# Package 'SOP'

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Maintainer Maria Xose Rodriguez-Alvarez <mxrodriguez@uvigo.gal></mxrodriguez@uvigo.gal>
<b>Description</b> Generalised additive P-spline regression models estimation using the separation of overlapping precision matrices (SOP) method. Estimation is based on the equivalence between P-splines and linear mixed models, and variance/smoothing parameters are estimated based on restricted maximum likelihood (REML). The package enables users to estimate P-spline models with overlapping penalties. Based on the work described in Rodriguez-Alvarez et al. (2015) <doi:10.1007 s11222-014-9464-2="">; Rodriguez-Alvarez et al. (2019) <doi:10.1007 s11222-018-9818-2="">, and Eilers and Marx (1996) <doi:10.1214 1038425655="" ss="">.</doi:10.1214></doi:10.1007></doi:10.1007>
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Author Maria Xose Rodriguez-Alvarez [aut, cre] (ORCID:
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Contents
SOP-package          ad          f

SOP-package

	plot.sop						 								 					6
	predict.sop														 					8
	print.sop						 								 					11
	rae														 					12
	sop														 					13
	sop.control .						 								 					16
	sop.fit						 								 	 				18
	summary.sop						 								 					20
Index																				22

SOP-package

Generalised Additive P-Spline Regression Models Estimation

## **Description**

Generalised additive P-spline regression models estimation using the separation of overlapping precision matrices (SOP) method. Estimation is based on the equivalence between P-splines and linear mixed models, and variance/smoothing parameters are estimated based on restricted maximum likelihood (REML). The package enables users to estimate P-spline models with overlapping penalties. Based on the work described in Rodriguez-Alvarez et al. (2015) <doi:10.1007/s11222-014-9464-2>; Rodriguez-Alvarez et al. (2019) <doi:10.1007/s11222-018-9818-2>, and Eilers and Marx (1996) <doi:10.1214/ss/1038425655>.

## **Details**

Index of help topics:

SOP-package	Generalised Additive P-Spline Regression Models
	Estimation
ad	Adaptive smooth terms in a SOP model formula
f	Defining smooth terms in SOP formulae
plot.sop	Default SOP plotting
predict.sop	Prediction from a fitted SOP model
print.sop	Print method for sop objects
rae	Defining random effects in SOP formula
sop	Estimation of generalised additive P-spline
	regression models with overlapping penalties.
sop.control	Function for controlling SOP fitting
sop.fit	Fitting generalised linear mixed models with
	overlapping precision matrices.
summary.sop	Summary method for a fitted SOP model.

This package incorporates the function sop() which enables users to estimate multidimensional generalised P-spline regression models with overlapping penalties. For a complete list of functions use library(help = SOP).

ad 3

#### Author(s)

NA

Maintainer: Maria Xose Rodriguez-Alvarez <mxrodriguez@uvigo.gal>

#### References

Eilers, P.H.C. and Marx, B.D. (1996). Flexible smoothing with B-splines and penalties. *Statistical Science*, **11** (2), 89–121.

Rodriguez-Alvarez, M.X., Lee, D. J., Kneib, T., Durban, M., and Eilers, P. (2015). Fast smoothing parameter separation in multidimensional generalized P-splines: the SAP algorithm. *Statistics and Computing*, **25** (5), 941–957.

Rodriguez-Alvarez, M.X., Durban, M., Lee, D. J. and Eilers, P. (2019). On the estimation of variance parameters in non-standard generalised linear mixed models: application to penalised smoothing. *Statistics and Computing*, **29** (3), 483–500.

ad

Adaptive smooth terms in a SOP model formula

## Description

Auxiliary function used to define adaptive smooth terms in a sop model formula. The function does not do any fitting but is used as part of a sop() model formula.

## Usage

```
ad(..., nseg = 10, pord = 2, degree = 3, nseg.sp = 5, degree.sp = 3)
```

#### **Arguments**

•••	the x-variable (continuous) to be used for adaptive smoothing. Currently, only one dimensional adaptive smoothers are allowed.
nseg	the number of segments for the B-spline basis used to represent the smooth term. The default value is 10.
pord	penalty order. The defauly value is 2 (second order penalty).
degree	the order of the polynomial for the B-spline basis for this term. The default value is 3 (cubic B-splines).
nseg.sp	the number of segments for the B-spline basis used to 'smooth' the smoothing parameters. The default value is 5.
degree.sp	the order of the polynomial for the B-spline basis used for smoothing of the smoothing parameters. The default value is 3 (cubic B-splines).

