
smooth.construct(object, data, knots)
```

# **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### Value

An object of class "tecxcx.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

## Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

# See Also

```
smooth.construct.tedmd.smooth.spec smooth.construct.tedecv.smooth.spec
smooth.construct.tedecx.smooth.spec smooth.construct.tecvcv.smooth.spec
smooth.construct.tecxcv.smooth.spec
```

## **Examples**

```
## Not run:
## tensor product `tecxcx' example
  ## simulating data...
   set.seed(2)
   n <- 30
   x1 \leftarrow sort(2*runif(n)-1)
   x2 \leftarrow sort(2*runif(n)-1)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
       { f1[i,j] <- 2*(x1[i]^2 + x2[j]^2)}
   f <- as.vector(t(f1))
   y \leftarrow f + rnorm(length(f)) * .05
   x11 \leftarrow matrix(0,n,n)
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
## fit model ...
   b < -scam(y < s(x1, x2, k = c(10, 10), b = "tecxcx"), data=dat)
   summary(b)
## plot results ...
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b,se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   vis.scam(b,theta=20,phi=20)
   ## plotting the truth...
   x11()
   x1 \leftarrow seq(min(x1), max(x1), length.out=30)
   x2 \leftarrow seq(min(x2), max(x2), length.out=30)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n) f1[i,j] \leftarrow 2*(x1[i]^2 + x2[j]^2)
   persp(x1, x2, f1, theta = 30, phi = 40)
## End(Not run)
```

smooth.construct.tedecv.smooth.spec

Tensor product smoothing constructor for bivariate function subject to mixed constraints: monotone decreasing constraint wrt the first covariate and concavity wrt the second one

# **Description**

This is a special method function for creating tensor product bivariate smooths subject to mixed constraints, monotone decreasing constraint wrt the first covariate and concavity wrt the second one,

which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths which are represented using the B-spline basis functions. This tensor product is specified by model terms such as  $s(x_1,x_2,k=c(q_1,q_2),b="tedecv",m=c(2,2))$ , where q1 and q2 denote the basis dimensions for the marginal smooths.

#### Usage

```
## S3 method for class 'tedecv.smooth.spec'
smooth.construct(object, data, knots)
```

# **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### Value

An object of class "tedecv.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

#### See Also

```
smooth.construct.tedmd.smooth.spec smooth.construct.temicx.smooth.spec
smooth.construct.tedecx.smooth.spec
```

```
## Not run:
## tensor product `tedecv' example
## simulating data...
set.seed(2)
n <- 30
x1 <- sort(runif(n)*4-1)
x2 <- sort(2*runif(n)-1)</pre>
```

```
f1 <- matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
       { f1[i,j] <- exp(4*x1[i])/(1+exp(4*x1[i]))- 4*x2[j]^2}
   f <- as.vector(t(f1))</pre>
   y <- f+rnorm(length(f))*0.1
   x11 <- matrix(0,n,n)</pre>
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
## fit model ...
   b \leftarrow scam(y \sim s(x1, x2, k = c(10, 10), b = "tedecv", m = 2), data = dat)
## plot results ...
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b, se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   vis.scam(b, theta=30)
   ## plotting the truth...
   x11()
   x1 \leftarrow seq(min(x1), max(x1), length.out=30)
   x2 \leftarrow seq(min(x2), max(x2), length.out=30)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n) f1[i,j] \leftarrow -\exp(4*x1[i])/(1+\exp(4*x1[i])) - 4*x2[j]^2
   persp(x1,x2,f1,theta = 30, phi = 40)
## End(Not run)
```

smooth.construct.tedecx.smooth.spec

Tensor product smoothing constructor for bivariate function subject to mixed constraints: monotone decreasing constraint wrt the first covariate and convexity wrt the second one

# Description

This is a special method function for creating tensor product bivariate smooths subject to mixed constraints, monotone decreasing constraint wrt the first covariate and convexity wrt the second one, which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths which are represented using the B-spline basis functions. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),bs="tedecx",m=c(2,2)), where q1 and q2 denote the basis dimensions for the marginal smooths.

# Usage

```
## S3 method for class 'tedecx.smooth.spec'
smooth.construct(object, data, knots)
```

# **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### Value

An object of class "tedecx.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p.ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

#### See Also

```
smooth.construct.tedmd.smooth.spec smooth.construct.tedecv.smooth.spec
```

```
## Not run:
## tensor product `tedecx' example
 ## simulating data...
   set.seed(2)
   n <- 30
   x1 \leftarrow sort(runif(n)*4-1)
   x2 \leftarrow sort(2*runif(n)-1)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
        f1[i,j] \leftarrow -exp(4*x1[i])/(1+exp(4*x1[i])) + 2*x2[j]^2
   f <- as.vector(t(f1))</pre>
   y <- f+rnorm(length(f))*0.05
   x11 <- matrix(0,n,n)</pre>
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 < - rep(x2,n)
   dat <- list(x1=x11, x2=x22, y=y)
## fit model ...
```

```
b \leftarrow scam(y\sim s(x1,x2,k=c(10,10),b="tedecx",m=2), not.exp=TRUE, data=dat)
## b1 <- scam(y \sim s(x1,bs="mpd",m=2)+s(x2,bs="cx",m=2), data=dat)
## plot results ...
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b, se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   x11()
   vis.scam(b,theta=20,phi=20)
   ## plotting the truth...
   x11()
   x1 \leftarrow seq(min(x1), max(x1), length.out=30)
   x2 \leftarrow seq(min(x2), max(x2), length.out=30)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n) f1[i,j] < -\exp(4*x1[i])/(1+\exp(4*x1[i])) + 2*x2[j]^2
   persp(x1, x2, f1, theta = 30, phi = 40)
## End(Not run)
```

smooth.construct.tedmd.smooth.spec

Tensor product smoothing constructor for bivariate function subject to double monotone decreasing constraint

# **Description**

This is a special method function for creating tensor product bivariate smooths subject to double monotone decreasing constraints which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths which are represented using the B-spline basis functions. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),b="tedmd",m=c(2,2)), where q1 and q2 denote the basis dimensions for the marginal smooths.

From scam version 1.2-15, the sum-to-zero contraint is now applied to all bivariate SCOP-splines after imposing the scop-constraints (including scop identifiability constraint). This simply shifts the smooth vertically, leaving the shape of the smooths unchanged.

#### Usage

