

Package ‘JOPS’

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Type Package

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Description Functions and data to reproduce all plots in the book ``Practical Smoothing. The Joys of P-splines'' by Paul H.C. Eilers and Brian D. Marx (2021, ISBN:978-1108482950).

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bbase	<i>Compute a B-spline basis matrix</i>
-------	--

Description

Compute a B-spline basis matrix using evenly spaced knots.

Usage

```
bbase(x, xl = min(x), xr = max(x), nseg = 10, bdeg = 3)
```

Arguments

x	a vector of argument values, at which the B-spline basis functions are to be evaluated.
xl	the lower limit of the domain of x; default is $\min(x)$.
xr	the upper limit of the domain of x; default is $\max(x)$.
nseg	the number of equally sized segments between xl and xr; default is 10.
bdeg	the degree of the splines, usually 1, 2, or 3 (default).

Details

If xl is larger than $\min(x)$, it will be adjusted to $\min(x)$ and a warning will be given. If xr is smaller than $\max(x)$, it will be adjusted to $\max(x)$ and a warning will be given. The values of the design parameters x, xl, xr, ndeg, bdeg and type = 'bbase' are added to the list of attributes of the matrix.

Value

A matrix with $\text{length}(x)$ rows and $\text{nseg} + \text{bdeg}$ columns.

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

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

Eilers, P.H.C. and B.D. Marx (2010). Splines, knots and penalties. *Wiley Interdisciplinary Reviews: Computational Statistics*. Wiley: NY. DOI: 10.1002/wics.125

Examples

```
# Compute and plot a B-spline basis matrix
x = seq(0, 360, by = 2)
B = bbase(x, 0, 360, nseg = 8, bdeg = 3)
matplot(x, B, type = 'l', lty = 1, lwd = 2, xlab = 'x', ylab = '')
```

binit	<i>Translated number vector to bin index.</i>
-------	---

Description

Translates number vector to bin index, given lower and upper limits of the domain and number of bins. A support function for (smoothing) histograms.

Usage

```
binit(x, xmin = min(x), xmax = max(x), nbin = 100)
```

Arguments

x	a numerical vector.
xmin	the lower limit of the domain.
xmax	the upper limit of the domain.
nbin	the number of bins (default=100).

Value

A list with components:

xbin	a vector of length(x) with elements giving the bin index.
xgrid	a vector of length(nbin) with the midpoints of the bins.
nbin	the number of bins.

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

bone_data	<i>Spinal bone relative mineral density</i>
-----------	---

Description

Relative spinal bone mineral density measurements on 261 North American adolescents. Each value is the difference in spnbmd taken on two consecutive visits, divided by the average. The age is the average age over the two visits.

Usage

```
data(bone_data)
```

Format

A dataframe with four columns:

idnum ID of the child

age age

gender male or female

spnbmd Relative Spinal bone mineral density.

Source

<https://web.stanford.edu/~hastie/ElemStatLearn/datasets/bone.data>

References

Bachrach, L.K., Hastie, T., Wang, M.-C., Narasimhan, B., Marcus, R. (1999). Bone Mineral Acquisition in Healthy Asian, Hispanic, Black and Caucasian Youth. A Longitudinal Study. *J Clin Endocrinol Metab* 84, 4702-12.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

CardioData

Female cardiovascular mortality data

Description

USA women, monthly exposures and deaths due to cardiovascular diseases.

Usage

`data(CardioData)`

Format

A list with two matrices:

Exposed Monthly exposures. Rows: ages 0 to 110, Columns: Jan 1933 to Dec 2005

Death Monthly deaths. Rows: ages 0 to 100. Columns: Jan 1959 to Dec 1998.

Source

Derived from USA Mortality Detail Files (deaths) and the Human Mortality Database by Roland Rau.

References

P.H.C. Eilers, J. Gampe, B.D. Marx, and R. Rau, "Modulation models for seasonal time series and incidence tables" *Statistics In Medicine* , 27, pp. 3430–3441, 2008.

cbase

*Compute a circular B-spline basis matrix***Description**

Computes a circular B-spline basis matrix using evenly spaced knots.

Usage

```
cbase(x, xl = min(x), xr = max(x), nseg = 10, bdeg = 3)
```

Arguments

x	a vector of argument values, at which the B-spline basis functions are to be evaluated.
xl	the lower limit of the domain of x; default is $\min(x)$.
xr	the upper limit of the domain of x; default is $\max(x)$.
nseg	the number of B-spline segments (default 10) between xl and xr.
bdeg	the degree of the basis, usually 1, 2, or 3 (default).

Details

If xl is larger than $\min(x)$, it will be adjusted to $\min(x)$ and a warning will be given. If xr is smaller than $\max(x)$, it will be adjusted to $\max(x)$ and a warning will be given.

The design parameters x, xl, xr, nseg, bdeg and type = 'cbase' are added to the list of attributes.

In a circular basis, the B-splines are wrapped around the boundaries of the domain. Use a circular basis for data like directions or angles. It should be combined with a circular penalty matrix, as computed by `cdiff()`.

Value

A matrix with $\text{length}(x)$ rows and nseg columns.

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Examples

```
# Compute and plot a circular B-spline basis matrix
x = seq(0, 360, by = 2)
B = cbase(x, 0, 360, nseg = 8, bdeg = 3)
matplot(x, B, type = 'l', lty = 1, lwd = 2, xlab = 'x', ylab = '')
title('Note how the ends connect smoothly meet at boundaries')
```

cdiff	<i>Compute a second order circular differencing matrix</i>
-------	--

Description

Compute difference matrix used for circular penalties.

Usage

```
cdiff(n)
```

Arguments

n number of rows (and columns) of the square differencing matrix.

Value

A square matrix with n rows and columns.

Author(s)

Paul Eilers

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Examples

```
# Compare standard and circular differencing matrix
n = 8
D1 = diff(diag(n), diff = 2)
D2 = cdiff(n)
oldpar = par(no.readonly = TRUE)
on.exit(par(oldpar))
par(mfrow = c(1, 2))
image(t(D1))
title('Linear differencing matrix')
image(t(D2))
title('Circular differencing matrix')
```

CGHsim

Simulation of CGH data

Description

A crude simulation of comparative genomic hybridization (CGH) data.

Usage

```
data(CGHsim)
```

Format

A data frame with 400 rows and two columns:

y Log R ratio

x Genomic position (but in fact the row number).

Source

The simulation program could not be located anymore. But the data have a very simple structure.

clone_base

Clone a B-spline basis for new x

Description

Extract basis parameters from an existing B-splines basis matrix, and use them for computing a new basis at new values of x.

Usage

```
clone_base(B, x)
```

Arguments

B a B-splines basis matrix, computed with `bbase()` or `cbase()`.

x a vector of new argument values.

Details

If values in x are outside the domain used for computing B, they will be discarded, with a warning.

Value

A matrix with number of rows=`length(xnew)`.

Author(s)

Paul Eilers

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Examples

```
x = seq(0, 10, length = 20)
n = length(x)
y = sin(x / 2) + rnorm(n) * 0.2
B = bbase(x)
nb = ncol(B)
D = diff(diag(nb), diff = 2)
lambda = 1
a = solve(t(B) %% B + lambda * t(D) %% D, t(B) %% y)
# Clone basis on finer grid
xg = seq(0, 10, length = 200)
Bg = clone_base(B, xg)
yg = Bg %% a
plot(x, y)
lines(xg, yg, col = 'blue')
```

col_one

Define constants for plotting (colors, linetype, palettes)

Description

Define constants for plotting (colors, linetype, palettes) #library(colorspace)

Usage

```
col_one
```

Format

An object of class character of length 1.

Complaints

Environmental complaints from the Rijnmond area of The Netherlands

Description

Environmental complaints about odors from the Rijnmond region (near Rotterdam in the Netherlands) in 1988.

Usage

```
data(Complaints)
```

Format

A dataframe with two columns:

freq The daily number of complaints.

count The number of days the specific complaint frequency occurred.

Details

In 1988, the Rijnmond Environmental Agency registered approximately 20,000 complaints about odors from regional inhabitants.

Source

Personal information from Paul Eilers.

Examples

```
plot(Complaints$freq, Complaints$count, type = 'h',  
     xlab = 'Number of complaints per day', ylab = 'Frequency')
```

count2d

Create a matrix of counts.

Description

Count the number of occurrences of pairs of positive integers in two vectors, producing a matrix.

Usage

```
count2d(xb, yb, nb)
```

Arguments

xb a vector of integers.

yb a vector of integers.

nb a vector of length 2 that provides the number of bins for the 2D histogram on x and y.

Details

This function builds a two-dimensional histogram, based on two two vectors of bin numbers (obtained with `binit`). Rows where `x[i] > nb[1]` or `y[i] > nb[2]` are discarded without a warning.

Value

A matrix with `nb[1]` rows and `nb[2]` columns with counts. It serves as the input for two-dimensional histogram smoothing.

dev_calc	<i>Deviance calculation for GLM P-spline fitting.</i>
----------	---

Description

Calculates the deviance and returns the ML estimated dispersion parameter for a variety of response distributions for P-spline fitting within the GLM framework.

Usage

```
dev_calc(
  family = "gaussian",
  y,
  mu,
  m_binomial = 0 * y + 1,
  r_gamma = 0 * y + 1
)
```

Arguments

family	the response distribution, e.g. "gaussian", "binomial", "poisson", "Gamma" distribution. Quotes are needed; default "family = gaussian".
y	the glm response vector of length m.
mu	the P-spline estimated mean for the glm response vector of length m.
m_binomial	a vector of binomial trials having length(y), when family = "binomial". Default is 1 vector.
r_gamma	a vector of gamma shape parameters, when family = "Gamma". Default is 1 vector.

Value

A list with two fields:

dev	the estimated deviance.
dispersion_parm	the ML estimated dispersion parameter.

Disks	<i>Prices of hard disk drives</i>
-------	-----------------------------------

Description

Prices and capacities of hard disk drives, as advertised in a Dutch computer monthly in 1999. Prices are given in Dutch guilders; the Euro did not yet exist.

Usage

```
data(Disks)
```

Format

A dataframe with six columns:

Year 1999-2000

Month month, 1-12

Size capacity in Gb

Buffer buffer size (Mb)

RPM rotating speed (rpm)

PriceDG in Dutch Guilders, divide by 2.2 for Euro.

Source

Personal information from Paul Eilers.

ECG

A section of an ECG (electrocardiogram)

Description

The data set includes two signals, respiration and the ECG. Both signals are distorted by strong 60Hz interference from the mains power.

Usage

data(ECG)

Format

A data frame with three columns:

time time in seconds

resp respiration, arbitrary units

ecg ECG, arbitrary units.