## **Details**

The function ad() can be use to fit an adaptive smooth function of x. An 'adaptive' smooth function is one in which the smoothing parameter is allowed to vary over the range of the explanatory variable x. Details can be found in Rodriguez-Alvarez *at. al* (2019).

4 ad

#### Value

The function is interpreted in the formula of a sop model and creates the right framework for fitting the adaptive smoother. List containing the following objects:

vars name of the covariates involved in the adaptive smooth term.

nseg the number of segments for the B-spline basis.

pord the penalty order.

degree the order of the polynomial for the B-Spline basis for this term.

nseg.sp the number of segments for the B-spline basis used to 'smooth' the smoothing

parameters.

degree.sp the order of the polynomial for the B-spline basis used for smoothing of the

smoothing parameters.

dim The dimension of the smoother - i.e. the number of covariates that it is a function

of.

label labels terms.

#### References

Rodriguez-Alvarez, M.X., Durban, M., Lee, D. J. and Eilers, P. (2019). On the estimation of variance parameters in non-standard generalised linear mixed models: application to penalised smoothing. *Statistics and Computing*, **29** (3), 483–500.

#### See Also

```
f, rae, sop
```

```
library(SOP)
# Simulate the data
set.seed(123)
n <- 1000
x <- runif(n, 0.0001, 1)
doppler.function <- function(x) sin(4 / (x + 0.1)) + 1.5
mu <- doppler.function(x)</pre>
sigma <- 0.2
y <- mu + sigma*rnorm(n)</pre>
dat <- data.frame(x = x, y = y)
# Fit the models
# With addaptive smoothing
m0 \leftarrow sop(formula = y \sim ad(x, nseg = 197, nseg.sp = 17), data = dat,
         control = list(trace = FALSE, epsilon = 1e-03))
# Without addaptive smoothing
m1 \leftarrow sop(formula = y \sim f(x, nseg = 197), data = dat,
         control = list(trace = FALSE, epsilon = 1e-03))
# Plot results
```

f 5

```
plot(y ~ x, data = dat)
ox <- order(dat$x)
lines(fitted(m0)[ox] ~ dat$x[ox], col = 2, lwd = 2)
lines(fitted(m1)[ox] ~ dat$x[ox], col = 4, lwd = 2)
legend("topright", c("Theoretical", "Adaptive", "Non Adaptive"),
      col = c(1,2,4), lty = 1, lwd = 2, bty = "n")</pre>
```

f

Defining smooth terms in SOP formulae

## Description

Auxiliary function used to define smooth terms within sop() model formulae. The function does not evaluate the smooth - it exists purely to help set up a model using P-spline based smoothers.

## Usage

```
f(..., nseg = 10, pord = 2, degree = 3)
```

## **Arguments**

... a list of up to three variables to construct the smooth term.

nseg the number of segments for the (marginal) B-spline bases used to represent the

smooth term. Numerical vector of length equal to the number of covariates.

Atomic values are also valid, being recycled. The default value is 10.

pord penalty order. Numerical vector of length equal to the number of covariates.

Atomic values are also valid, being recycled. The default value is 2 (second-

order penalty).

degree the order of the polynomial for the (marginal) B-spline bases for this term. Nu-

merical vector of length equal to the number of covariates. Atomic values are

also valid, being recycled. The default value is 3 (cubic B-splines).

#### **Details**

The functions f() is designed to represent either a one dimensional smooth functions for main effects of an continuous explanatory variable or two or three dimensional smooth functions representing two way and three way interactions of continuous variables. By default, the values of the arguments nseg, pord and degree are repeated to the length of the explanatory covariates. The two and three dimensional smooth terms are constructed using the tensor-product of marginal (one-dimensional) B-spline bases and anisotropic penalties are considered.

#### Value

The function is interpreted in the formula of a sop model and creates the right framework for fitting the smoother. List containing the following elements:

vars names of the covariates involved in the smooth term.

6 plot.sop

the number of segments for the (marginal) B-spline basis for each covariate.

the penalty order (numerical vector of length equal to the number of covariates).

the order of the polynomial for the (marginal) B-Spline bases for this term (numerical vector of length equal to the number of covariates).

dim

The dimension of the smoother - i.e. the number of covariates that it is a function of.

label labels terms.