```
## S3 method for class 'tedmd.smooth.spec'
smooth.construct(object, data, knots)
```

#### **Arguments**

object	A smooth specification object, generated by an s term in a GAM formula.
data	A data frame or list containing the values of the elements of object\$term, with names given by object\$term.
knots	An optional list containing the knots corresponding to object\$term. If it is NULL then the knot locations are generated automatically.

#### Value

An object of class "tedmd. smooth". In addition to the usual elements of a smooth class documented under smooth. construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parameters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

## Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.tedmi.smooth.spec
```

```
## Not run:
## tensor product `tedmd' example
 ## simulating data...
  require(scam)
  set.seed(2)
  n <- 30
  x1 \leftarrow sort(runif(n)*4-1)
  x2 <- sort(runif(n))</pre>
  f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
       { f1[i,j] <- -exp(4*x1[i])/(1+exp(4*x1[i]))-2*exp(x2[j]-0.5)}
   f <- as.vector(t(f1))</pre>
  y <- f+rnorm(length(f))*0.1
  x11 \leftarrow matrix(0,n,n)
  x11[,1:n] <- x1
  x11 \leftarrow as.vector(t(x11))
  x22 < - rep(x2,n)
  dat <- list(x1=x11,x2=x22,y=y)
## fit model ...
  b < -scam(y \sim s(x1, x2, k = c(10, 10), b = "tedmd"), data=dat)
   summary(b)
## plot results ...
  par(mfrow=c(2,2), mar=c(4,4,2,2))
  plot(b, se=TRUE)
  plot(b,pers=TRUE,theta = 80, phi = 40)
  plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
```

```
## End(Not run)
```

smooth.construct.tedmi.smooth.spec

Tensor product smoothing constructor for bivariate function subject to double monotone increasing constraint

# Description

This is a special method function for creating tensor product bivariate smooths subject to double monotone increasing constraints which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths which are represented using the B-spline basis functions. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),b="tedmi",m=c(2,2)), where q1 and q2 denote the basis dimensions for the marginal smooths.

## Usage

```
## S3 method for class 'tedmi.smooth.spec'
smooth.construct(object, data, knots)
```

#### **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

# Value

An object of class "tedmi.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.tedmd.smooth.spec
```

## **Examples**

```
## Not run:
## tensor product `tedmi' example
  ## simulating data...
   set.seed(1)
   n <- 30
   x1 <- sort(runif(n)*4-1)</pre>
   x2 <- sort(runif(n))</pre>
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
       \{f1[i,j] \leftarrow exp(4*x1[i])/(1+exp(4*x1[i]))+2*exp(x2[j]-0.5)\}
   f <- as.vector(t(f1))</pre>
   y <- f+rnorm(length(f))*0.1
   x11 <- matrix(0,n,n)</pre>
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 < - rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
## fit model ...
   b \leftarrow scam(y^s(x1,x2,k=c(10,10),b="tedmi"), data=dat,optimizer="efs")
## plot results ...
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b, se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
## End(Not run)
```

smooth.construct.temicv.smooth.spec

Tensor product smoothing constructor for bivariate function subject to mixed constraints: monotone increasing constraint wrt the first covariate and concavity wrt the second one

#### **Description**

This is a special method function for creating tensor product bivariate smooths subject to mixed constraints, monotone increasing constraint wrt the first covariate and concavity wrt the second one, which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths which are represented using the B-spline basis functions. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),bs="temicv",m=c(2,2)), where q1 and q2 denote the basis dimensions for the marginal smooths.

#### **Usage**

```
## S3 method for class 'temicv.smooth.spec'
smooth.construct(object, data, knots)
```

## **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### Value

An object of class "temicv.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

#### See Also

```
smooth. construct. tedmd. smooth. spec smooth. construct. temicx. smooth. spec smooth. \\
```

```
x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
## fit model ...
   b <- scam(y \sim s(x1, x2, k = c(10, 10), b = "temicv"), data=dat)
## plot results ...
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b, se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   x11()
   vis.scam(b, theta=30, phi = 40)
   ## plotting the truth...
   x1 \leftarrow seq(min(x1), max(x1), length.out=30)
   x2 \leftarrow seq(min(x2), max(x2), length.out=30)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n) f1[i,j] \leftarrow exp(4*x1[i])/(1+exp(4*x1[i])) - 4*x2[j]^2
   persp(x1,x2,f1,theta = 30, phi = 40)
## End(Not run)
```

smooth.construct.temicx.smooth.spec

Tensor product smoothing constructor for bivariate function subject to mixed constraints: monotone increasing constraint wrt the first covariate and convexity wrt the second one

#### **Description**

This is a special method function for creating tensor product bivariate smooths subject to mixed constraints, monotone increasing constraint wrt the first covariate and convexity wrt the second one, which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths which are represented using the B-spline basis functions. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),bs="temicx",m=c(2,2)), where q1 and q2 denote the basis dimensions for the marginal smooths.

#### Usage

```
## S3 method for class 'temicx.smooth.spec'
smooth.construct(object, data, knots)
```

## **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

A data frame or list containing the values of the elements of object\$term, with names given by object\$term.

Knots An optional list containing the knots corresponding to object\$term. If it is NULL then the knot locations are generated automatically.

#### Value

An object of class "temicx.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parameters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

#### See Also