Source

<https://physionet.org/content/fantasia/1.0.0/>

References

Iyengar N, Peng C-K, Morin R, Goldberger AL, Lipsitz LA. Age-related alterations in the fractal scaling of cardiac interbeat interval dynamics. *Am J Physiol*, 1996; 271: 1078-1084.

Standard citation for PhysioNet: Goldberger AL, Amaral LAN, Glass L, Hausdorff JM, Ivanov PCh, Mark RG, Mietus JE, Moody GB, Peng C-K, Stanley HE. PhysioBank, PhysioToolkit, and PhysioNet: Components of a New Research Resource for Complex Physiologic Signals (2003). *Circulation*. 101(23):e215-e220.

fitampl

*Fit amplitude coefficients in the bundle model for expectiles***Description**

There are two functions for fitting the expectile bundle model, one for estimating asymmetry parameters (`fitasy`), the other for estimating the amplitude function, `fitampl`, this function. See the details below.

Usage

```
fitampl(y, B, alpha, p, a, pord = 2, lambda)
```

Arguments

<code>y</code>	a response vector.
<code>B</code>	a proper B-spline basis matrix, see <code>bbase()</code> .
<code>alpha</code>	a vector of B-spline coefficients.
<code>p</code>	a vector of asymmetries.
<code>a</code>	a vector of asymmetry parameters.
<code>pord</code>	the order of the difference penalty, default is 2.
<code>lambda</code>	the positive tuning parameter for the penalty.

Details

The expectile bundle model determines a set of expectile curves for a point cloud with data vectors x and y , as $\psi_j x_i = a_j g(x_i)$. Here a_j is the asymmetry parameter corresponding to a given asymmetry p_j . A vector of asymmetries with all $0 < p_j < 1$ is specified by the user.

The asymmetric least squares objective function is

$$\sum_j \sum_i w_{ij} (y_i - \sum_j a_j g_j(x_i))^2.$$

The function $g(\cdot)$ is called the amplitude. The weights depend on the residuals:

$$w_{ij} = p_j$$

if $y_i > a_j g(x_i)$ and $w_{ij} = 1 - p_j$ otherwise.

The amplitude function is a sum of B-splines with coefficients `alpha`. There is no direct solution, so `alpha` and the asymmetry parameters `a` must be updated alternately. See the example.

Value

a vector of estimated B-spline coefficients.

Note

This is a simplification of the model described in the reference. There is no explicit term for the trend.

Author(s)

Paul Eilers

References

Schnabel, S.K. and Eilers, P.H.C. (2013) A location-scale model for non-crossing expectile curves. *Stat 2*: 171–183.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
# Get the data
data(bone_data)
x = bone_data$age
y = bone_data$spnbmd
m <- length(x)

# Set asymmetry levels
p = c(0.005, 0.01, 0.02, 0.05, 0.2, 0.5, 0.8, 0.9, 0.95, 0.98, 0.99, 0.995)
np <- length(p)

# Set P-spline parameters
x0 <- 5
x1 <- 30
ndx <- 20
bdeg <- 3
pord <- 2

# Compute bases
B <- bbase(x, x0, x1, ndx, bdeg)
xg <- seq(from = min(x), to = max(x), length = 100)
Bg <- clone_base(B, xg)
n <- ncol(B)

lambda = 1
alpha <- rep(1,n)
a = p
for (it in 1:20){
  alpha <- fitampl(y, B, alpha, p, a, pord, lambda)
  alpha <- alpha / sqrt(mean(alpha ^ 2))
  anew <- fitasy(y, B, alpha, p, a)
  da = max(abs(a - anew))
  a = anew
  cat(it, da, '\n')
  if (da < 1e-6) break
}

# Compute bundle on grid
ampl <- Bg %*% alpha
Z <- ampl %*% a

# Plot data and bundle
plot(x, y, pch = 15, cex = 0.7, col = 'grey', xlab = 'Age', ylab = 'Density')
cols = colorspace::rainbow_hcl(np, start = 10, end = 350)
matlines(xg, Z, lty = 1, lwd = 2, col = cols)
```

fitasy

*Fit asymmetry parameters in the expectile bundle model***Description**

There are two functions for fitting the expectile bundle model, the present one for estimating asymmetry parameters (`fitasy`), the other for estimating the amplitude function, `fitampl`. See the details below.

Usage

```
fitasy(y, B, b, p, c0)
```

Arguments

<code>y</code>	a response vector.
<code>B</code>	a proper B-spline basis matrix, see <code>bbase()</code> .
<code>b</code>	a vector of B-spline coefficients.
<code>p</code>	a vector of asymmetries with values between 0 and 1.
<code>c0</code>	a vector.

Details

The expectile bundle model determines a set of expectile curves for a point cloud with data vectors x and y , as $\psi_j x_i = a_j g(x_i)$. Here a_j is the asymmetry parameter corresponding to a given asymmetry p_j . A vector of asymmetries with all $0 < p_j < 1$ is specified by the user.

The asymmetric least squares objective function is

$$\sum_j \sum_i w_{ij} (y_i - \sum_j a_j g_j(x_i))^2.$$

The function $g(\cdot)$ is called the amplitude. The weights depend on the residuals:

$$w_{ij} = p_j$$

if $y_i > a_j g(x_i)$ and $w_{ij} = 1 - p_j$ otherwise.

The amplitude function is a sum of B-splines with coefficients `alpha`. There is no direct solution, so `alpha` and the asymmetry parameters `a` must be updated alternately. See the example.

Value

a vector of estimated asymmetry parameters .

Note

This is a simplification of the model described in the reference. There is no explicit term for the trend.

Author(s)

Paul Eilers

References

Schnabel, S.K. and Eilers, P.H.C. (2013) A location-scale model for non-crossing expectile curves. *Stat 2*: 171–183.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
# Get the data
data(bone_data)
x = bone_data$age
y = bone_data$spnbmd
m <- length(x)

# Set asymmetry levels
p = c(0.005, 0.01, 0.02, 0.05, 0.2, 0.5, 0.8, 0.9, 0.95, 0.98, 0.99, 0.995)
np <- length(p)

# Set P-spline parameters
x0 <- 5
x1 <- 30
ndx <- 20
bdeg <- 3
pord <- 2

# Compute bases
B <- bbase(x, x0, x1, ndx, bdeg)
xg <- seq(from = min(x), to = max(x), length = 100)
Bg <- clone_base(B, xg)
n <- ncol(B)

lambda = 1
alpha <- rep(1,n)
a = p
for (it in 1:20){
  alpha <- fitampl(y, B, alpha, p, a, pord, lambda)
  alpha <- alpha / sqrt(mean(alpha ^ 2))
  anew <- fitasy(y, B, alpha, p, a)
  da = max(abs(a - anew))
  a = anew
  cat(it, da, '\n')
  if (da < 1e-6) break
}

# Compute bundle on grid
ampl <- Bg %*% alpha
Z <- ampl %*% a

# Plot data and bundle
plot(x, y, pch = 15, cex = 0.7, col = 'grey', xlab = 'Age', ylab = 'Density')
cols = colorspace::rainbow_hcl(np, start = 10, end = 350)
matlines(xg, Z, lty = 1, lwd = 2, col = cols)
```

G519C18

Chromosome G519C18 data

Description

An extract of the data set G519 in the Bioconductor package Vega, for chromosome 18.

Usage

```
data(G519C18)
```

Format

A dataframe with two columns:

y Probe position

x Log R Ratio.

References

<https://www.bioconductor.org/packages/release/bioc/html/Vega.html>

Examples

```
plot(G519C18$x, G519C18$y, type = 'l', ylab = 'LRR', xlab = 'Position', main = 'Chromosome 18')
```

Greece_deaths

Deaths in Greece in 1960.

Description

Deaths in Greece in 1960.

Usage

```
data(Greece_deaths)
```

Format

A dataframe with three columns:

Age 0 - 85

Male male deaths

Female female deaths.

Details

All counts for ages above 84 have been grouped to one number for age 85.

Source

Personal information from Aris Perperoglou.

Hepatitis	<i>Prevalence of Hepatitis among a sample of Bulgarian males.</i>
-----------	---

Description

Prevalence of Hepatitis among a sample of Bulgarian males.

Usage

```
data(Hepatitis)
```

Format

A data frame with three columns:

Age years

Infected number of infected persons

Sampled number of sampled persons.

Source

Table 2 in Keiding (1991).

References

N. Keiding (1991) Age-Specific Incidence and Prevalence: A Statistical Perspective. *JRSS-A* 154, 371-396.

hist2d	<i>Compute a 2D histogram</i>
--------	-------------------------------

Description

Compute a two-dimesnional histogram from two vectors (of the same length), x and y.

Usage

```
hist2d(x, y, nb = c(100, 100), xlim = range(x), ylim = range(y))
```

Arguments

x	a numeric vector.
y	a numeric vector of the same length as x.
nb	a vector c(nbx, nby), or a scalar nb, providing the number of bins for x, and y; default is 100; see details.
xlim	a vector c(xmin, xmax) containing the limits of the domain of x; default range(x).
ylim	a vector c(ymin, ymax) containing the limits of the domain of y; default range(y).

Details

If `nb` is scalar, it is extended to `c(nb, nb)`, so that both dimensions will have the same number of bins.

Elements of `x` (`y`) that fall outside the range specified by `xlim` (`ylim`) are not counted.

Value

A list with components:

<code>H</code>	a matrix of dimension <code>nbx</code> by <code>nby</code> containing bin counts.
<code>xgrid</code>	a vector of length <code>nbx</code> representing centers of the bins for <code>x</code> .
<code>ygrid</code>	a vector of length <code>nby</code> representing centers of the bins for <code>y</code> .
<code>xbin</code>	a vector giving the bin number of each element of <code>x</code> .
<code>ybin</code>	a vector giving the bin number of each element of <code>y</code> .