#### See Also

```
ad, rae, sop
```

## **Examples**

```
library(SOP)
# Simulate the data
set.seed(123)
n <- 1000
sigma <- 0.5
x <- runif(n)</pre>
f0 <- function(x) 2*sin(pi*x)</pre>
f \leftarrow f0(x)
y \leftarrow f + rnorm(n, 0, sigma)
dat \leftarrow data.frame(x = x, y = y)
# Fit the model
m0 <- sop(formula = y \sim f(x, nseg = 10), data = dat)
summary(m0)
# Plot results
plot(y \sim x, data = dat)
ox <- order(dat$x)</pre>
lines(f[ox] \sim dat$x[ox], lwd = 2)
lines(fitted(m0)[ox] \sim dat$x[ox], col = "red", lwd = 2)
```

plot.sop

Default SOP plotting

## **Description**

Takes a fitted sop object produced by sop() and plots the component smooth functions that make it up, on the scale of the linear predictor.

#### Usage

```
## S3 method for class 'sop'
plot(x, rug = TRUE, pages = 0, select = NULL, grid, ...)
```

plot.sop 7

## **Arguments**

X	a fitted sop object as produced by sop().
rug	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. Setting to FALSE will speed up plotting for large datasets.
pages	(default 0) the number of pages over which to spread the output. For example, 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 smooth term to be selected for printing. e.g. if you just want the plot for the second smooth term set select = 2.
grid	number of covariate values used for each 1-d plot - for a nice smooth plot this needs to be several times the estimated degrees of freedom for the smooth. Default value 100.
• • •	other graphics parameters to pass on to plotting commands. See details for smooth plot specific options.

#### **Details**

Produces default plot showing the smooth and random components of a fitted SOP.

For smooth terms plot . sop actually calls plot method functions depending on the dimension of the smooth function.

For plots of smooths in one dimension, the x axis of each plot is labelled with the covariate name, while the y axis is labelled 'f(cov), edf' where cov is the covariate name, and edf the estimated degrees of freedom of the smooth.

Several smooth plots methods using image will accept a colors argument, which can be anything documented in topo.colors (in which case something like colors=rainbow(50) is appropriate), or the grey function (in which case something like colors=grey(0:50/50) is needed).

## Value

The function main purpose is to generate plots. It also (silently) returns a list of the data used to produce the plots for the smooth terms. This function is inspired by the plot.gam function of the same name described in mgcv package (but is not a clone).

#### See Also

```
sop, predict.sop
```

```
library(SOP)
## Simulate the data
set.seed(123)
n <- 1000
sigma <- 0.5
x <- runif(n)
f0 <- function(x) 2*sin(pi*x)</pre>
```

8 predict.sop

```
f \leftarrow f0(x)
y \leftarrow f + rnorm(n, 0, sigma)
dat \leftarrow data.frame(x = x, y = y)
# Fit the model
m0 \leftarrow sop(formula = y \sim f(x, nseg = 10), data = dat)
summary(m0)
# Plot results
plot(m0)
## An example of use of SOP package with tensor product B-splines in 2D
# Simulate the data
set.seed(123)
n <- 1000
sigma <- 0.1
x1 <- runif(n, -1, 1)
x2 <- runif(n, -1, 1)
f0 \leftarrow function(x1, x2) cos(2*pi*sqrt((x1 - 0.5)^2 + (x2 - 0.5)^2))
f < -f0(x1, x2)
y \leftarrow f + rnorm(n, 0, sigma)
dat \leftarrow data.frame(x1 = x1, x2 = x2, y = y)
m0 \leftarrow sop(formula = y \sim f(x1, x2, nseg = 10), data = dat,
         control = list(trace = FALSE))
summary(m0)
plot(m0, col = topo.colors(100))
plot(m0, col = grey(0:100/100))
aux <- plot(m0)</pre>
names(aux)
```

predict.sop

Prediction from a fitted SOP model

## **Description**

The function takes a fitted sop object and produces predictions for the original data if the argument newdata is not set or predictions for new data if newdata is specified. Predictions can be accompanied by standard errors, based on the Bayesian posterior distribution of the model coefficients.

## Usage

predict.sop 9

#### **Arguments**

object a fitted sop object as produced by sop().

newdata a data frame 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 the data frame newdata is provided then it should contain all the variables needed for prediction: a warning is generated if not. If newdata contains a variable offset, it is included into the predictions when

type = "link" and type = "response".

type When this has the value "link" the linear predictor fitted values or predictions

(possibly with associated standard errors) are returned. When type = "terms" each component of the linear predictor is returned separately (possibly with approximate standard errors): this includes parametric model components, followed by each smooth component, but excludes any offset and any intercept. When type = "response" (default) fitted values or predictions on the scale of

the response are returned (possibly with approximate standard errors).

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

prediction.

