Package ‘lmeSplines’

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Title Add Smoothing Spline Modelling Capability to `nlme`
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Description Adds smoothing spline modelling capability to nlme. Fits smoothing spline terms in Gaussian linear and nonlinear mixed-effects models.
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approx.Z Interpolating in smoothing spline Z-matrix columns

Description

Function to interpolate the Z-matrix for LME smoothing spline fits from one set of values of the time covariate to another.

Usage

approx.Z(oldtimes, newtimes)
Arguments

- **Z**: A Z-matrix with rows corresponding to the sorted unique values of the time covariate.
- **oldtimes**: Original (sorted) values for time covariate, corresponding to the rows of **Z**.
- **newtimes**: New (sorted) values for time covariate.

Details

Uses linear interpolation of each column of the Z-matrix, regarded as a function of time, with the times given by `oldtimes`.

Value

A matrix corresponding to an interpolated spline matrix. Can be used with `smspline()` for fitting LME splines with random effects corresponding to a different set of values of the time covariate than those represented in the data, or as part of the 'newdata' argument prediction from an existing model, to obtain predictions at points not represented in the data using `predict.lme()`.

Note

Linear interpolation works well here because the spline basis functions are approximately piecewise linear.

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See Also

- `smspline`
- `nlme`

Examples

```r
times1 <- 1:10
Zt1 <- smspline(~ times1)
times2 <- seq(1,10,by=0.1)
Zt2 <- approx.Z(Zt1,oldtimes=times1,newtimes=times2)
```

Description

Functions to generate matrices for a smoothing spline covariance structure, to enable fitting smoothing spline terms in LME/NLME.
smspline

Usage

smspline(formula, data)
smspline.v(time)

Arguments

formula model formula with right hand side giving the spline covariate
data optional data frame
time spline ‘time’ covariate to smooth over

Details

A smoothing spline can be represented as a mixed model (Speed 1991, Verbyla 1999). The generated Z-matrix from smspline() can be incorporated in the user’s dataframe, then used in model formulae for LME random effects terms at any level of grouping (see examples). The spline random terms are fitted in LME using an identity ‘pdIdent’ structure of the form pdIdent(~Z - 1). The model formulation for a spline in time (t) is as follows (Verbyla 1999):

\[ y = X_s \beta_s + Z_s u_s + e \]

where \( X_s = [1|t] \), \( Z_s = Q(t(Q)Q)^{-1} \), and \( u_s \sim N(0, G_s) \), is a set of random effects. We transform the set of random effects \( u_s \) to independence with \( u_s = Lv_s \), where \( v_s \sim N(0, I \sigma_s^2) \)

is a set of independent random effects. The Z-matrix is transformed accordingly to \( Z = Z_s L \), where \( L \) is the lower triangle of the Choleski decomposition of \( G_s \).

The function smspline.v() is called by smspline(), and can be used to access the matrices \( X_s, Q, G_s \). See Verbyla (1999) for further information.

Value

For smspline(), a Z-matrix with the same number of rows as the data frame. After fitting, the LME model output gives a standard deviation parameter for the random effects, estimating \( \sigma_s \). The smoothing parameter from the penalised likelihood formulation is

\[ \lambda = \frac{\sigma^2}{\sigma_s^2} \]

For smspline.v(), a list of the form

- \( Xs \) X-matrix for fixed effects part of the model
- \( Zs \) Z-matrix for random effects part of the model
- \( Q, Gs, R \) Matrices \( Q, G_s, R \) associated to the mixed-model form of the smoothing spline.

Note

The time points for the smoothing spline basis are, by default, the unique values of the time covariate. This is the easiest approach, and model predictions at the fitted data points, can be obtained using predict.lme. By interpolation, using approx.Z, the Z-matrix can be obtained for any set of time points and can be used for fitting and/or prediction. (See examples). Synopsis:

```
data$Z <- smspline(formula1, data); fit <-lme(formula2, data, random= ...)```
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References

The correspondence between penalized likelihood formulations of smoothing splines and mixed models was pointed out by Speed (1991). The formulation used here for the mixed smoothing spline matrices are given in Verbyla (1999). LME/NLME modelling is introduced in Pinheiro and Bates (2000).


See Also

approx.Z nlme

Examples

# smoothing spline curve fit
data(smSplineEx1)
# variable 'all' for top level grouping
smSplineEx1$all <- rep(1,nrow(smSplineEx1))
# setup spline Z-matrix
smSplineEx1$Zt <- smspline(~ time, data=smSplineEx1)
fit1s <- lme(y ~ time, data=smSplineEx1,
            random=list(all=pdIdent(~Zt - 1)))
summary(fit1s)
plot(smSplineEx1$time,smSplineEx1$y,pch="o",type="n",
     main="Spline fits: lme(y ~ time, random=list(all=pdIdent(~Zt-1)))",
     xlab="time",ylab="y")
points(smSplineEx1$time,smSplineEx1$y,col=1)
lines(smSplineEx1$time, smSplineEx1$y.true,col=1)
lines(smSplineEx1$time, fitted(fit1s),col=2)

# fit model with cut down number of spline points
times20 <- seq(1,100,length=20)
Zt20 <- smspline(times20)
smSplineEx1$Zt20 <- approx.Z(Zt20,times20,smSplineEx1$time)
fit1s20 <- lme(y ~ time, data=smSplineEx1,
              random=list(all=pdIdent(~Zt20 - 1)))
# note: virtually identical df, loglik.
anova(fit1s,fit1s20)
summary(fit1s20)

# model predictions on a finer grid
times200 <- seq(1,100,by=0.5)
pred.df <- data.frame(all=rep(1,length(times200)),time=times200)
pred.df$Zt20 <- approx.Z(Zt20, times20, times200)
yp20.200 <- predict(fit1s20, newdata=pred.df)
lines(times200, yp20.200+0.02, col=4)

# mixed model spline terms at multiple levels of grouping
data(Spruce)
Spruce$Zday <- smspline(~ days, data=Spruce)
Spruce$all <- rep(1, nrow(Spruce))
# overall spline term, random plot and Tree effects
spruce.fit1 <- lme(logSize ~ days, data=Spruce,
    random=list(all= pdIdent(~Zday -1),
                plot= ~1, Tree= ~1))
# try overall spline term plus plot level linear + spline term
spruce.fit2 <- lme(logSize ~ days, data=Spruce,
    random=list(all= pdIdent(~Zday -1),
                plot= pdBlocked(list(~ days,pdIdent(~Zday -1))),
                Tree = ~1))
anova(spruce.fit1, spruce.fit2)
summary(spruce.fit1)

---

smSplineEx1  Simulated data about a smooth curve

Description

Simulated data to demonstrate smoothing spline curve fitting with \texttt{smspline} and \texttt{lme}

Usage

data(smSplineEx1)

Format

A data frame with 100 observations on the following 4 variables.

- \textbf{time} time covariate
- \textbf{y} simulated response values
- \textbf{y.true} true response values

Details

100 data points were simulated about the curve \( y = 10 - 6 \times \exp(-4t/100) \), with iid normal random errors with standard deviation 1.

Examples

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