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
data(faithful)
x = faithful$eruptions
y = faithful$waiting
C = hist2d(x, y, c(50,50))
image(C$xgrid, C$ygrid, C$H, xlab='Eruption length (min)', ylab='Waiting time (min)')
title('Old Faithful geyser')
```

hist2dsm

Smooth a 2D histogram

Description

Fit a 2D smooth P-spline surface to a matrix of counts, assuming Poisson distributed observations.

Usage

```
hist2dsm(
  Y,
  nsegx = 10,
  nsegy = nsegx,
  bdeg = 3,
  lambdax = 10,
  lambday = lambdax,
  dx = 3,
  dy = dx,
  Mu = Y + 0.01,
  kappa = 1e-04,
  tol = 1e-05
)
```

Arguments

Y	a matrix of counts.
nsegx	the number of knots along x (default=10).
nsegy	the number of evenly spaced knots along y for Tensor product B-spline basis (default=10).
bdeg	the degree of the basis, default is 3.
lambdax	the positive number for the tuning parameter along x.
lambday	the positive number for the tuning parameter along y.
dx	the order of the difference penalty along x, default is 3.
dy	the order of the difference penalty along y, default is 3.
Mu	the initialization of the mean (default $Y + 0.01$).
kappa	a (small, positive) number for ridge tuning parameter to stabilize estimation (default $1e-4$).
tol	the convergence criterion (default $1e-5$).

Value

A list with elements:

ed	the effective dimension of the smooth 2D surface.
Mu	a matrix with the smooth estimates, with dimensions of $\dim(Y)$
pen	the numerical value of the penalty.

Author(s)

Paul Eilers

References

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
x = faithful$eruptions
y = faithful$waiting
h = hist2d(x, y, c(100, 100))
sm = hist2dsm(h$H, nsegx = 25, nsegy = 25, bdeg = 3, lambdax = 10, lambday = 10)
image(h$xgrid, h$ygrid, sm$Mu, xlab = 'Eruption length (min)',
      ylab = 'Waiting time (min)', main = 'Old Faithful')
```

indiumoxide	<i>An X-ray diffractogram.</i>
-------------	--------------------------------

Description

An X-ray diffractogram.

Usage

```
data(indiumoxide)
```

Format

A matrix with two columns:

angle the angles (degrees) of diffraction

count corresponding photon counts.

Details

An X-ray diffractogram of Indium-Tin oxide.

These data have been taken from the source of package *Diffraction*, which is no longer available from CRAN in binary form.

Source

P.L. Davies, U. Gather, M. Meise, D. Mergel, T. Mildenerger (2008). Residual based localization and quantification of peaks in x-ray diffractograms, *Annals of Applied Statistics*, Vol. 2, No. 3, 861-886.

Examples

```
angle = indiumoxide[,1]
photon = indiumoxide[,2]
plot(angle, type = 'l', photon, xlab = 'Angle', ylab = 'Photon count')
```

inverse_link	<i>Inverse link function, used for GLM fitting.</i>
--------------	---

Description

Inverse link function, used for GLM fitting.

Usage

```
inverse_link(x, link)
```

Arguments

x	scalar, vector, or matrix input.
link	the link function, one of "identity", "log", "sqrt", "logit", "probit", "cloglog", "loglog", "reciprocal"; quotes are needed (default "identity").

Value

The inverse link function applied to x. If link is not in the above list of allowed names, NULL will be returned.

 JOPS

Joys of P-Splines

Description

A package for working with and learning about P-splines. P-splines combine B-splines with discrete penalties to build a very flexible and effective smooth models. They can handle non-normal data in the style of generalized linear models.

This package provides functions for constructing B-spline bases and penalty matrices. It solves the penalized likelihood equations efficiently.

Several methods are provided to determine the values of penalty parameters automatically, using cross-validation, AIC, mixed models or fast Bayesian algorithms.

This package is a companion to the book by Eilers and Marx (2021). The book presents the underlying theory and contains many examples and the code R for each example is available on the website <https://psplines.bitbucket.io>

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

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

 JOPS_colors

Custom color ramp.

Description

Custom color ramp.

Usage

```
JOPS_colors(n)
```

Arguments

n	number of steps.
---	------------------

Value

custom color ramp.

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

JOPS_point	<i>Themeing functions used to unify ggplot features</i>
------------	---

Description

Custom size and color of points.

Usage

```
JOPS_point(s_size = 1.5)
```

Arguments

`s_size` point size parameter for ggplot2 (default = 1.5).

Value

themeing function for ggplot2 features.

JOPS_theme	<i>Custom theme for ggplot</i>
------------	--------------------------------

Description

Set a ggplot theme in black and white, with centered titles.

Set a ggplot theme in black and white, with centered titles.

Usage

```
JOPS_theme(h_just = 0.5)
```

```
JOPS_theme(h_just = 0.5)
```

Arguments

`h_just` horizontal justification for ggplot2.

Value

custom theme for ggplot.

Custom theming function used to unify ggplot features.

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

LAPS_dens

Bayesian density estimation

Description

Bayesian density estimation with P-splines and Laplace approximation.

Usage

```
LAPS_dens(B, P, y, loglambdas, tol = 1e-05, mon = FALSE)
```

Arguments

B	matrix (m by n) with B-spline basis, see <code>bbase()</code> .
P	penalty matrix (n by n).
y	vector (length m) of counts, usually a histogram.
loglambdas	a vector of values of logarithms of lambda to explore.
tol	convergence tolerance (relative change in coefficients), default 1e-5.
mon	TRUE or FALSE to monitor the iteration history (default FALSE).

Details

The B-spline basis should be based on the midpoints of the histogram bins. See the example below. This function is based on the paper of Gressani and Lambert (2018) and code input by Oswaldo Gressani.

Value

A list with elements:

alpha	P-spline coefficients of length n.
weights	weights from the Laplace approximation, which sum to 1 and are the same length as loglambdas.
mu	a vector of length m of expected values.
Cov	covariance matrix (m by m) of log(mu).
lambda	the penalty parameter.
ed	the effective model dimension.

Author(s)

Paul Eilers

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Gressani, O. and Lambert, P. (2018). Fast Bayesian inference using Laplace approximations in a flexible promotion time cure model based on P-splines. *Computational Statistics and Data Analysis* 124, 151-167.

Examples

```
# Smoothing a histogram of Old Faithful eruption durations
data(faithful)
durations = faithful[, 1] # Eruption length

# Histogram with narrow bin widths
bw = 0.05
hst = hist(durations, breaks = seq(1, 6, by = bw), plot = TRUE)
x = hst$mids
y = hst$counts

# B-spline basis matrices, for fitting and plotting
nseg = 30
B = bbase(x, nseg = nseg)
xg = seq(min(x), max(x), by = 0.01)
Bg = bbase(xg, nseg = nseg)
n = ncol(B)

# Penalty matrix
D2 = diff(diag(n), diff = 2)
P2 = t(D2) %*% D2

# Fit the model
loglambs = seq(-1, 2, by = 0.05)
laps2 = LAPS_dens(B, P2, y, loglambs, mon = FALSE)
fhat2 = exp(Bg %*% laps2$alpha)
lines(xg, fhat2, col = "blue", lwd = 2)
```

Mixture

Mixture Data

Description

The mixture data were obtained in an unpublished experiment in 2001 by Zhenyu Wang at University of Amsterdam, under the supervision of Age Smilde. We are grateful for the permission to use the data.

Usage

```
data(Mixture)
```

Format

A list consisting of the following:

`fractions` a 34 x 3 matrix of mixture fractions (rows sum to unity): Water (subboiled demi water (self made)), 1,2ethanediol (99.8% Sigma-Aldrich Germany), 3amino1propanol (99% Merk Schuchardt Germany)

`xspectra` spectra array, 34 (observations) x 401 (wavelenths channels) x 12 (temperatures (C): 30, 35, 37.5, 40, 45, 47.5, 50, 55, 60, 62.5, 65, 70)

`wl` wavelenghts for the spectra, 700 to 1100 (nm), by 1nm.

Details

The following instruments and chemicals were used in the experiment: HP 8453 spectrophotometer (Hewlett-Packard, Palo Alto, CA); 2cm closed quartz cuvette with glass thermostatable jacket; Pt-100 temperature sensor; Neslab microprocessor EX-111 circulator bath; UV-visible Chemstation software (Rev A.02.04) on a Hewlett-Packard Vectra XM2 PC.

References

Eilers, P. H. C., and Marx, B. D. (2003). Multivariate calibration with temperature interaction using two-dimensional penalized signal regression. *Chemometrics and Intelligent Laboratory Systems*, 66, 159–174.

Marx, B. D., Eilers, P. H. C., and Li, B. (2011). Multidimensional single-index signal regression. *Chemometrics and Intelligent Laboratory Systems*, 109(2), 120–130. [see the Appendix within]

Zhenyou Wang and Age Smilde, Univeristy of Amsterdam, The Netherlands. Personal communication.

pclm

Fit a composite link model

Description

Fit a smooth latent distribution using the penalized composite link model (PCLM).

Usage

```
pclm(y, C, B, lambda = 1, pord = 2, itmax = 50, show = FALSE)
```

Arguments

<code>y</code>	a vector of counts, length <code>m</code> .
<code>C</code>	a composition matrix, <code>m</code> by <code>q</code> .
<code>B</code>	a B-spline basis matrix, <code>q</code> by <code>n</code> .
<code>lambda</code>	the penalty parameter.
<code>pord</code>	the the order of the difference penalty (default = 2).
<code>itmax</code>	the maximum number of iterations (default = 50).
<code>show</code>	Set to TRUE or FALSE to display iteration history (default = FALSE).

Details

The composite link model assumes that $E(y) = \mu = C \exp(B\alpha)$, where $\exp(B\alpha)$ is a latent discrete distribution, usually on a finer grid than that for y .

Note that `sum(gamma) == sum(mu)`.

Value

A list with the following items:

alpha	the estimated B-spline coefficients, length n.
gamma	the estimated latent distribution, length q.
mu	estimated values of y, length m.
dev	the deviance of the model.
ed	the effective model dimension.
aic	Akaike's Information Criterion.