```
smooth.construct.tedmd.smooth.spec
```

```
## Not run:
## tensor product `temicx' example
  ## simulating data...
   set.seed(1)
   n <- 30
   x1 <- sort(runif(n)*4-1)</pre>
   x2 \leftarrow sort(2*runif(n)-1)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
         f1[i,j] \leftarrow exp(4*x1[i])/(1+exp(4*x1[i])) + 2*x2[j]^2
   f <- as.vector(t(f1))</pre>
   y <- f+rnorm(length(f))*0.1
   x11 \leftarrow matrix(0,n,n)
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 < - rep(x2,n)
   dat <- list(x1=x11, x2=x22, y=y)
## fit model ...
   b \leftarrow scam(y \sim s(x1, x2, k = c(10, 10), b = "temicx", m = 2), data = dat)
## plot results ...
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b, se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   vis.scam(b, theta = 30, phi = 40)
   ## plotting the truth...
   x11()
```

```
x1 <- seq(min(x1),max(x1),length.out=30)
x2 <- seq(min(x2),max(x2),length.out=30)
f1 <- matrix(0,n,n)
for (i in 1:n) for (j in 1:n) f1[i,j] <- exp(4*x1[i])/(1+exp(4*x1[i])) + 2*x2[j]^2
persp(x1,x2,f1,theta = 30, phi = 40)
## End(Not run)</pre>
```

```
smooth.construct.tescv.smooth.spec
```

Tensor product smoothing constructor for a bivariate function concave in the second covariate

# Description

This is a special method function for creating tensor product bivariate smooths concave in the second covariate which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),b="tescv",m=c(2,2)), where the basis for the first marginal smooth is specified in the second element of bs.

#### Usage

```
## S3 method for class 'tescv.smooth.spec'
smooth.construct(object, data, knots)
```

# Arguments

object	A smooth specification object, generated by an s term in a GAM formula.
data	A data frame or list containing the values of the elements of object\$term, with names given by object\$term.
knots	An optional list containing the knots corresponding to object\$term. If it is NULL then the knot locations are generated automatically.

# Value

An object of class "tescv.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parameters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

## Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

#### See Also

```
smooth.construct.temicv.smooth.spec smooth.construct.temicx.smooth.spec
smooth.construct.tedecv.smooth.spec smooth.construct.tedecx.smooth.spec
smooth.construct.tescx.smooth.spec
```

```
## Not run:
## tensor product `tescv' example
  ## simulating data...
   set.seed(5)
   n <- 30
   x1 <- sort(runif(n))</pre>
   x2 \leftarrow sort(2*runif(n)-1)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
         f1[i,j] \leftarrow sin(2*x1[i]) - 4*x2[j]^2
   f1 \leftarrow as.vector(t(f1))
   f \leftarrow (f1-min(f1))/(max(f1)-min(f1))
   y \leftarrow f+rnorm(length(f))*0.1
   x11 <- matrix(0,n,n)</pre>
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11, x2=x22, y=y)
## fit model ...
   b <- scam(y \sim s(x1, x2, k = c(10, 10), b = "tescv", m = 2),
             family=gaussian(), data=dat)
## plot results ...
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b,se=TRUE)
   plot(b,pers=TRUE, theta = 50, phi = 20)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   vis.scam(b, theta = 50, phi = 20)
   ## plotting the truth...
   x11()
   x1 \leftarrow seq(min(x1), max(x1), length.out=30)
   x2 \leftarrow seq(min(x2), max(x2), length.out=30)
   f1 \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n) f1[i,j] <- \sin(2*x1[i]) - 4*x2[j]^2
   persp(x1, x2, f1, theta = 50, phi = 20)
## End(Not run)
```

smooth.construct.tescx.smooth.spec

Tensor product smoothing constructor for a bivariate function convex in the second covariate

# Description

This is a special method function for creating tensor product bivariate smooths convex in the second covariate which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),b="tescx",m=c(2,2)), where the basis for the first marginal smooth is specified in the second element of bs.

#### **Usage**

```
## S3 method for class 'tescx.smooth.spec'
smooth.construct(object, data, knots)
```

#### **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### Value

An object of class "tescx.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p.ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

# Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

# See Also

```
smooth.construct.temicv.smooth.spec smooth.construct.temicx.smooth.spec
smooth.construct.tedecv.smooth.spec smooth.construct.tedecx.smooth.spec
smooth.construct.tescv.smooth.spec
```

# **Examples**

```
## Not run:
## tensor product `tescx' example
  ## simulating data...
   set.seed(2)
   n <- 30
   x1 <- sort(runif(n))</pre>
   x2 \leftarrow sort(2*runif(n)-1)
   f1 <- matrix(0,n,n)</pre>
   for (i in 1:n) for (j in 1:n)
        f1[i,j] \leftarrow sin(x1[i]) + 2*x2[j]^2
   f1 \leftarrow as.vector(t(f1))
   f \leftarrow (f1-min(f1))/(max(f1)-min(f1))
   y <- f+rnorm(length(f))*0.1
   x11 \leftarrow matrix(0,n,n)
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
   ## fit model \dots
   b <- scam(y \sim s(x1, x2, k = c(10, 10), b = "tescx", m = 2),
             family=gaussian(), data=dat)
   ## plot results ...
   par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b, se=TRUE)
   plot(b,pers=TRUE, theta = 50, phi = 20)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   x11()
   vis.scam(b, theta = 50, phi = 20)
   ## plotting the truth...
   x1 \leftarrow seq(min(x1), max(x1), length.out=30)
   x2 <- seq(min(x2), max(x2), length.out=30)</pre>
   f1 <- matrix(0,n,n)
   for (i in 1:n) for (j in 1:n) f1[i,j] \leftarrow sin(x1[i]) + 2*x2[j]^2
   persp(x1,x2,f1,theta = 50, phi = 20)
## End(Not run)
```

smooth.construct.tesmd1.smooth.spec

Tensor product smoothing constructor for a bivariate function monotone decreasing in the first covariate

#### **Description**

This is a special method function for creating tensor product bivariate smooths monotone decreasing in the first covariate which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),b="tesmd1",m=2). The default basis for the second marginal smooth is P-spline. Cyclic cubic regression spline ("cc") is implemented in addition to the P-spline. See an example below on how to call for it.

#### Usage