... other arguments. Not yet implemented.

#### Value

A vector/matrix (or list, with elements fit and se.fit, is se = TRUE) equal to:

"link" a vector of linear predictor values.

"response" a vector of linear predictor values on the scale of the response.

"terms" a matrix with a column per term, and may have an attribute "constant".

## See Also

```
sop, plot.sop
```

```
library(SOP)
## Example training/set
# Simulate the data
set.seed(123)
n <- 1000
sigma <- 0.5
x <- runif(n)
f0 <- function(x)2*sin(pi*x)
f <- f0(x)
y <- f + rnorm(n, 0, sigma)
da <- data.frame(x = x, y = y)# all data
rand <- sample(2, 610, replace=TRUE, prob=c(0.6,0.4))
traindata <- da[rand==1,] # training data
valdata <- da[rand=2,] # validation data
plot(y ~ x, data = traindata, pch = 20, col = gray(.7))</pre>
```

10 predict.sop

```
points(y \sim x, data = valdata, pch = 20, col = gray(.2))
# Fit the model in the training data
m0 \leftarrow sop(formula = y \sim f(x, nseg = 10), data = traindata)
lines(fitted(m0)[order(traindata$x)]~traindata$x[order(traindata$x)],
       col="red", lwd=2)
# Predict and plot in the data used for the fit
po <- predict(m0)</pre>
plot(y \sim x, data = traindata, pch = 20, col = gray(.7))
lines(po[order(traindata$x)] ~ traindata$x[order(traindata$x)],
      col="red", lwd=2)
# Predict and plot in new data
pn <- predict(m0, newdata = valdata)</pre>
plot(y \sim x, data = traindata, pch = 20, col = gray(.7))
lines(pn[order(valdata$x)] ~ valdata$x[order(valdata$x)], col = "yellow", lwd = 2)
# Example Gamma distribution
# Simulate the data
set.seed(123)
n <- 1000
alpha <- 0.75
x0 <- runif(n)</pre>
x1 <- x0*alpha + (1-alpha)*runif(n)
x2 <- runif(n)</pre>
x3 <- x2*alpha + (1-alpha)*runif(n)
x4 <- runif(n)
x5 <- runif(n)
f0 <- function(x)2*sin(pi*x)</pre>
f1 <- function(x)exp(2*x)</pre>
f2 \leftarrow function(x) \ 0.2*x^11*(10*(1-x))^6+10*(10*x)^3*(1-x)^10
f \leftarrow f0(x0) + f1(x1) + f2(x2)
y \leftarrow rgamma(f,exp(f/4),scale=1.2)
df \leftarrow data.frame(y = y, x0 = x0, x1 = x1, x2 = x2, x3 = x3, x4 = x4, x5 = x5)
# Fit the model
m1 <- sop(formula = y \sim f(x0, nseg = 17) + f(x1, nseg = 17) +
      f(x2, nseg = 17) + f(x3, nseg = 17) +
      f(x4, nseg = 17) + f(x5, nseg = 17),
      family = Gamma(link = log), data = df)
summary(m1)
# Predict in a new dataframe
x \leftarrow seq(max(c(min(x1), min(x3))), min(c(max(x1), max(x3))), l = 100)
df.p \leftarrow data.frame(x0 = x, x1 = x, x2 = x, x3 = x, x4 = x, x5 = x)
p <- predict(m1, type = "terms", newdata = df.p)</pre>
colnames(p)
# Plot the different smooth terms
```

print.sop 11

```
op <- par(mfrow = c(2,3))
plot(m1, select = 1)
lines(x, p[,1], col = "red")
plot(m1, select = 2)
lines(x, p[,2], col = "red")
plot(m1, select = 3)
lines(x, p[,3], col = "red")
plot(m1, select = 4)
lines(x, p[,4], col = "red")
plot(m1, select = 5)
lines(x, p[,5], col = "red")
plot(m1, select = 6)
lines(x, p[,6], col = "red")
par(op)</pre>
```

print.sop

Print method for sop objects

## Description

Print method for sop objects

## Usage

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

## **Arguments**

x an object of class sop as produced by sop()

... further arguments passed to or from other methods. Not yet implemented.

#### Value

Prints some summary statistics of the fitted model.

#### See Also

sop

```
library(SOP)
# Simulate the data
set.seed(123)
n <- 1000
sigma <- 0.5
x <- runif(n)
f0 <- function(x) 2*sin(pi*x)</pre>
```

12 rae

```
f <- f0(x)
y <- f + rnorm(n, 0, sigma)
dat <- data.frame(x = x, y = y)

# Fit the model
m0 <- sop(formula = y ~ f(x, nseg = 10), data = dat)
m0</pre>
```

rae

Defining random effects in SOP formula

## Description

Auxiliary function used to define random effects terms in a sop model formula.