Author(s)

Paul Eilers and Jutta Gampe

References

Eilers, P. H. C. (2007). III-posed problems with counts, the composite link model and penalized likelihood. *Statistical Modelling*, 7(3), 239–254.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
# Left and right boundaries, and counts, of wide intervals of the data
cb <- c( 0, 20, 30, 40, 50, 60)
ce <- c(20, 30, 40, 50, 60, 70)
y <- c(79, 54, 19, 1, 1, 0)

# Construct the composition matrix
m <- length(y)
n <- max(ce)
C <- matrix(0, m, n)
for (i in 1:m) C[i, cb[i]:ce[i]] <- 1

mids = (cb + ce) / 2 - 0.5
widths = ce - cb + 1
dens = y / widths / sum(y)
x = (1:n) - 0.5
B = bbase(x)
fit = pclm(y, C, B, lambda = 2, pord = 2, show = TRUE)
gamma = fit$gamma / sum(fit$gamma)
# Plot density estimate and data
plot(x, gamma, type = 'l', lwd = 2, xlab = "Lead Concentration", ylab = "Density")
rect(cb, 0, ce, dens, density = rep(10, 6), angle = rep(45, 6))
```

plot.ps2dglm *Plotting function for ps2DGLM*

Description

Plotting function for 2D P-spline (GLM) smoothing (using ps2DGLM with class ps2dglm).

Usage

```
## S3 method for class 'ps2dglm'
plot(x, ..., xlab = " ", ylab = " ", Resol = 100, se = 2)
```

Arguments

x	the P-spline object, usually from ps2DGLM.
...	other parameters.
xlab	label for the x-axis, e.g. "my x" (quotes required).
ylab	label for the y-axis, e.g. "my y" (quotes required).
Resol	resolution for plotting, default Resol = 100.
se	a scalar, e.g. se = 2 to produce twice se surfaces, set se > 0 (or set se = 0 to suppress).

Value

Plot a plot of the mean (inverse link) 2D P-spline (GLM) smooth surface.

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Examples

```
library(fields)
library(JOPS)
# Extract data
library(rpart)
Kyphosis <- kyphosis$Kyphosis
Age <- kyphosis$Age
Start <- kyphosis$Start
y <- 1 * (Kyphosis == "present") # make y 0/1
fit <- ps2DGLM(
  Data = cbind(Start, Age, y),
  Pars = rbind(c(1, 18, 10, 3, .1, 2), c(1, 206, 10, 3, .1, 2)),
  family = "binomial"
```

```

)
plot(fit, xlab = "Start", ylab = "Age")
#title(main = "Probability of Kyphosis")

```

plot.ps2dnormal	<i>Plotting function for ps2DNormal</i>
-----------------	---

Description

Plotting function for 2D P-spline smoothing (using ps2DNormal with class ps2dnormal).

Usage

```

## S3 method for class 'ps2dnormal'
plot(x, ..., xlab = " ", ylab = " ", Resol = 100)

```

Arguments

x	the P-spline object, usually from ps2DNormal.
...	other parameters.
xlab	label for the x-axis, e.g. "my x" (quotes required).
ylab	label for the y-axis, e.g. "my y" (quotes required).
Resol	resolution for plotting, default Resol = 100.

Value

Plot	a plot of the smooth 2D P-spline smooth surface.
------	--

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Examples

```

library(SemiPar)
library(fields)
library(spam)
library(JOPS)

# Get the data
data(ethanol)
x <- ethanol$C
y <- ethanol$E
z <- ethanol$NOx

```

```
# Set parameters for domain
xlo <- 7
xhi <- 19
ylo <- 0.5
yhi <- 1.25

# Set P-spline parameters, fit and compute surface
xpars <- c(xlo, xhi, 10, 3, 3, 1)
ypars <- c(ylo, yhi, 10, 3, 3, 1)
Pars1 <- rbind(xpars, ypars)
fit <- ps2DNormal(cbind(x, y, z), Pars = Pars1)
plot(fit, xlab = "C", ylab = "E")
```

plot.ps2dsignal

Plotting function for ps2DSignal

Description

Plotting function for 2D P-spline signal regression coefficients (using ps2DSignal with class ps2dsignal). Although standard error surface bands can be computed they are intentionally left out as they are not interpretable, and there is generally little data to steer such a high-dimensional parameterization.

Usage

```
## S3 method for class 'ps2dsignal'
plot(x, ..., xlab = " ", ylab = " ", Resol = 200)
```

Arguments

x	the P-spline object, usually from ps2DSignal.
...	other parameters.
xlab	label for the x-axis, e.g. "my x" (quotes required).
ylab	label for the y-axis, e.g. "my y" (quotes required).
Resol	Resolution of bgrid (default Resol = 200).

Value

Plot	a plot of the 2D P-spline signal coefficient surface.
------	---

Author(s)

Paul Eilers and Brian Marx

References

Marx, B.D. and Eilers, P.H.C. (2005). Multidimensional penalized signal regression, *Technometrics*, 47: 13-22.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```

library(fields)
library(JOPS)

# Get the data
x0 <- Sugar$X
x0 <- x0 - apply(x0, 1, mean) # center Signal
y <- as.vector(Sugar$y[, 3]) # Response is Ash

# Inputs for two-dimensional signal regression
nseg <- c(7, 37)
pord <- c(3, 3)
min_ <- c(230, 275)
max_ <- c(340, 560)
M1_index <- rev(c(340, 325, 305, 290, 255, 240, 230))
M2_index <- seq(from = 275, to = 560, by = .5)
p1 <- length(M1_index)
p2 <- length(M2_index)

# Fit optimal model based on L00CV
opt_lam <- c(8858.6679, 428.1332) # Found via svcm
Pars_opt <- rbind(
  c(min_[1], max_[1], nseg[1], 3, opt_lam[1], pord[1]),
  c(min_[2], max_[2], nseg[2], 3, opt_lam[2], pord[2]))

fit <- ps2DSignal(y, x0, p1, p2, "unfolded", M1_index, M2_index,
  Pars_opt, int = FALSE, ridge_adj = 1e-4 )

# Plotting coefficient image
plot(fit)

```

plot.pspfit

*Plotting function for psNormal, psPoisson, psBinomial***Description**

Plotting function for P-spline smooth with normal, Poisson, or binomial responses (class pspfit), with or without standard error bands.

Usage

```

## S3 method for class 'pspfit'
plot(x, ..., se = 2, xlab = "", ylab = "", col = "black", pch = 1)

```

Arguments

x	the P-spline object, usually from psNormal, psPoisson, psBinomial.
...	other parameters.
se	a scalar, e.g. se = 2 to produce twice se bands, set se > 0 (or set se=0 to supress).
xlab	label for the x-axis.
ylab	label for the y-axis.
col	color for points.
pch	point character.

Value

Plot a plot of the mean (inverse link) smoothed normal, Poisson, or binomial responses, with or without se bands.

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Examples

```
library(JOPS)
#Extract data
library(MASS)
# Get the data
data(mcycle)
x = mcycle$times
y = mcycle$accel
fit1 = psNormal(x, y, nseg = 20, bdeg = 3, pord = 2, lambda = .8)
plot(fit1, se = 2, xlab = "time (ms)", ylab = "accel")

library(JOPS)
library(boot)
# Extract the data
Count = hist(coal$date, breaks=c(1851:1963), plot = FALSE)$counts
Year = c(1851:1962)
xl = min(Year)
xr = max(Year)

# Poisson smoothing
nseg = 20
bdeg = 3
fit1=psPoisson(Year, Count, xl, xr, nseg, bdeg, pord = 2,
lambda = 1)
names(fit1)
plot(fit1, xlab = "Year", ylab = "Count", se = 2)

library(JOPS)
#Extract data
library(rpart)
Kyphosis = kyphosis$Kyphosis
Age =kyphosis$Age
y = 1 * (Kyphosis == "present") # make y 0/1
# Binomial smoothing
fit1 = psBinomial(Age, y, xl = min(Age), xr = max(Age), nseg = 20,
bdeg = 3, pord = 2, lambda = 1)
names(fit1)
plot(fit1, xlab = "Age", ylab = '0/1', se = 2)
```

plot.pssignal	<i>Plotting function for psSignal</i>
---------------	---------------------------------------

Description

Plotting function for signal regression P-spline smooth coefficients (using psSignal with class pssignal), with or without standard error bands.

Usage

```
## S3 method for class 'pssignal'
plot(x, ..., se = 2, xlab = "", ylab = "", col = "black", lty = 1)
```

Arguments

x	the P-spline x, usually from psSignal.
...	other parameters.
se	a scalar, e.g. se = 2 to produce twice se bands, set se > 0 (or set se = 0 to suppress).
xlab	label for the x-axis, e.g. "my x" (quotes required).
ylab	label for the y-axis, e.g. "my y" (quotes required).
col	color.
lty	line type for plotting e.g. lty = 2.

Value

Plot	a plot of the smooth P-spline signal coefficient vector, with or without standard error bands.
------	--

Author(s)

Paul Eilers and Brian Marx

References

Marx, B.D. and Eilers, P.H.C. (1999). Generalized linear regression for sampled signals and curves: A P-spline approach. *Technometrics*, 41(1): 1-13.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(JOPS)
# Get the data
library(fds)
data(nirc)
iindex=nirc$x
X=nirc$y
sel= 50:650 #1200 <= x & x<= 2400
X=X[sel, ]
```

```

iindex=iindex[sel]
dX=diff(X)
diindex=iindex[-1]
y=as.vector(labc[1,1:40])
oout = 23
dX=t(dX[, -oout])
y=y[-oout]
fit2 = psSignal(y, dX, diindex, nseg = 25, lambda = 0.0001)
plot(fit2, se = 2, xlab = 'Coefficient Index', ylab= "ps Smooth Coeff")
title(main='25 B-spline segments with tuning=0.0001')
names(fit2)

```

plot.psvcsignal

Plotting function for psVCSignal

Description

Plotting function for varying-coefficient signal regression P-spline smooth coefficients (using psVCSignal with class psvcsignal). Although se surface bands can be computed they are intentionally left out as they are not interpretable, and there is generally little data to steer such a high-dimensional parameterization.

Usage

```

## S3 method for class 'psvcsignal'
plot(x, ..., xlab = " ", ylab = " ", Resol = 100)

```

Arguments

x	the P-spline object, usually from psVCSignal.
...	other parameters.
xlab	label for the x-axis, e.g. "my x" (quotes required).
ylab	label for the y-axis, e.g. "my y" (quotes required).
Resol	resolution for plotting, default Resol = 100.

Value

Plot	a two panel plot, one of the 2D P-spline signal coefficient surface and another that displays several slices of the smooth coefficient vectors at fixed levels of the varying index.
------	--

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P. H. C. and Marx, B. D. (2003). Multivariate calibration with temperature interaction using two-dimensional penalized signal regression. *Chemometrics and Intelligent Laboratory Systems*, 66, 159–174.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```

library(fds)
data(nirc)
iindex <- nirc$x
X <- nirc$y
sel <- 50:650 # 1200 <= x & x<= 2400
X <- X[sel, ]
iindex <- iindex[sel]
dX <- diff(X)
diindex <- iindex[-1]
y <- as.vector(labc[1, 1:40]) # percent fat
t_var <- as.vector(labc[4, 1:40]) # percent flour
oout <- 23
dX <- t(dX[, -oout])
y <- y[-oout]
t_var = t_var[-oout]
Pars = rbind(c(min(diindex), max(diindex), 25, 3, 1e-7, 2),
c(min(t_var), max(t_var), 20, 3, 0.0001, 2))
fit1 <- psVCSignal(y, dX, diindex, t_var, Pars = Pars,
family = "gaussian", link = "identity", int = TRUE)
plot(fit1, xlab = "Coefficient Index", ylab = "VC: % Flour")
names(fit1)

```

plot.simpsr

*Plotting function for sim_psr***Description**

Plotting function for single-index signal regression with tensor product P-splines (using `sim_psr` with class `simpsr`).