```
## S3 method for class 'tesmd1.smooth.spec'
smooth.construct(object, data, knots)
```

## **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### Value

An object of class "tesmd1.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

margin.bs A two letter character string indicating the (penalized) smoothing basis to use

for the second unconstrained marginal smooth. (eg "ps" for P-splines).

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.tesmd2.smooth.spec
```

```
## Not run:
## tensor product `tesmd1' example
  ## simulating data...
  require(scam)
   set.seed(2)
   n <- 30
   x1 <- sort(runif(n)*4-1); x2 <- sort(runif(n))</pre>
   f \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
        f[i,j] \leftarrow -\exp(4*x1[i])/(1+\exp(4*x1[i]))+2*\sin(pi*x2[j])
   f <- as.vector(t(f))</pre>
   y <- f+rnorm(length(f))*.2</pre>
   x11 \leftarrow matrix(0,n,n)
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
  x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
## fit model ...
  b \leftarrow scam(y\sim s(x1,x2,bs="tesmd1",k=10),data=dat)
## plot results ...
   old.par <- par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b,se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   par(old.par)
   vis.scam(b,theta=40,phi=20)
## example with cyclic cubic regression spline along the second covariate...
   set.seed(2)
  n <- 30
   x1 \leftarrow sort(runif(n)*4-1); x2 \leftarrow sort(runif(n))
   f \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
        f[i,j] \leftarrow -\exp(4*x1[i])/(1+\exp(4*x1[i]))+\sin(2*pi*x2[j])
   f <- as.vector(t(f))</pre>
   y <- f+rnorm(length(f))*.2
   x11 \leftarrow matrix(0,n,n)
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 < - rep(x2,n)
  dat <- list(x1=x11, x2=x22, y=y)
## fit model ...
   b1 \leftarrow scam(y\sim s(x1,x2,bs="tesmd1",xt=list("cc"),k=10), data=dat)
## plot results ...
   old.par <- par(mfrow=c(2,2))
   plot(b1,se=TRUE)
   plot(b1,pers=TRUE,theta = 30, phi = 40)
   plot(y,b1$fitted.values,xlab="Simulated data",ylab="Fitted data")
   par(old.par)
   vis.scam(b1,theta=40,phi=20)
```

```
## End(Not run)
```

smooth.construct.tesmd2.smooth.spec

Tensor product smoothing constructor for a bivariate function monotone decreasing in the second covariate

#### **Description**

This is a special method function for creating tensor product bivariate smooths monotone decreasing in the second covariate which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),b="tesmd2",m=c(2,2)). The default basis for the first marginal smooth is P-spline. Cyclic cubic regression spline ("cc") is implemented in addition to the P-spline. See an example below on how to call for it.

# Usage

```
## S3 method for class 'tesmd2.smooth.spec'
smooth.construct(object, data, knots)
```

## **Arguments**

object	A smooth specification object, generated by an s term in a GAM formula.
data	A data frame or list containing the values of the elements of object\$term, with names given by object\$term.
knots	An optional list containing the knots corresponding to object\$term. If it is NULL then the knot locations are generated automatically.

#### Value

An object of class "tesmd2.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p.ident A vector of 0's and 1's for model parameter identification: 1's indicate parameters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

margin.bs A two letter character string indicating the (penalized) smoothing basis to use

for the first unconstrained marginal smooth. (eg "ps" for P-splines).

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.tesmd1.smooth.spec
```

```
## Not run:
## tensor product `tesmd2' example
  ## simulating data...
   require(scam)
   set.seed(2)
   n <- 30
   x1 \leftarrow sort(runif(n)); x2 \leftarrow sort(runif(n)*4-1)
   f \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
        f[i,j] \leftarrow 2*sin(pi*x1[i])-exp(4*x2[j])/(1+exp(4*x2[j]))
   f <- as.vector(t(f))</pre>
   y <- f+rnorm(length(f))*.2</pre>
   x11 \leftarrow matrix(0,n,n)
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 < - rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
## fit model ...
   b \leftarrow scam(y\sim s(x1,x2,bs="tesmd2",k=10),data=dat)
## plot results ...
   old.par <- par(mfrow=c(2,2), mar=c(4,4,2,2))
   plot(b,se=TRUE)
   plot(b, scheme=1, theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   par(old.par)
   vis.scam(b, theta = 40, phi = 20)
## example with cyclic cubic regression spline along the 1st covariate...
   set.seed(4)
   n <- 30
   x1 <- sort(runif(n)); x2 <- sort(runif(n)*4-1)</pre>
   f \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
        f[i,j] \leftarrow \sin(2*pi*x1[i]) - \exp(4*x2[j])/(1+\exp(4*x2[j]))
   f <- as.vector(t(f))
   y <- f+rnorm(length(f))*.2
   x11 <- matrix(0,n,n)</pre>
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
```

```
x22 <- rep(x2,n)
dat <- list(x1=x11,x2=x22,y=y)
## fit model ...
b1 <- scam(y~s(x1,x2,bs="tesmd2",xt=list("cc"),k=10), data=dat)
## plot results ...
old.par <-par(mfrow=c(2,2))
plot(b1,se=TRUE)
plot(b1,scheme=1,theta = 30, phi = 40)
plot(y,b1$fitted.values,xlab="Simulated data",ylab="Fitted data")
par(old.par)
vis.scam(b1,theta=40,phi=20)
## End(Not run)</pre>
```

smooth.construct.tesmi1.smooth.spec

Tensor product smoothing constructor for a bivariate function monotone increasing in the first covariate

#### **Description**

This is a special method function for creating tensor product bivariate smooths monotone increasing in the first covariate which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),b="tesmi1",m=2). The basis for the second marginal smooth can be specified as a two letter character string of the argument xt (eg xt="cc" to specify cyclic cubic regression spline). See example below. The default basis for the second marginal smooth is P-spline. Cyclic cubic regression spline ("cc") is implemented in addition to the P-spline. See an example below on how to call for it.

# Usage