#### **Usage**

rae(x)

#### **Arguments**

Х

the x-variable (factor) that defines the random effects term.

#### **Details**

The functions is designed to represent random effects in SOP formulae.

## Value

The function is interpreted in the formula of a sop model and creates the right framework for fitting the random effect. List containing the following elements:

x name of the covariate involved.

## See Also

```
f, ad, sop
```

```
library(SOP)
require(SpATS)
## An example of use of SOP package for the analysis of field trials experiments.
## Taken from the SpATS package.
data(wheatdata)

# Create factor variable for row and columns
wheatdata$R <- as.factor(wheatdata$row)
wheatdata$C <- as.factor(wheatdata$col)</pre>
```

sop 13

```
# package SOP
m0 <- sop(formula = yield ~ colcode + rowcode +
  f(col, row, nseg = c(10, 10)) +
  rae(geno) + rae(R) + rae(C), data = wheatdata)
summary(m0)
plot(m0, col = topo.colors(100))</pre>
```

sop

Estimation of generalised additive P-spline regression models with overlapping penalties.

## **Description**

The function sop() fits generalised additive regression models. For the smooth terms, it uses P-splines (Eilers and Marx, 1996) and it can cope with one, two and three dimensional smooth terms. The innovation of the function is that smoothing/variance parameters are estimated on the basis of the SOP method; see Rodriguez-Alvarez *et al.* (2015) and Rodriguez-Alvarez *et al.* (2019) for details. This speeds up the fit.

## Usage

```
sop(formula, data = list(), family = gaussian(), weights = NULL, offset = NULL,
    control = sop.control(), fit = TRUE)
```

## Arguments

formula	a sop formula. This is exactly like the formula for a GLM except that (1) P-splines in one, two and three dimensions (f), (2)spatially adaptive P-splines in 1 dimension (ad); and (3) random effects (rae) can be added to the right hand side of the formula.
data	a data frame containing the model response variable and covariates required by the formula.
family	object of class family specifying the distribution and link function.
weights	prior weights on the contribution of the data to the log likelihood. Note that a weight of 2, for example, is equivalent to having made exactly the same observation twice. If you want to reweight the contributions of each datum without changing the overall magnitude of the log likelihood, then you should normalize the weights e.g. weights <- weights/mean(weights)). If NULL (default), the weights are considered to be one.
offset	this can be used to specify an a priori known component to be included in the linear predictor during fitting. This should be NULL or a numeric vector of length equal to the number of observations.
control	a list of control values to replace the default values returned by the function sop.control.
fit	logical. If TRUE, the model is fitted.

14 sop

#### **Details**

The sop() can be used to fit generalised additive models. It works similarly to the function gam() of the package **mgcv**. The function sop() uses P-splines (Eilers and Marx, 1996), one of the option on gam(). Estimation is based on the equivalence between P-splines and linear mixed models, and variance/smoothing parameters are estimated based on restricted maximum likelihood (REML) using the separation of overlapping precision matrices (SOP) method described in Rodriguez-Alvarez *et al.* (2015) and Rodriguez-Alvarez *et al.* (2019). The function sop() can be seen as a faster alternative to gam() for some data sets.

#### Value

An object of class 'sop'. It is a list containing the following objects:

b.fixed the estimated fixed effect coefficients (present if fit = TRUE). b.random the predicted random effect coefficients (present if fit = TRUE).

fitted.values the fitted values (present if fit = TRUE).

linear.predictor

the values of the linear predictor (present if fit = TRUE).

residuals the (deviance) residuals (present if fit = TRUE).

X the fixed effect design matrix.

Z the random effect design matrix.

G a list containing information about the precision/penalty matrices (one for each

smoothing/variance parameter in the model).

y the response
weights the prior weights.
family the distribution family.

out a list with i) tol.ol tolerance parameter (outer loop); ii) it.ol number of iter-

ation (outer loop); iii) tol.il tolerance parameter (inner loop); it.il (number of iteration (inner loop)), iv) vc variance components estimates, v) edf effective

degrees of freedom (present if fit = TRUE).

deviance the deviance (present if fit = TRUE).
null.deviance the null deviance (present if fit = TRUE).