Usage

```

## S3 method for class 'simpsr'
plot(x, ..., xlab = " ", ylab = " ", Resol = 100)

```

Arguments

<code>x</code>	the P-spline object, usually from <code>sim_psr</code> .
<code>...</code>	other parameters.
<code>xlab</code>	label for the x-axis, e.g. "my x" (quotes required).
<code>ylab</code>	label for the y-axis, e.g. "my y" (quotes required).
<code>Resol</code>	resolution for plotting, default <code>Resol = 100</code> .

Value

`Plot` a two panel plot, one for the estimated P-spline signal coefficient vector, and another for the estimated (unkown) P-spline smooth link function.

Author(s)

Paul Eilers, Brian Marx, and Bin Li

References

Eilers, P.H.C., B. Li, B.D. Marx (2009). Multivariate calibration with single-index signal regression, *Chemometrics and Intelligent Laboratory Systems*, 96(2), 196-202.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(JOPS)
# Get the data
library(fds)
data(nirc)
iindex <- nirc$x
X <- nirc$y
sel <- 50:650 # 1200 <= x & x<= 2400
X <- X[sel, ]
iindex <- iindex[sel]
dX <- diff(X)
diindex <- iindex[-1]
y <- as.vector(labc[1, 1:40])
oout <- 23
dX <- t(dX[, -oout])
y <- y[-oout]

pords <- c(2, 2)
nsegs <- c(27, 7)
bdegs = c(3, 3)
lambdas <- c(1e-6, .1)
max_iter <- 100

# Single-index model
fit <- sim_psr(y, dX, diindex, nsegs, bdegs, lambdas, pords,
              max_iter)
plot(fit, xlab = "Wavelength (nm)", ylab = " ")
```

plot.simvcpsr

Plotting function for sim_vcpsr

Description

Plotting function for varying-coefficient single-index signal regression using tensor P-splines (using sim_vcpsr with class simvcpsr).

Usage

```
## S3 method for class 'simvcpsr'
plot(x, ..., xlab = " ", ylab = " ", Resol = 100)
```

Arguments

x	the P-spline object, usually from sim_vcpsr.
...	other parameters.
xlab	label for the x-axis, e.g. "my x" (quotes required).
ylab	label for the y-axis, e.g. "my y" (quotes required).
Resol	resolution for plotting, default Resol = 100.

Value

Plot	a plot of the estimated 2D P-spline signal coefficient surface along with the companion plot of the estimated 2D P-spline varying link function surface. Slices of these plots, at fixed levels of the indexing covariate, are also provided.
------	---

Author(s)

Paul Eilers and Brian Marx

References

Marx, B. D. (2015). Varying-coefficient single-index signal regression. *Chemometrics and Intelligent Laboratory Systems*, 143, 111–121.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

```
# @examples # Load libraries library(fields) # Needed for plotting
# Get the data Dat <- Mixture
# Dimensions: observations, temperature index, signal m <- 34 p1 <- 401 p2 <- 12
# Stacking mixture data, each mixture has 12 signals stacked # The first differenced spectra are also
# computed. mixture_data <- matrix(0, nrow = p2 * m, ncol = p1) for (ii in 1:m)
mixture_data[((ii - 1) * p2 + 1):(ii * p2), 1:p1] <- t(as.matrix(Dat$xspectra[ii, ])) d_mixture_data
<- t(diff(t(mixture_data)))
# Response (typo fixed) and index for signal y_mixture <- Dat$fractions y_mixture[17, 3] <- 0.1501
index_mixture <- Dat$w1
# Select response and replicated for the 12 temps # Column 1: water; 2: ethanediol; 3: amino-1-
# propanol y <- as.vector(y_mixture[, 2]) y <- rep(y, each = p2)
bdegs = c(3, 3, 3, 3) pords <- c(2, 2, 2, 2) nsegs <- c(12, 5, 5, 5) # Set to c(27, 7, 7, 7) for given
# lambdas mins <- c(700, 30) maxs <- c(1100, 70) lambdas <- c(1e-11, 100, 0.5, 1) # based on svcm
# search x_index <- seq(from = 701, to = 1100, by = 1) # for dX t_var_sub <- c(30, 35, 37.5, 40, 45,
# 47.5, 50, 55, 60, 62.5, 65, 70) t_var <- rep(t_var_sub, m) max_iter <- 2 # Set higher in practice, e.g.
# 100 int <- TRUE
# Defining x as first differenced spectra, number of channels. x <- d_mixture_data
# Single-index VC model using optimal tuning fit <- sim_vcpsr(y, x, t_var, x_index, nsegs, bdegs,
# lambdas, pords, max_iter = max_iter, mins = mins, maxs = maxs)
plot(fit, xlab = "Wavelength (nm)", ylab = "Temp C")
```

predict.ps2dglm *Predict function for ps2DGLM*

Description

Prediction function which returns both linear predictor and inverse link predictions at arbitrary (x, y) data locations (using ps2DGLM with class ps2dglm).

Usage

```
## S3 method for class 'ps2dglm'
predict(object, ..., XY, type = "mu")
```

Arguments

object	an object using ps2DGLM.
...	other parameters.
XY	a matrix of arbitrary (x, y) locations for desired prediction.
type	the mean value type = "mu" (default) or linear predictor type = "eta".

Value

pred	the estimated mean (inverse link function) (default) or the linear predictor prediction with type = "eta", for arbitrary (x, y) locations in XY.
------	--

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(fields)
library(JOPS)
# Extract data
library(rpart)
Kyphosis <- kyphosis$Kyphosis
Age <- kyphosis$Age
Start <- kyphosis$Start
y <- 1 * (Kyphosis == "present") # make y 0/1
fit <- ps2DGLM(
  Data = cbind(Start, Age, y),
  Pars = rbind(c(1, 18, 10, 3, .1, 2), c(1, 206, 10, 3, .1, 2)),
  family = "binomial", link = "logit")
predict(fit, XY = cbind(Start, Age)[1:5,])
```

predict.ps2dnormal *Predict function for ps2DNormal*

Description

Prediction function which returns linear predictions at arbitrary (x, y) data locations (using ps2DNormal with class ps2dnormal).

Usage

```
## S3 method for class 'ps2dnormal'  
predict(object, ..., XY)
```

Arguments

object	an object using ps2DNormal.
...	other parameters.
XY	a matrix of arbitrary (x, y) locations for desired prediction.

Value

pred	the estimated mean at (x, y) locations, in XY.
------	--

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(SemiPar)  
library(fields)  
library(spam)  
library(JOPS)  
  
# Get the data  
data(ethanol)  
x <- ethanol$C  
y <- ethanol$E  
z <- ethanol$NOx  
  
# Set parameters for domain  
xlo <- 7  
xhi <- 19  
ylo <- 0.5  
yhi <- 1.25
```

```
# Set P-spline parameters, fit and compute surface
xpars <- c(xlo, xhi, 10, 3, 0.01, 1)
ypars <- c(ylo, yhi, 10, 3, 0.1, 1)
Pars1 <- rbind(xpars, ypars)
fit <- ps2DNormal(cbind(x, y, z), Pars = Pars1)
predict(fit, XY = cbind(x, y)[1:5, ])
```

predict.ps2dsignal *Predict function for ps2DSignal*

Description

Prediction function which returns both linear predictor and inverse link predictions for arbitrary 2D signals (using ps2DSignal with class ps2dsignal).

Usage

```
## S3 method for class 'ps2dsignal'
predict(object, ..., M_pred, M_type = "unfolded", type = "mu")
```

Arguments

object	an object using ps2DSignal.
...	other parameters.
M_pred	a matrix of q arbitrary "stacked" or "unfolded" signal matrices of dimension (q by p1) by p2 or q by (p1 by p2, respectively, for desired prediction (default "unfolded").
M_type	"stacked" or "unfolded" (default).
type	the mean value type = "mu" (default) or linear predictor type = "eta".

Value

pred	the estimated mean (inverse link function) or the linear predictor prediction with type = "eta", for arbitrary 2D signals in M_pred.
------	--

Author(s)

Paul Eilers and Brian Marx

References

Marx, B.D. and Eilers, P.H.C. (2005). Multidimensional penalized signal regression, *Technometrics*, 47: 13-22.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```

library(fields)
library(JOPS)

# Get the data
x0 <- Sugar$X
x0 <- x0 - apply(x0, 1, mean) # center Signal
y <- as.vector(Sugar$y[, 3]) # Response is Ash

# Inputs for two-dimensional signal regression
nseg <- c(7, 37)
pord <- c(3, 3)
min_ <- c(230, 275)
max_ <- c(340, 560)
M1_index <- rev(c(340, 325, 305, 290, 255, 240, 230))
M2_index <- seq(from = 275, to = 560, by = .5)
p1 <- length(M1_index)
p2 <- length(M2_index)

# Fit optimal model based on L00CV
opt_lam <- c(8858.6679, 428.1332) # Found via svcm
Pars_opt <- rbind(
  c(min_[1], max_[1], nseg[1], 3, opt_lam[1], pord[1]),
  c(min_[2], max_[2], nseg[2], 3, opt_lam[2], pord[2])
)
fit <- ps2DSignal(y, x0, p1, p2, "unfolded", M1_index, M2_index,
  Pars_opt, int = TRUE, ridge_adj = 0.0001,
  M_pred = x0 )

predict(fit, M_pred= x0, type = "mu", M_type = "unfolded")

```

predict.pspfit

Predict function for psNormal, psBinomial, psPoisson

Description

Prediction function which returns both linear predictor and inverse link predictions at arbitrary data locations (using psNormal, psBinomial, psPoisson with class pspfit).

Usage

```

## S3 method for class 'pspfit'
predict(object, ..., x, type = "mu")

```

Arguments

object	an object using psNormal, psBinomial, or psPoisson .
...	other parameters.
x	a scalar or vector of arbitrary x locations for desired prediction.
type	the mean value type = "mu" (default) or linear predictor type = "eta".

Value

pred the estimated mean (inverse link function) (default) or the linear predictor prediction with `type = "eta"`, at arbitrary `x` locations.