```
## S3 method for class 'tesmi1.smooth.spec'
smooth.construct(object, data, knots)
```

# **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

A data frame or list containing the values of the elements of object\$term, with names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

# Value

An object of class "tesmi1.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p.ident	A vector of 0's and 1's for model parameter identification: 1's indicate parameters which will be exponentiated, 0's - otherwise.
Zc	A matrix of identifiability constraints.
margin.bs	A two letter character string indicating the (penalized) smoothing basis to use for the second unconstrained marginal smooth. (eg "cc" for cyclic cubic regression spline).

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

```
smooth.construct.tesmi2.smooth.spec
```

```
## Not run:
## tensor product `tesmi1' example...
  ## simulating data...
   require(scam)
   set.seed(2)
   n <- 30
   x1 <- sort(runif(n)*4-1)</pre>
   x2 <- sort(runif(n))</pre>
   f \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
        f[i,j] \leftarrow \exp(4*x1[i])/(1+\exp(4*x1[i]))+2*\sin(pi*x2[j])
   f <- as.vector(t(f))</pre>
   y <- f+rnorm(length(f))*.3</pre>
   x11 <- matrix(0,n,n)</pre>
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 < - rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)</pre>
## fit model ...
   b <- scam(y \le (x1, x2, bs = "tesmi1", k = c(10, 10)), data = dat)
## plot results ...
   old.par<- par(mfrow=c(2,2))
   plot(b,se=TRUE)
   plot(b,pers=TRUE,theta = 30, phi = 40)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   par(old.par)
   vis.scam(b,theta=40,phi=20)
```

```
## example with cyclic cubic regression spline along the second covariate...
   set.seed(2)
   n <- 30
   x1 <- sort(runif(n)*4-1)</pre>
   x2 <- sort(runif(n))</pre>
   f \leftarrow matrix(0,n,n)
   for (i in 1:n) for (j in 1:n)
        f[i,j] \leftarrow \exp(4*x1[i])/(1+\exp(4*x1[i]))+\sin(2*pi*x2[j])
   f <- as.vector(t(f))</pre>
   y <- f+rnorm(length(f))*.2
   x11 \leftarrow matrix(0,n,n)
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11,x2=x22,y=y)
## fit model ...
   b1 \leftarrow scam(y\sim s(x1,x2,bs="tesmi1",xt=list("cc"),k=10), data=dat)
## plot results ...
   old.par<- par(mfrow=c(2,2))
   plot(b1, se=TRUE)
   plot(b1,pers=TRUE,theta = 30, phi = 40)
   plot(y,b1$fitted.values,xlab="Simulated data",ylab="Fitted data")
   par(old.par)
   vis.scam(b1,theta=40,phi=20)
## End(Not run)
```

smooth.construct.tesmi2.smooth.spec

Tensor product smoothing constructor for a bivariate function monotone increasing in the second covariate

# Description

This is a special method function for creating tensor product bivariate smooths monotone increasing in the second covariate which is built by the mgcv constructor function for smooth terms, smooth.construct. It is constructed from a pair of single penalty marginal smooths. This tensor product is specified by model terms such as s(x1,x2,k=c(q1,q2),b="tesmi2",m=c(2,2)). The default basis for the first marginal smooth is P-spline. Cyclic cubic regression spline ("cc") is implemented in addition to the P-spline. See an example below on how to call for it.

# Usage

```
## S3 method for class 'tesmi2.smooth.spec'
smooth.construct(object, data, knots)
```

## Arguments

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### Value

An object of class "tesmi2.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

margin.bs A two letter character string indicating the (penalized) smoothing basis to use

for the first unconstrained marginal smooth. (eg "cc" for cyclic cubic regression

spline).

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

# See Also

```
smooth.construct.tesmi1.smooth.spec
```

```
x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 \leftarrow rep(x2,n)
   dat <- list(x1=x11, x2=x22, y=y)
## fit model ...
   b \leftarrow scam(y \sim s(x1, x2, bs = "tesmi2", k = c(10, 10)), data = dat)
## plot results ...
   old.par <- par(mfrow=c(2,2),mar=c(4,4,2,2))
   plot(b, se=TRUE)
   plot(b,pers=TRUE, theta = 50, phi = 20)
   plot(y,b$fitted.values,xlab="Simulated data",ylab="Fitted data")
   par(old.par)
   vis.scam(b,theta=50,phi=20)
## example with cyclic cubic regression spline along the 1st covariate...
   set.seed(2)
   n <- 30
   x1 <- sort(runif(n)); x2 <- sort(runif(n)*4-1)</pre>
   f <- matrix(0,n,n)</pre>
   for (i in 1:n) for (j in 1:n)
        f[i,j] \leftarrow \sin(2*pi*x1[i]) + \exp(4*x2[j])/(1+exp(4*x2[j]))
   f <- as.vector(t(f))</pre>
   y <- f+rnorm(length(f))*.3</pre>
   x11 \leftarrow matrix(0,n,n)
   x11[,1:n] <- x1
   x11 \leftarrow as.vector(t(x11))
   x22 < - rep(x2,n)
   dat <- list(x1=x11, x2=x22, y=y)
## fit model ...
   b1 <- scam(y\sim s(x1,x2,bs="tesmi2",xt=list("cc"),k=10), data=dat)
## plot results ...
   old.par <- par(mfrow=c(2,2))
   plot(b1,se=TRUE)
   plot(b1,pers=TRUE,theta = 50, phi = 20)
   plot(y,b1$fitted.values,xlab="Simulated data",ylab="Fitted data")
   par(old.par)
   vis.scam(b1,theta=40,phi=20)
## End(Not run)
```

smooth.construct.tismd.smooth.spec

Tensor product interaction with decreasing constraint along the first covariate and unconstrained along the second covariate

#### **Description**

This is a special method function for creating tensor product bivariate interaction smooths with decreasing constraint in the first covariate, appropriate when the main effects (and any lower interactions) are also present. It is built by the mgcv constructor function for smooth terms, smooth.construct,

and constructed from a pair of single penalty marginal smooths. This tensor product is specified by model terms such as  $s(x_1, x_2, k=c(q_1, q_2), b="tismd")$ . See example below.

#### Usage