Vp Bayesian posterior covariance matrix for the coefficients (present if fit = TRUE).

call the function call.

data the data.

formula the model formula.

lin a list containing information about the parametric/linear.random a list containing information about the random effects.f a list containing information about the smoothers.

na.action vector with the observations (position) deleted due to missingness.

names.terms the terms used in the formula.
model.terms the explanatory variables.

nterms the number of linear, random and smooth terms in the formula.

sop 15

#### References

Eilers, P.H.C. and Marx, B.D. (1996). Flexible smoothing with B-splines and penalties. *Statistical Science*, **11** (2), 89–121.

Rodriguez-Alvarez, M.X., Lee, D. J., Kneib, T., Durban, M., and Eilers, P. (2015). Fast smoothing parameter separation in multidimensional generalized P-splines: the SAP algorithm. *Statistics and Computing*, **25** (5), 941–957.

Rodriguez-Alvarez, M.X., Durban, M., Lee, D. J. and Eilers, P. (2019). On the estimation of variance parameters in non-standard generalised linear mixed models: application to penalised smoothing. *Statistics and Computing*, **29** (3), 483–500.

```
library(SOP)
## An example of use of SOP package with tensor product B-splines in 2D
# Simulate the data
set.seed(123)
n <- 1000
sigma <- 0.1
x1 <- runif(n, -1, 1)
x2 <- runif(n, -1, 1)
f0 \leftarrow function(x1, x2) cos(2*pi*sqrt((x1 - 0.5)^2 + (x2 - 0.5)^2))
f < -f0(x1, x2)
y <- f + rnorm(n, 0, sigma)
dat \leftarrow data.frame(x1 = x1, x2 = x2, y = y)
# Theoretical surface
np <- 50
x1p \leftarrow seq(-1, 1, length = np)
x2p \leftarrow seq(-1, 1, length = np)
fp <- cos(2 * pi * sqrt(outer((x1p - 0.5) ^ 2, (x2p - 0.5) ^ 2, '+')))
image(x1p, x2p, matrix(fp, np, np), main = 'f(x1,x2) - Theor',
     col = topo.colors(100)
# Fit the model
m0 \leftarrow sop(formula = y \sim f(x1, x2, nseg = 10), data = dat,
        control = list(trace = FALSE))
summary(m0)
plot(m0, col = topo.colors(100))
## An example of use of SOP package with several smooth terms and Gamma distribution
# Simulate the data
set.seed(123)
n <- 1000
alpha <- 0.75
x0 <- runif(n)</pre>
x1 <- x0*alpha + (1-alpha)*runif(n)
x2 <- runif(n)</pre>
x3 <- x2*alpha + (1-alpha)*runif(n)
```

sop.control

```
x4 <- runif(n)
x5 <- runif(n)
f0 <- function(x)2*sin(pi*x)</pre>
f1 <- function(x)exp(2*x)</pre>
f2 \leftarrow function(x) \ 0.2*x^11*(10*(1-x))^6+10*(10*x)^3*(1-x)^10
f \leftarrow f0(x0) + f1(x1) + f2(x2)
y \leftarrow rgamma(f,exp(f/4),scale=1.2)
df \leftarrow data.frame(y = y, x0 = x0, x1 = x1, x2 = x2, x3 = x3, x4 = x4, x5 = x5)
# Fit the model
m1 <- sop(formula = y \sim f(x0, nseg = 17) +
                              f(x1, nseg = 17) +
                              f(x2, nseg = 17) +
                              f(x3, nseg = 17) +
                              f(x4, nseg = 17) +
                              f(x5, nseg = 17), family = Gamma(link = log), data = df)
summary(m1)
plot(m1)
## An example of use of SOP package for the analysis of field trials experiments.
## Taken from the SpATS package.
require(SpATS)
data(wheatdata)
# Create factor variable for row and columns
wheatdata$R <- as.factor(wheatdata$row)</pre>
wheatdata$C <- as.factor(wheatdata$col)</pre>
# package SOP
m2 <- sop(formula = yield ~ colcode + rowcode +
  f(col, row, nseg = c(10, 10)) +
  rae(geno) + rae(R) + rae(C), data = wheatdata)
summary(m2)
plot(m2, col = topo.colors(100), pages = 1)
# Package SpATS: more adequate for this analysis.
# SpATS has been explicitly developed for the analysis field trials experiments.
m3 <- SpATS(response = "yield",
    spatial = \sim SAP(col, row, nseg = c(10,10), degree = 3, pord = 2, center = TRUE),
    genotype = "geno",
    genotype.as.random = TRUE,
    fixed = ~ colcode + rowcode, random = ~ R + C, data = wheatdata,
    control = list(tolerance = 1e-06))
summary(m3)
plot(m3)
```

sop.control 17

#### **Description**

The function controls some of the fitting parameters of sop. Typically only used when calling sop().