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(JOPS)
library(boot)

# Extract the data
Count <- hist(coal$date, breaks = c(1851:1963), plot = FALSE)$counts
Year <- c(1851:1962)
xl <- min(Year)
xr <- max(Year)

# Poisson smoothing
nseg <- 20
bdeg <- 3
fit1 <- psPoisson(Year, Count, xl, xr, nseg, bdeg, pord = 2, lambda = 1)
names(fit1)
plot(fit1, xlab = "Year", ylab = "Count", se = 2)
predict(fit1, x = fit1$x[1:5])
predict(fit1, x = fit1$x[1:5], type = "eta")
```

predict.pssignal *Predict function for psSignal*

Description

Prediction function which returns both linear predictor and inverse link predictions, for an arbitrary matrix of signals (using `psSignal` with class `pssignal`).

Usage

```
## S3 method for class 'pssignal'
predict(object, ..., X_pred, type = "mu")
```

Arguments

object	an object using psSignal.
...	other parameters.
X_pred	a matrix of arbitrary signals with $\text{ncol}(X) == \text{length}(x_index)$ locations for desired prediction.
type	the mean value type = "mu" (default) or linear predictor type = "eta".

Value

pred	the estimated mean (inverse link function) (default) or the linear predictor prediction with type = "eta", for a matrix of signals in X_pred.
------	---

Author(s)

Paul Eilers and Brian Marx

References

Marx, B.D. and Eilers, P.H.C. (1999). Generalized linear regression for sampled signals and curves: A P-spline approach. *Technometrics*, 41(1): 1-13.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(JOPS)
# Get the data
library(fds)
data(nirc)
iindex=nirc$x
X=nirc$y
sel= 50:650 #1200 <= x & x<= 2400
X=X[sel,]
iindex=iindex[sel]
dX=diff(X)
diindex=iindex[-1]
y=as.vector(labc[1,1:40])
oout=23
dX=t(dX[, -oout])
y=y[-oout]
fit1 = psSignal(y, dX, diindex, nseg = 25, lambda = 0.0001)
predict(fit1, X_pred = dX[1:5, ])
predict(fit1, X_pred = dX[1:5, ], type = 'eta')
```

predict.psvcsignal *Predict function for psVCSignal*

Description

Prediction function which returns both linear predictor and inverse link predictions for an arbitrary matrix of signals with their vector of companion indexing covariates (using psVCSignal with class psvcsignal).

Usage

```
## S3 method for class 'psvcsignal'
predict(object, ..., X_pred, t_pred, type = "mu")
```

Arguments

object	an object using psVCSignal.
...	other parameters.
X_pred	a matrix of q arbitrary signal vectors of dimension q by p1 for desired prediction.
t_pred	a q vector for the varying index variable associated with X_pred.
type	the mean value type = "mu" (default) or linear predictor type = "eta".

Value

pred	the estimated mean (inverse link function) (default) or the linear predictor prediction with type = "eta", at signals in matrix X_pred and covariates in vector t_pred.
------	---

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P. H. C. and Marx, B. D. (2003). Multivariate calibration with temperature interaction using two-dimensional penalized signal regression. *Chemometrics and Intelligent Laboratory Systems*, 66, 159–174.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(fds)
data(nirc)
iindex <- nirc$x
X <- nirc$y
sel <- 50:650 # 1200 <= x & x<= 2400
X <- X[sel, ]
iindex <- iindex[sel]
dX <- diff(X)
diindex <- iindex[-1]
y <- as.vector(labc[1, 1:40]) # percent fat
t_var <- as.vector(labc[4, 1:40]) # percent flour
oout <- 23
dX <- t(dX[, -oout])
y <- y[-oout]
t_var = t_var[-oout]
Pars = rbind(c(min(diindex), max(diindex), 25, 3, 1e-7, 2),
c(min(t_var), max(t_var), 20, 3, 0.0001, 2))
fit1 <- psVCSignal(y, dX, diindex, t_var, Pars = Pars,
family = "gaussian", link = "identity", int = TRUE)
predict(fit1, X_pred = dX[1:5,], t_pred = t_var[1:5])
```

predict.simsr	<i>Predict function for sim_psr</i>
---------------	-------------------------------------

Description

Prediction function which returns single-index inverse link linear predictions at arbitrary data locations (using `sim_psr` with class `simsr`).

Usage

```
## S3 method for class 'simsr'
predict(object, ..., X_pred)
```

Arguments

object	an object using <code>sim_psr</code> .
...	other parameters.
X_pred	a matrix of arbitrary signals with <code>ncol(X_pred) = length(x_index)</code> locations for desired prediction.

Value

pred	the estimated (inverse single-index) mean for the signals in <code>X_pred</code> .
------	--

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C., B. Li, B.D. Marx (2009). Multivariate calibration with single-index signal regression, *Chemometrics and Intelligent Laboratory Systems*, 96(2), 196-202.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(JOPS)
# Get the data
library(fds)
data(nirc)
iindex <- nirc$x
X <- nirc$y
sel <- 50:650 # 1200 <= x & x<= 2400
X <- X[sel, ]
iindex <- iindex[sel]
dX <- diff(X)
diindex <- iindex[-1]
y <- as.vector(labc[1, 1:40])
oout <- 23
dX <- t(dX[, -oout])
y <- y[-oout]
```

```

pords <- c(2, 2)
nsegs <- c(27, 7)
bdegs = c(3, 3)
lambdas <- c(1e-6, .1)
max_iter <- 100

# Single-index model
fit <- sim_psr(y, dX, diindex, nsegs, bdegs, lambdas, pords,
              max_iter)
predict(fit, X_pred = dX)

```

predict.simvcpsr	<i>Predict function for sim_vcpsr</i>
------------------	---------------------------------------

Description

Prediction function which returns varying-coefficient single-index inverse link linear predictions at arbitrary data locations (using `sim_vcpsr` with class `simvcpsr`).

Usage

```

## S3 method for class 'simvcpsr'
predict(object, ..., X_pred, t_pred)

```

Arguments

<code>object</code>	an object using <code>sim_vcpsr</code> .
<code>...</code>	other parameters.
<code>X_pred</code>	a matrix of arbitrary signals with <code>ncol(X_pred) = length(x_index)</code> locations for desired prediction.
<code>t_pred</code>	a <code>q</code> vector for the VC index variable associated with <code>X_pred</code> .

Value

<code>pred</code>	the estimated (inverse single-index) mean for the signals in the matrix <code>X_pred</code> , with the companion vector of indexing covariates in <code>t_pred</code> .
-------------------	---

Author(s)

Paul Eilers and Brian Marx

References

Marx, B. D. (2015). Varying-coefficient single-index signal regression. *Chemometrics and Intelligent Laboratory Systems*, 143, 111–121.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```

# Load libraries
library(fields) # Needed for plotting

# Get the data
Dat <- Mixture

# Dimensions: observations, temperature index, signal
m <- 34
p1 <- 401
p2 <- 12

# Stacking mixture data, each mixture has 12 signals stacked
# The first differenced spectra are also computed.
mixture_data <- matrix(0, nrow = p2 * m, ncol = p1)
for (ii in 1:m)
{
  mixture_data[((ii - 1) * p2 + 1):(ii * p2), 1:p1] <-
    t(as.matrix(Dat$spectra[ii, ]))
  d_mixture_data <- t(diff(t(mixture_data)))
}

# Response (typo fixed) and index for signal
y_mixture <- Dat$fractions
y_mixture[17, 3] <- 0.1501
index_mixture <- Dat$w1

# Select response and replicated for the 12 temps
# Column 1: water; 2: ethanediol; 3: amino-1-propanol
y <- as.vector(y_mixture[, 2])
y <- rep(y, each = p2)

bdegs = c(3, 3, 3, 3)
pords <- c(2, 2, 2, 2)
nsegs <- c(12, 5, 5, 5) # Set to c(27, 7, 7, 7) for given lambdas
mins <- c(700, 30)
maxs <- c(1100, 70)
lambdas <- c(1e-11, 100, 0.5, 1) # based on svcm search
x_index <- seq(from = 701, to = 1100, by = 1) # for dX
t_var_sub <- c(30, 35, 37.5, 40, 45, 47.5, 50, 55, 60, 62.5, 65, 70)
t_var <- rep(t_var_sub, m)
max_iter <- 2 # Set higher in practice, e.g. 100
int <- TRUE

# Defining x as first differenced spectra, number of channels.
x <- d_mixture_data

# Single-index VC model using optimal tuning
fit <- sim_vcpsr(y, x, t_var, x_index, nsegs, bdegs, lambdas, pords,
  max_iter = max_iter, mins = mins, maxs = maxs)

predict(fit, X_pred = x, t_pred = t_var)

```

ps2DGLM	<i>Two-dimensional smoothing of scattered normal or non-normal (GLM) responses using tensor product P-splines.</i>
---------	--

Description

ps2DGLM is used to smooth scattered normal or non-normal responses, with anisotropic penalization of tensor product P-splines.

Usage

```
ps2DGLM(
  Data,
  Pars = rbind(c(min(Data[, 1]), max(Data[, 1]), 10, 3, 1, 2), c(min(Data[, 2]),
    max(Data[, 2]), 10, 3, 1, 2)),
  ridge_adj = 0,
  XYpred = Data[, 1:2],
  z_predicted = NULL,
  se_pred = 2,
  family = "gaussian",
  link = "default",
  m_binomial = rep(1, nrow(Data)),
  wts = rep(1, nrow(Data)),
  r_gamma = rep(1, nrow(Data))
)
```

Arguments

Data	a matrix of 3 columns x, y, z of equal length; the response is z .
Pars	a matrix of 2 rows, where the first and second row sets the P-spline parameters for x and y , respectively. Each row consists of: min max nseg bdeg lambda pord. The min and max set the ranges, nseg (default 10) is the number of evenly spaced segments between min and max, bdeg is the degree of the basis (default 3 for cubic), lambda is the (positive) tuning parameter for the penalty (default 1), pord is the number for the order of the difference penalty (default 2).
ridge_adj	a ridge penalty tuning parameter, usually set to small value, e.g. $1e-8$ to stabilize estimation (default 0).
XYpred	a matrix with two columns (x, y) that give the coordinates of (future) prediction; the default is the data locations.
z_predicted	a vector of responses associated with XYpred, useful for external validation with family = "gaussian".
se_pred	a scalar, default se_pred = 2 to produce se surfaces, set se_pred > 0. Used for CIs for XYpred locations.
family	"gaussian", "binomial", "poisson", "Gamma" (quotes needed). Default is "gaussian".
link	the link function, one of "identity", "log", "sqrt", "logit", "probit", "cloglog", "loglog", "reciprocal"; quotes are needed (default "identity").
m_binomial	vector of binomial trials, default is vector of ones with family = "binomial", NULL otherwise.

wts	non-negative weights, which can be zero (default ones).
r_gamma	gamma scale parameter, default is vector ones with family = "Gamma", NULL otherwise.

Details

Support functions needed: pspline_fitter, bbase, and pspline_2dchecker.

Value

pcoef	a vector of length $(\text{Pars}[1,3] + \text{Pars}[1,4]) * (\text{Pars}[2,3] + \text{Pars}[2,4])$ of (un-folded) estimated P-spline coefficients.
mu	a vector of length(z) of smooth estimated means (at the x, y locations).
dev	the deviance of fit.
eff_df	the approximate effective dimension of fit.
aic	AIC.
df_resid	approximate df residual.
cv	leave-one-out standard error prediction, when family = 'gaussian'.
cv_predicted	standard error prediction for y_predict, when family = 'gaussian'.
avediff_pred	mean absolute difference prediction, when family = 'gaussian'.
Pars	the design and tuning parameters (see arguments above).
dispersion_parm	estimate of dispersion, dev/df_resid.
summary_predicted	inverse link prediction vectors, and se_pred bands.
eta_predicted	estimated linear predictor of length(z).
press_mu	leave-one-out prediction of mean, when family = 'gaussian'.
bin_percent_correct	percent correct classification based on 0.5 cut-off (when family = "binomial").
Data	a matrix of 3 columns x, y, z of equal length; the response is z.
Q	the tensor product B-spline basis.
qr	the Q-R of the model.

Author(s)

Paul Eilers and Brian Marx

References

- Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.
- Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

See Also

ps2DNormal

Examples