```
## S3 method for class 'tismd.smooth.spec'
smooth.construct(object, data, knots)
```

#### **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### **Details**

In some cases, it is helpful to consider models with a main-effects + interactions structure, for example,

$$f_1(x) + f_2(z) + f_3(x,z)$$

where  $f_1$  and  $f_2$  are smooth 'main effects' and  $f_3$  is a smooth 'interaction' subject to decreasing constraint wrt x ( $f_1$  can be subject to decreasing constraint).

Constructing such functional ANOVA decomposition recognises the fact that the tensor produc basis construction is exactly the same as the construction used for any interaction in a linear model. tismd produce tensor product interactions with decreasing constraint along the first covariate from which the main effects have been excluded, under the assumption that they will be included separately. For example, the  $\sim s(x) + s(z) + s(x,z,bs="tismd")$  would produce the above main effects + interaction structure. Specifically, the marginal smooths of a tensor product, tismd, are subject to identifiability constraints before constructing the tensor product basis. This results in the interaction smooths that do not include the corresponding main effects. tismd apply SCOP identifiability constraints to the first marginal and sum-to-zero constraints to the second unconstrained marginal. See Wood (2017, section 5.6.3) for ANOVA decompositions of unconstrained smooths.

#### Value

An object of class "tismd.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

margin.bs A two letter character string indicating the (penalized) smoothing basis to use for

the second unconstrained marginal smooth. (eg "cc" for cyclic cubic regression

spline).

# Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Wood S.N. (2017) Generalized Additive Models: An Introduction with R (2nd edition). Chapman and Hall/CRC Press.

#### See Also

```
smooth.construct.tesmd1.smooth.spec
smooth.construct.tismi.smooth.spec
```

```
## Not run:
## tensor product `tismd' example...
  ## simulating data...
require(scam)
test <- function(x,z){
  -\exp(4*x)/(1+\exp(4*x))-2*\sin(pi*z)-(x+1)^0.6*z
set.seed(7)
n <- 600
x <- runif(n)*4-1
z <- runif(n)</pre>
xs \leftarrow seq(-1,3,length=30); zs \leftarrow seq(0,1,length=30)
pr \leftarrow data.frame(x=rep(xs,30),z=rep(zs,rep(30,30)))
truth <- matrix(test(pr$x,pr$z),30,30)</pre>
f \leftarrow test(x,z)
y < -f + rnorm(n)*0.3
bi <- scam(y^{-}ti(x)+ti(z)+s(x,z,bs="tismd"))
summary(bi)
old.par <- par(mfrow=c(2,2))</pre>
persp(xs,zs,truth);title("truth")
vis.scam(bi);title("tismd")
## fitting with "tesmd1" instead...
bc <- scam(y\sim s(x,z,bs="tesmd1"))
vis.scam(bc);title("tesmd1")
par(old.par)
plot(bi,pages=1,scheme=2)
plot(bi, select=3, scheme=1, zlim=c(-3,3))
## End(Not run)
```

smooth.construct.tismi.smooth.spec

Tensor product interaction with increasing constraint along the first covariate and unconstrained along the second covariate

# **Description**

This is a special method function for creating tensor product bivariate interaction smooths with increasing constraint in the first covariate, appropriate when the main effects (and any lower interactions) are also present. It is built by the mgcv constructor function for smooth terms, smooth.construct, and constructed from a pair of single penalty marginal smooths. This tensor product is specified by model terms such as s(x1, x2, k=c(q1, q2), b="tismi"). See example below.

## Usage

```
## S3 method for class 'tismi.smooth.spec'
smooth.construct(object, data, knots)
```

#### **Arguments**

object A smooth specification object, generated by an s term in a GAM formula.

data A data frame or list containing the values of the elements of object\$term, with

names given by object\$term.

knots An optional list containing the knots corresponding to object\$term. If it is

NULL then the knot locations are generated automatically.

#### **Details**

In some cases, it is helpful to consider models with a main-effects + interactions structure, for example,

$$f_1(x) + f_2(z) + f_3(x,z)$$

where  $f_1$  and  $f_2$  are smooth 'main effects' and  $f_3$  is a smooth 'interaction' subject to increasing constraint wrt x ( $f_1$  can be subject to increasing constraint).

Constructing such functional ANOVA decomposition recognises the fact that the tensor produc basis construction is exactly the same as the construction used for any interaction in a linear model. tismi produce tensor product interactions with increasing constraint along the first covariate from which the main effects have been excluded, under the assumption that they will be included separately. For example, the  $\sim s(x) + s(z) + s(x,z,bs="tismi")$  would produce the above main effects + interaction structure. Specifically, the marginal smooths of a tensor product, tismi, are subject to identifiability constraints before constructing the tensor product basis. This results in the interaction smooths that do not include the corresponding main effects. tismi apply SCOP identifiability constraints to the first marginal and sum-to-zero constraints to the second unconstrained marginal. See Wood (2017, section 5.6.3) for ANOVA decompositions of unconstrained smooths.

#### Value

An object of class "tismi.smooth". In addition to the usual elements of a smooth class documented under smooth.construct of the mgcv library, this object contains:

p. ident A vector of 0's and 1's for model parameter identification: 1's indicate parame-

ters which will be exponentiated, 0's - otherwise.

Zc A matrix of identifiability constraints.

margin.bs A two letter character string indicating the (penalized) smoothing basis to use for

the second unconstrained marginal smooth. (eg "cc" for cyclic cubic regression

spline).

#### Author(s)

Natalya Pya <nat.pya@gmail.com>

#### References

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Wood S.N. (2017) Generalized Additive Models: An Introduction with R (2nd edition). Chapman and Hall/CRC Press

#### See Also