## Usage

```
sop.control(maxit = 200, epsilon = 1e-6, trace = FALSE)
```

## **Arguments**

maxit numerical value indicating the maximum number of iterations. Default set to

200 (see Details).

epsilon numerical value indicating the tolerance for the convergence criterion. Default

set to 1e-6 (see Details).

trace logical indicating if output should be produced for each iteration.

#### **Details**

For Gaussian response variables, the implemented algorithm is an iterative procedure, with the fixed and random effects as well as the variance components being updated at each iteration. To check the convergence of this iterative procedure, the (REML) deviance is monitored. For non-Gaussian response variables, estimation is based on Penalized Quasi-likelihood (PQL) methods. Here, the algorithm is a two-loop algorithm: the outer loop corresponds to the Fisher-Scoring algorithm (monitored on the basis of the change in the linear predictor between consecutive iterations), and the inner loop corresponds to that described for the Gaussian case.

## Value

A list with the arguments as components.

#### References

Rodriguez-Alvarez, M.X., Lee, D. J., Kneib, T., Durban, M., and Eilers, P. (2015). Fast smoothing parameter separation in multidimensional generalized P-splines: the SAP algorithm. *Statistics and Computing*, **25** (5), 941–957.

Rodriguez-Alvarez, M.X., Durban, M., Lee, D. J. and Eilers, P. (2019). On the estimation of variance parameters in non-standard generalised linear mixed models: application to penalised smoothing. *Statistics and Computing*, **29** (3), 483–500.

## See Also

sop.

```
library(SOP)
# Simulate the data
set.seed(123)
n <- 1000</pre>
```

18 sop.fit

```
sigma <- 0.5
x <- runif(n)
f0 <- function(x) 2*sin(pi*x)
f <- f0(x)
y <- f + rnorm(n, 0, sigma)
dat <- data.frame(x = x, y = y)

# Fit the model
m0 <- sop(formula = y ~ f(x, nseg = 10), data = dat, control = list(trace = FALSE))
summary(m0)</pre>
```

sop.fit

Fitting generalised linear mixed models with overlapping precision matrices.

## Description

This is an internal function of package SOP. It is used to fit SOP models by specifying the design matrices for the fixed and random effects as well as the precision matrices for each variance component in the model.

## Usage

```
sop.fit(y, X, Z, weights = NULL, G = NULL, vcstart = NULL,
  etastart = NULL, mustart = NULL, offset = NULL,
  family = gaussian(), control = sop.control())
```

## **Arguments**

У	vector of observations of length n.
Χ	design matrix for the fixed effects (dimension n x p).
Z	design matrix for the random effects (of dimension n x q).
weights	an optional vector of 'prior weights' to be used in the fitting process. If NULL (default), the weights are considered to be one.
G	a list with the diagonal elements of the precision matrices for each variance component in the model. Each element of the list is a vector of the same length as the number of columns in Z (i.e. q). The vector can be padded out with zeroes to indicate random coefficient not 'affected' by the variance component (see details).
vcstart	optional numeric vector. Initial values for the variance components (including the error variance as the first element of the vector). If NULL, all variance components are initialised to one.
etastart	initial values for the linear predictor.
mustart	initial values for the expected response.

sop.fit 19

offset this can be used to specify an a priori known component to be included in the

linear predictor during fitting. This should be NULL or a numeric vector of

length equal to the number of observations.

family object of class family specifying the distribution and link function.

control a list of control values to replace the default values returned by the function

sop.control.

#### Details

sop.fit is the workhorse function: it is typically not normally called directly but can be more efficient where the response vector 'y', design matrixs 'X' and 'Z', and precision matrices 'G' have already been calculated. Currently, the function only allows for diagonal precision matrices (possibly overlappping).

#### Value

A list containing the following objects:

b. fixed the estimated fixed effect coefficients.b. random the predicted random effect coefficients.

residuals the (deviance) residuals.

fitted.values the fitted values.

linear.predictor

the values of the linear predictor.

X the fixed effect design matrix.Z the random effect design matrix.

y the response.
weights the prior weights.
family the distribution family.

out a list with i) tol.ol tolerance parameter (outer loop); ii) it.ol number of iter-

ation (outer loop); iii) tol.il tolerance parameter (inner loop); it.il (number of iteration (inner loop)), iv) vc variance components estimates, v) edf effective

degrees of freedom.

deviance the deviance.
null.deviance the null deviance.