```

library(fields)
library(JOPS)
# Extract data
library(rpart)
Kyphosis <- kyphosis$Kyphosis
Age <- kyphosis$Age
Start <- kyphosis$Start
y <- 1 * (Kyphosis == "present") # make y 0/1
fit <- ps2DGLM(
  Data = cbind(Start, Age, y),
  Pars = rbind(c(1, 18, 10, 3, .1, 2), c(1, 206, 10, 3, .1, 2)),
  family = "binomial", link = "logit")
plot(fit, xlab = "Start", ylab = "Age")
#title(main = "Probability of Kyphosis")

```

ps2DNormal

*Two-dimensional smoothing scattered (normal) data using P-splines.***Description**

ps2DNormal is used to smooth scattered (normal) data, with anisotropic penalization of tensor product P-splines.

Usage

```

ps2DNormal(
  Data,
  Pars = rbind(c(min(Data[, 1]), max(Data[, 1]), 10, 3, 1, 2), c(min(Data[, 2]),
    max(Data[, 2]), 10, 3, 1, 2)),
  XYpred = expand.grid(Data[, 1], Data[, 2])
)

```

Arguments

Data	a matrix of 3 columns x, y, z of equal length; the response is z .
Pars	a matrix of 2 rows, where the first and second row sets the P-spline parameters for x and y , respectively. Each row consists of: min max nseg bdeg lambda pord . The min and max set the ranges, nseg (default 10) is the number of evenly spaced segments between min and max , bdeg is the degree of the basis (default 3 for cubic), lambda is the (positive) tuning parameter for the penalty (default 1), pord is the number for the order of the difference penalty (default 2),
XYpred	a matrix with two columns (x, y) that give the coordinates of (future) prediction; the default is the data locations.

Details

Support functions needed: `pspline_fitter`, `bbase`, and `pspline_2dchecker`.

Value

coef	a vector of length $(\text{Pars}[1,3] + \text{Pars}[1,4]) * (\text{Pars}[2,3] + \text{Pars}[2,4])$ of (un- folded) estimated P-spline coefficients.
fit	a vector of length(y) of smooth estimated means (at the x, y locations).
pred	a vector of length nrow(XYpred) of (future) predictions.
Pars	the design and tuning parameters (see arguments above).
cv	leave-one-out standard error of prediction or root average PRESS.
h	"hat" diagonals of tensor P-spline fit.
B	tensor product B-spline basis used for fitting.

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

See Also

ps2DGLM

Examples

```
library(SemiPar)
library(fields)
library(spam)
library(JOPS)

# Get the data
data(ethanol)
x <- ethanol$C
y <- ethanol$E
z <- ethanol$NOx

# Set parameters for domain
xlo <- 7
xhi <- 19
ylo <- 0.5
yhi <- 1.25

# Set P-spline parameters, fit and compute surface
xpars <- c(xlo, xhi, 10, 3, 3, 1)
ypars <- c(ylo, yhi, 10, 3, 3, 1)
Pars1 <- rbind(xpars, ypars)
fit <- ps2DNormal(cbind(x, y, z), Pars = Pars1)
plot(fit, xlab = "C", ylab = "E")
```

ps2DSignal

*Two-dimensional penalized signal regression using P-splines.***Description**

ps2DSignal is a function used to regress a (glm) response onto a two-dimensional signal or image, with anisotropic penalization of tensor product P-splines.

Usage

```
ps2DSignal(
  y,
  M,
  p1,
  p2,
  M_type = "stacked",
  M1_index = c(1:p1),
  M2_index = c(1:p2),
  Pars = rbind(c(1, p1, 10, 3, 1, 2), c(1, p2, 10, 3, 1, 2)),
  ridge_adj = 1e-06,
  M_pred = M,
  y_predicted = NULL,
  family = "gaussian",
  link = "default",
  m_binomial = 1 + 0 * y,
  wts = 1 + 0 * y,
  r_gamma = 1 + 0 * y,
  int = TRUE,
  se_pred = 2
)
```

Arguments

y	a response vector of length m, usually continuous, binary/binomial or counts.
M	The signal/image regressors, which are either "stacked" or "unfolded", with dimensions (m * p1) by p2 (i.e. m stacked matrices each of p1 by p2) or with dimensions m by (p1 * p2) (i.e. regressor matrix with m regressor rows, each with column length p1 * p2), respectively.
p1	the row dimension of the image.
p2	the column dimension of the image.
M_type	"stacked" (signal as matrix) or "unfolded" (signal as vector).
M1_index	an index of length p1 for rows of regressor matrix (default is a simple sequence).
M2_index	an index of length p2 for columns of regressor matrix (default is a simple sequence).
Pars	a matrix of 2 rows, where the first and second row sets the P-spline parameters for x and y, respectively. Each row consists of: min max nseg bdeg lambda pord. The min and max set the ranges, nseg (default 10) is the number of evenly spaced segments between min and max, bdeg is the degree of the basis (default 3 for cubic), lambda is the (positive) tuning parameter for the penalty (default 1), pord is the number for the order of the difference penalty (default 2).

ridge_adj	A ridge penalty tuning parameter (usually set to small value, default 1e-6, to stabilize estimation).
M_pred	(e.g. stacked (q * p1) by p2 signal inputs or (unfolded) q by (p1 * p2) signal inputs for q new predictions.
y_predicted	a vector of responses from a cv data set (assoc. with M_pred), when family = "gaussian".
family	the response distribution, e.g. "gaussian", "binomial", "poisson", "Gamma" distribution. Quotes are needed. Default is "gaussian".
link	the link function, one of "identity", "log", "sqrt", "logit", "probit", "cloglog", "loglog", "reciprocal"; quotes are needed (default "identity").
m_binomial	a vector of binomial trials having length(y). Default is 1 vector for family = "binomial", NULL otherwise.
wts	the weight vector of length(y). Default is 1.
r_gamma	a vector of gamma shape parameters. Default is 1 vector for for family = "Gamma", NULL otherwise.
int	set to TRUE or FALSE to include intercept term in linear predictor (default TRUE).
se_pred	a scalar, e.g. se = 2 (default) to produce twice se surfaces, set se > 0. Used for CIs at XYpred locations.

Details

Support functions needed: pspline_fitter, bbase, and pspline_2dchecker.

Value

pcoef	a vector of length (Pars[1,3]+Pars[1,4])*(Pars[2,3]+Pars[2,4]) of (unfolded) estimated P-spline coefficients for tensor surface.
summary_predicted	inverse link prediction vectors, and standard error surfaces.
dev	deviance of fit.
eff_df	the approximate effective dimension of fit.
aic	AIC.
df_resid	approximate df residual.
cv	leave-one-out standard error prediction, when family = "gaussian".
cv_predicted	standard error prediction for y_predict, when family = "gaussian".
avediff_pred	mean absolute difference prediction, when family = 'gaussian'.
Pars	design and tuning parameters (see above arguments).
Dispersion_parm	estimate of dispersion, dev/df_resid.
summary_predicted	inverse link prediction vectors at M_pred, and standard error bands.
eta_predicted	estimated linear predictor of length(y).
press_mu	leave-one-out prediction of mean, when family = "gaussian".
bin_percent_correct	percent correct classification based on 0.5 cut-off, when family = "binomial", NULL otherwise.

B	Tensor basis ($p_1 \times p_2$) by ($n_1 \times n_2$) for 2D signal regression.
Q	Effective regressors (m by $n_1 * n_2$) for 2D signal regression.
Ahat	smooth P-spline coefficient vector of length $p_1 \times p_2$, constructed by <code>B %*% pcoef</code> .
M	the signal/image regressors.
y	the response vector.
M1index	index of length p_1 for rows of regressor matrix.
M2index	index of length p_2 for columns of regressor matrix.
M_type	"stacked" or "unfolded".
w	GLM weight vector of length m .
h	"hat" diagonals.
ridge_adj	additional ridge tuning parameter to stabilize estimation.

Author(s)

Paul Eilers and Brian Marx

References

Marx, B.D. and Eilers, P.H.C. (2005). Multidimensional penalized signal regression, *Technometrics*, 47: 13-22.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(fields)
library(JOPS)

# Get the data
x0 <- Sugar$X
x0 <- x0 - apply(x0, 1, mean) # center Signal
y <- as.vector(Sugar$y[, 3]) # Response is Ash

# Inputs for two-dimensional signal regression
nseg <- c(7, 37)
pord <- c(3, 3)
min_ <- c(230, 275)
max_ <- c(340, 560)
M1_index <- rev(c(340, 325, 305, 290, 255, 240, 230))
M2_index <- seq(from = 275, to = 560, by = .5)
p1 <- length(M1_index)
p2 <- length(M2_index)

# Fit optimal model based on LOOCV
opt_lam <- c(8858.6679, 428.1332) # Found via svcm
Pars_opt <- rbind(
  c(min_[1], max_[1], nseg[1], 3, opt_lam[1], pord[1]),
  c(min_[2], max_[2], nseg[2], 3, opt_lam[2], pord[2])
)
fit <- ps2DSignal(y, x0, p1, p2, "unfolded", M1_index, M2_index,
  Pars_opt,int = TRUE, ridge_adj = 0.0001,
```

```

M_pred = x0 )

# Plotting coefficient image
plot(fit)

```

ps2D_PartialDeriv	<i>Partial derivative two-dimensional smoothing scattered (normal) data using P-splines.</i>
-------------------	--

Description

ps2D_PartialDeriv provides the partial derivative P-spline surface along x , with anisotropic penalization of tensor product B-splines.