```
smooth.construct.tismd.smooth.spec
smooth.construct.tesmi1.smooth.spec
```

```
## Not run:
## tensor product `tismi' example...
require(scam)
test <- function(x,z){</pre>
  \exp(4*x)/(1+\exp(4*x))+2*\sin(pi*z)+(x+1)^0.6*z
set.seed(7)
n <- 600
x \leftarrow runif(n)*4-1
z <- runif(n)</pre>
xs \leftarrow seq(-1,3,length=30); zs \leftarrow seq(0,1,length=30)
pr <- data.frame(x=rep(xs,30),z=rep(zs,rep(30,30)))</pre>
truth <- matrix(test(pr$x,pr$z),30,30)</pre>
f \leftarrow test(x,z)
y < -f + rnorm(n)*0.3
bi <- scam(y^* ti(x)+ti(z)+ s(x,z,bs="tismi"))
summary(bi)
old.par <- par(mfrow=c(2,2))</pre>
persp(xs,zs,truth);title("truth")
vis.scam(bi);title("tismi")
```

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```
## fitting with "tesmi1"...
bc <- scam(y~s(x,z,bs="tesmi1"))
vis.scam(bc);title("tesmi1")
par(old.par)

plot(bi,pages=1,scheme=2)
plot(bi,select=3,scheme=1,zlim=c(-5,5))

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

summary.scam

Summary for a SCAM fit

# Description

Takes a fitted scam object produced by scam() and produces various useful summaries from it. The same code as in summary.gam of the mgcv package is used here with slight modifications to accept the exponentiated parameters of the shape constrained smooth terms and the corresponding covariance matrix.

# Usage

# **Arguments**

object	a fitted scam object as produced by scam().
X	a summary.scam object produced by summary.scam().
dispersion	A known dispersion parameter. NULL to use estimate or default (e.g. $1$ for Poisson).
freq	By default p-values for individual terms are calculated using the Bayesian estimated covariance matrix of the parameter estimators. If this is set to TRUE then the frequentist covariance matrix of the parameters is used instead.
digits	controls number of digits printed in output.
signif.stars	Should significance stars be printed alongside output.

other arguments.

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#### Value

summary.scam produces the same list of summary information for a fitted scam object as in the unconstrained case summary.gam except for the last element BFGS termination condition.

p.coeff is an array of estimates of the strictly parametric model coefficients.

p.t is an array of the p.coeff's divided by their standard errors.

p.pv is an array of p-values for the null hypothesis that the corresponding parameter

is zero. Calculated with reference to the t distribution with the estimated residual degrees of freedom for the model fit if the dispersion parameter has been

estimated, and the standard normal if not.

m The number of smooth terms in the model.

chi.sq An array of test statistics for assessing the significance of model smooth terms.

See details.

s.pv An array of approximate p-values for the null hypotheses that each smooth term

is zero. Be warned, these are only approximate.

se array of standard error estimates for all parameter estimates.

r.sq The adjusted r-squared for the model. Defined as the proportion of variance

explained, where original variance and residual variance are both estimated using unbiased estimators. This quantity can be negative if your model is worse than a one parameter constant model, and can be higher for the smaller of two nested models! Note that proportion null deviance explained is probably more

appropriate for non-normal errors.

dev.expl The proportion of the null deviance explained by the model. edf array of estimated degrees of freedom for the model terms.

residual.df estimated residual degrees of freedom.

n number of data.

gcv minimized GCV score for the model, if GCV used.

ubre minimized UBRE score for the model, if UBRE used.

scale estimated (or given) scale parameter.

family the family used.

formula the original scam formula.

dispersion the scale parameter.

pTerms.df the degrees of freedom associated with each parameteric term (excluding the

constant).

pTerms.chi.sq a Wald statistic for testing the null hypothesis that the each parametric term is

zero.

pTerms.pv p-values associated with the tests that each term is zero. For penalized fits these

are approximate. The reference distribution is an appropriate chi-squared when

the scale parameter is known, and is based on an F when it is not.

cov.unscaled The estimated covariance matrix of the parameters (or estimators if freq=TRUE),

divided by scale parameter.

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The estimated covariance matrix of the parameters (estimators if freq=TRUE). cov.scaled significance table for parameters p.table s.table significance table for smooths pTerms.table significance table for parametric model terms BFGS termination condition

> the value of the maximum component of the scaled GCV/UBRE gradient used as stopping condition. This value is printed if the termination code of the BFGS optimization process is not '1' (not full convergence) (see bfgs\_gcv.ubrefor

details)

#### WARNING

The p-values are approximate.

## Author(s)

Natalya Pya <nat.pya@gmail.com> based on mgcv by Simon Wood

#### References

Wood S.N. (2006) Generalized Additive Models: An Introduction with R. Chapman and Hall/CRC Press.

Pya, N. and Wood, S.N. (2015) Shape constrained additive models. Statistics and Computing, 25(3), 543-559

Pya, N. (2010) Additive models with shape constraints. PhD thesis. University of Bath. Department of Mathematical Sciences

#### See Also

scam