Vp Bayesian posterior covariance matrix for the coefficients.

#### References

Rodriguez-Alvarez, M.X., Lee, D. J., Kneib, T., Durban, M., and Eilers, P. (2015). Fast smoothing parameter separation in multidimensional generalized P-splines: the SAP algorithm. *Statistics and Computing*, **25** (5), 941–957.

Rodriguez-Alvarez, M.X., Durban, M., Lee, D. J. and Eilers, P. (2019). On the estimation of variance parameters in non-standard generalised linear mixed models: application to penalised smoothing. *Statistics and Computing*, **29** (3), 483–500.

20 summary.sop

## **Examples**

```
library(SOP)
# Simulate the data
set.seed(123)
n <- 1000
sigma <- 0.1
x1 <- runif(n, -1, 1)
x2 <- runif(n, -1, 1)
f0 \leftarrow function(x1, x2) cos(2*pi*sqrt((x1 - 0.5)^2 + (x2 - 0.5)^2))
f < -f0(x1, x2)
y \leftarrow f + rnorm(n, 0, sigma)
dat \leftarrow data.frame(x1 = x1, x2 = x2, y = y)
# Save but not fit the model
m0_nfit <- sop(formula = y \sim f(x1, x2, nseg = 10), data = dat,
     fit = FALSE)
# Now fit using sop.fit()
m0 <- sop.fit(X = m0_nfit$X, Z = m0_nfit$Z, G = m0_nfit$G,</pre>
y = m0_nfit$y, weights = m0_nfit$weights,
   control = list(trace = FALSE))
names(m0)
```

summary.sop

Summary method for a fitted SOP model.

#### **Description**

Summary method for a fitted SOP model.

## Usage

```
## S3 method for class 'sop'
summary(object, ...)
```

## Arguments

object an object of class sop as produced by sop().
... further arguments passed to or from other methods. Not yet implemented.

#### Value

The function summary.sop computes and returns a list of summary statistics of the fitted model given in object, using the components (list elements) "call" and "terms" from its argument, plus

call the matched call.

b.random a vector with the predicted random effects coefficients.

summary.sop 21

b. fixed a vector with the estimated fixed effects coefficients.

r.sq.adj the (adjusted)  $R^2$ , i.e., 'fraction of variance explained by the model',

$$R^2 = 1 - \frac{\sum_i R_i^2 / (n - df)}{\sum_i (y_i - y^*)^2 / (n - 1)},$$

where  $R_i = w_i(y_i - \mu_i)$  and  $y^*$  is the (weighted) mean of  $y_i$ .

deviance the deviance.

null.deviance the null deviance.

dev.expl proportion of the null deviance explained by the model.

n number of data.
iter number of iterations.

residual.df residual degrees of freedom.

edf a vector with the estimated degrees of freedom for the (smooth and random)

model terms.

formula the model formula. family the family used.

na.action vector with the observations (position) deleted due to missingness.

#### See Also

sop, summary

```
library(SOP)
# Simulate the data
set.seed(123)
n <- 1000
sigma <- 0.5
x <- runif(n)
f0 <- function(x) 2*sin(pi*x)
f <- f0(x)
y <- f + rnorm(n, 0, sigma)
dat <- data.frame(x = x, y = y)
# Fit the model
m0 <- sop(formula = y ~ f(x, nseg = 10), data = dat)
summary(m0)</pre>
```

## **Index**

```
* hplot
                                                    SOP (SOP-package), 2
    plot.sop, 6
                                                    sop, 4, 6, 7, 9, 11, 12, 13, 17, 21
* \ models \\
                                                    SOP-package, 2
    ad, 3
                                                    sop.control, 13, 16, 19
    f, 5
                                                    sop.fit, 18
    predict.sop, 8
                                                    summary, 21
    rae, 12
                                                    summary.sop, 20
* package
                                                    topo.colors, 7
    SOP-package, 2
* regression
    ad, 3
    f, 5
    plot.sop, 6
    predict.sop, 8
    rae, 12
    sop, 13
    sop.control, 16
    sop.fit, 18
* smooth
    ad, 3
    f, 5
    plot.sop, 6
    predict.sop, 8
    print.sop, 11
    rae, 12
    summary.sop, 20
ad, 3, 6, 12, 13
f, 4, 5, 12, 13
family, 13, 19
grey, 7
image, 7
plot.sop, 6, 9
predict.sop, 7, 8
print.sop, 11
rae, 4, 6, 12, 13
```