```
## Not run:
## simulating data...
require(scam)
n <- 200
set.seed(1)
x1 <- runif(n)*6-3
f1 <- 3*exp(-x1^2) # unconstrained smooth term
x2 <- runif(n)*4-1;</pre>
f2 \leftarrow \exp(4*x2)/(1+\exp(4*x2)) # monotone increasing smooth
x3 <- runif(n)*5;
f3 < -\log(x3)/5 # monotone decreasing smooth
f <- f1+f2+f3
y \leftarrow f + rnorm(n)*.3
dat <- data.frame(x1=x1, x2=x2, x3=x3, y=y)
## fit model ...
b < -scam(y \sim s(x1, k=15, bs="cr", m=2) + s(x2, k=30, bs="mpi", m=2) + s(x3, k=30, bs="mpd", m=2),
```

vis.scam

```
data=dat)
summary(b)
plot(b,pages=1,shade=TRUE)
## End(Not run)
```

vis.scam

Visualization of SCAM objects

# **Description**

Produces perspective or contour plot views of scam model predictions. The code is a clone of vis.gam of the mgcv package.

# Usage

# **Arguments**

The documentation below is the same as in documentation object vis.gam.

X	a scam object, produced by scam()
view	an array containing the names of the two main effect terms to be displayed on the x and y dimensions of the plot. If omitted the first two suitable terms will be used.
cond	a named list of the values to use for the other predictor terms (not in view). Variables omitted from this list will have the closest observed value to the median for continuous variables, or the most commonly occuring level for factors. Parametric matrix variables have all the entries in each column set to the observed column entry closest to the column median.
n.grid	The number of grid nodes in each direction used for calculating the plotted surface.
too.far	plot grid nodes that are too far from the points defined by the variables given in view can be excluded from the plot. too.far determines what is too far. The grid is scaled into the unit square along with the view variables and then grid nodes more than too.far from the predictor variables are excluded.
col	The colours for the facets of the plot. If this is NA then if se>0 the facets are transparent, otherwise the colour scheme specified in color is used. If col is not NA then it is used as the facet colour.
color	the colour scheme to use for plots when se<=0. One of "topo", "heat", "cm", "terrain", "gray" or "bw". Schemes "gray" and "bw" also modify the colors used when se>0.

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sets the colour of contours when using plot.type="contour". Default scheme contour.col used if NULL. if less than or equal to zero then only the predicted surface is plotted, but if se greater than zero, then 3 surfaces are plotted, one at the predicted values minus se standard errors, one at the predicted values and one at the predicted values plus se standard errors. "link" to plot on linear predictor scale and "response" to plot on the response type plot.type one of "contour" or "persp". zlim a two item array giving the lower and upper limits for the z-axis scale. NULL to choose automatically. The number of colors to use in color schemes. nCo1 other options to pass on to persp, image or contour. . . .

#### Value

Simply produces a plot.

# Author(s)

Simon Wood <simon.wood@r-project.org>

#### See Also

```
persp, vis.gam, and scam.
```

```
library(scam)
# Example with factor variable
set.seed(0)
fac<-rep(1:4,20)
x <- runif(80)*5;
y < - fac + log(x)/5 + rnorm(80) * 0.1
fac <- factor(fac)</pre>
b <- scam(y~fac+s(x,bs="mpi"))</pre>
vis.scam(b,theta=-35,color="heat") # factor example
# Example with "by" variable
z<-rnorm(80)*0.4
y<-as.numeric(fac)+log(x)*z+rnorm(80)*0.1
b < -scam(y - fac + s(x, by = z))
g \leftarrow gam(y^fac+s(x,by=z))
vis.scam(b,theta=-35,color="terrain",cond=list(z=1)) # by variable example
vis.scam(b,view=c("z","x"),theta= 65) # plot against by variable
```

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```
## compare with gam(mgcv)...
vis.gam(g,theta=-35,color="terrain",cond=list(z=1)) # by variable example
vis.gam(g,view=c("z","x"),theta= 65) # plot against by variable
## all three smooths are increasing...
set.seed(2)
n <- 400
x <- runif(n, 0, 1)
f1 < - \log(x *5)
f2 \leftarrow exp(2 * x) - 4
f3 <- 5* sin(x)
e <- rnorm(n, 0, 2)
fac <- as.factor(sample(1:3,n,replace=TRUE))</pre>
fac.1 <- as.numeric(fac==1)</pre>
fac.2 <- as.numeric(fac==2)</pre>
fac.3 <- as.numeric(fac==3)</pre>
y <- f1*fac.1 + f2*fac.2 + f3*fac.3 + e
dat \leftarrow data.frame(y=y,x=x,fac=fac,f1=f1,f2=f2,f3=f3)
b1 <- scam(y ~ s(x,by=fac,bs="mpi"),data=dat,optimizer="efs")
plot(b1,pages=1,scale=0,shade=TRUE)
summary(b1)
vis.scam(b1,theta=-40,color="terrain",cond=list(z=1))
## note that the preceding, b1, fit is the same as....
b2 \leftarrow scam(y \sim s(x,by=as.numeric(fac==1),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==2),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.numeric(fac==3),bs="mpi")+s(x,by=as.nume
          s(x,by=as.numeric(fac==3),bs="mpi"),data=dat,optimizer="efs")
summary(b2)
## Note that as in gam() when using factor 'by' variables, centering
## constraints are applied to the smooths, which usually means that the 'by'
## variable should be included as a parametric term, as well.
## The difference with scam() is that here a 'zero intercept' constraint is
## applied in place of 'centering' (although scam's fitted smooths are centred for plotting).
## compare with the gam() fits..
g1 \leftarrow gam(y \sim fac+s(x,by=fac),data=dat)
g2 \leftarrow gam(y \sim s(x,by=fac),data=dat)
summary(g1)
summary(g2)
plot(g1,pages=1,scale=0,shade=TRUE)
```

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