Usage

```

ps2D_PartialDeriv(
  Data,
  Pars = rbind(c(min(Data[, 1]), max(Data[, 1]), 10, 3, 1, 2), c(min(Data[, 2]),
    max(Data[, 2]), 10, 3, 1, 2)),
  XYpred = cbind(Data[, 1], Data[, 2])
)

```

Arguments

Data	a matrix of 3 columns x, y, z of equal length; the response is z .
Pars	a matrix of 2 rows, where the first and second row sets the P-spline paramters for x and y , respectively. Each row consists of: min max nseg bdeg lambda pord. The min and max set the ranges, nseg (default 10) is the number of evenly spaced segments between min and max, bdeg is the degree of the basis (default 3 for cubic), lambda is the (positive) tuning parameter for the penalty (default 1), pord is the number for the order of the difference penalty (default 2).
XYpred	a matrix with two columns (x, y) that give the coordinates of (future) prediction; the default is the data locations.

Details

This is support function for `sim_vcpsr`.

Value

coef	a vector of length $(\text{Pars}[1, 3] + \text{Pars}[1, 4]) * (\text{Pars}[1, 3] + \text{Pars}[1, 4])$. of (unfolded) estimated P-spline coefficients.
B	the tensor product B-spline matrix of dimensions m by $\text{length}(\text{coef})$.
fit	a vector of length (y) of smooth estimated means (at the x, y locations).
pred	a vector of length $nrow(\text{XYpred})$ of (future) predictions.
d_coef	a vector of length $(\text{Pars}[1, 3] + \text{Pars}[1, 4] - 1) * (\text{Pars}[1, 3] + \text{Pars}[1, 4])$. of (unfolded) partial derivative estimated P-spline coefficients.
B_d	the tensor product B-spline matrix of dimensions m by $\text{length}(\text{d_coef})$, associated with the partial derivative of the tensor basis.

d_fit	a vector of length(y) of partial derivative (along x) of the smooth estimated means (at the x, y locations).
d_pred	a vector of length nrow(XYpred) of partial derivative (future) predictions.
Pars	a matrix of 2 rows, where each the first (second) row sets the P-spline paramters for x (y): min max nseg bdeg lambda pord. See the argument above.
cv	root leave-one-out CV or root average PRESS.
XYpred	a matrix with two columns (x, y) that give the coordinates of (future) prediction; the default is the data locations.

Author(s)

Brian Marx

References

Marx, B. D. (2015). Varying-coefficient single-index signal regression. *Chemometrics and Intelligent Laboratory Systems*, 143, 111–121.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

psBinomial

Smoothing scattered binomial data using P-splines.

Description

psBinomial is used to smooth scattered binomial data using P-splines using a logit link function.

Usage

```
psBinomial(
  x,
  y,
  xl = min(x),
  xr = max(x),
  nseg = 10,
  bdeg = 3,
  pord = 2,
  lambda = 1,
  ntrials = 0 * y + 1,
  wts = NULL,
  show = FALSE,
  iter = 100,
  xgrid = 100
)
```

Arguments

x	the vector for the continuous regressor of length(y) and the abscissae, on which the B-spline basis is constructed.
y	the response vector, usually 0/1 or binomial counts.
x1	the lower limit for the domain of x (default is min(x)).
xr	the upper limit for the domain of x (default is max(x)).
nseg	the number of evenly spaced segments between x1 and xr.
bdeg	the number of the degree of the basis, usually 1, 2 (default), or 3.
pord	the number of the order of the difference penalty, usually 1, 2, or 3 (default).
lambda	the (positive) number for the tuning parameter for the penalty.
ntrials	the vector for the number of binomial trials (default = 1).
wts	the vector of weights, default is 1, zeros allowed.
show	Set to TRUE or FALSE to display iteration history.
iter	a scalar to set the maximum number of iterations, default iter = 100.
xgrid	a scalar or a vector that gives the x locations for prediction, useful for plotting. If a scalar (default 100) is used then a uniform grid of this size along (x1, xr).

Value

pcoef	a vector of length n of estimated P-spline coefficients.
p	a vector of length m of estimated probabilities.
muhat	a vector of length m of estimated means (ntrials*p).
dev	deviance
effdim	effective dimension of the smooth.
aic	AIC
wts	a vector of preset weights (default = 1).
nseg	the number of B-spline segments.
bdeg	the degree of the B-spline basis.
pord	the order of the difference penalty.
family	the GLM family (response distribution).
link	the link function.
y	the binomial response.
x	the regressor on which the basis is constructed.
P	"half" of the penalty matrix, $P'P = \lambda D'D$.
B	the B-spline basis.
lambda	the positive tuning parameter.
dispersion	dispersion parameter estimated $dev/(m-effdim)$.
xgrid	gridded x values, useful for plotting.
ygrid	gridded fitted linear predictor values, useful for plotting.
pgrid	gridded (inverse link) fitted probability values, useful for plotting.
se_eta	gridded standard errors for the linear predictor.

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Examples

```
library(JOPS)
# Extract data
library(rpart)
Kyphosis <- kyphosis$Kyphosis
Age <- kyphosis$Age
y <- 1 * (Kyphosis == "present") # make y 0/1
fit1 <- psBinomial(Age, y,
  xl = min(Age), xr = max(Age), nseg = 20,
  bdeg = 3, pord = 2, lambda = 10
)
names(fit1)
plot(fit1, xlab = "Age", ylab = "0/1", se = 2)
```

psNormal

Smoothing scattered (normal) data using P-splines.

Description

psNormal is used to smooth scattered (normal) data using P-splines (with identity link function).

Usage

```
psNormal(
  x,
  y,
  xl = min(x),
  xr = max(x),
  nseg = 10,
  bdeg = 3,
  pord = 2,
  lambda = 1,
  wts = NULL,
  xgrid = 100
)
```

Arguments

x	the vector for the continuous regressor of length(y) and the abscissae used to build the B-spline basis.
y	the response vector, usually continuous data.
x1	the number for the min along x (default is min(x)) .
xr	the number for the max along x (default is max(x)).
nseg	the number of evenly spaced segments between x1 and xr.
bdeg	the number of the degree of the basis, usually 1, 2 (default), or 3.
pord	the number of the order of the difference penalty, usually 1, 2, or 3 (default).
lambda	the (positive) number for the tuning parameter for the penalty (default 1).
wts	the vector of general weights, default is 1; zero allowed.
xgrid	a scalar or a vector that gives the x locations for prediction, useful for plotting. If a scalar (default 100) is used then a uniform grid of this size along (x1, xr).

Value

pcoeff	a vector of length n of estimated P-spline coefficients.
muhat	a vector of length m of smooth estimated means.
B	a matrix of dimension m by n for the B-spline basis matrix.
wts	a vector of length m of weights.
effdim	estimated effective dimension.
ed_resid	approximate df residual.
sigma	square root of MSE.
cv	standard error of leave-one-out prediction or root average PRESS.
nseg	the number of B-spline segments.
bdeg	the degree of the B-spline basis.
pord	the order of the difference penalty.
lambda	the positive tuning parameter.
xgrid	gridded x values, useful for plotting.
ygrid	gridded fitted mean values, useful for plotting.
se_eta	gridded standard errors for the fitted mean values, useful for plotting.
P	"half" of the penalty, such that $P'P = \lambda D'D$.

Author(s)

Paul Eilers and Brian Marx

References

- Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.
- Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Examples

```

library(JOPS)
library(MASS)
data(mcycle)
x <- mcycle$times
y <- mcycle$accel
fit1 <- psNormal(x, y, nseg = 20, bdeg = 3, pord = 2, lambda = .8)
plot(fit1, se = 2, xlab = "Time (ms)", ylab = "Acceleration")

```

psNormal_Deriv

Derivative for a P-spline fit of scattered (normal) data.

Description

psNormal_Deriv provides the derivative P-spline fit along x.

Usage

```

psNormal_Deriv(
  x,
  y,
  x1 = min(x),
  xr = max(x),
  nseg = 10,
  bdeg = 3,
  pord = 2,
  lambda = 1,
  wts = rep(1, length(y)),
  xgrid = x
)

```

Arguments

x	the vector for the continuous regressor of length(y) and the abscissae of fit.
y	the response vector, usually continuous data.
x1	the number for the min along x (default is min(x)).
xr	the number for the max along x (default is max(x)).
nseg	the number of evenly spaced segments between x1 and xr.
bdeg	the number of the degree of the basis, usually 1, 2, or 3 (default).
pord	the number of the order of the difference penalty, usually 1, 2 (default), or 3.
lambda	the positive tuning parameter (default 1).
wts	the vector of weights, default is 1; 0/1 allowed.
xgrid	a scalar or a vector that gives the x locations for prediction, useful for plotting. If a scalar (default 100) is used then a uniform grid of this size along (x1, xr).

Details

This is also a support function needed for sim_psr and sim_vcpsr. SISR (Eilers, Li, Marx, 2009).

Value

coef	a vector of length(nsegs + bdeg) of estimated P-spline coefficients.
B	The B-spline matrix of dimensions m by length(coef).
fit	a vector of length(y) of smooth estimated means (at the x locations).
pred	a vector of length(xgrid) of (future) predictions.
d_coef	a vector of length(nsegs + bdeg -1) of differenced (derivative) estimated P-spline coefficients.
B_d	The first derivative B-spline matrix of dimensions m by length(d_coef).
d_fit	a vector of length(y) of partial derivative (along x) of the smooth estimated means (at the x locations).
d_pred	a vector of length length(xgrid) of partial derivative (future) predictions.
xl	the number for the min along x (default is min(x)).
xr	the number for the max along x (default is max(x)).
nseg	the number of evenly spaced segments between xl and xr.
bdeg	the number of the degree of the basis, usually 1, 2, or 3 (default).
pord	the number of the order of the difference penalty, usually 1, 2 (default), or 3.
lambda	the positive tuning parameter (default 1).

Author(s)

Paul Eilers and Brian Marx

References

- Marx, B. D. (2015). Varying-coefficient single-index signal regression. *Chemometrics and Intelligent Laboratory Systems*, 143, 111–121.
- Eilers, P.H.C., B. Li, B.D. Marx (2009). Multivariate calibration with single-index signal regression, *Chemometrics and Intellegent Laboratory Systems*, 96(2), 196-202.
- Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

See Also

sim_psr sim_vcpsr

pspline2d_checker *P-spline 2D tensor product checking algorithm for the GLM.*

Description

pspline_2dchecker checks to see if all the 2D tensor inputs associated for P-spines are properly defined.

Usage

```
pspline2d_checker(
  family,
  link,
  bdeg1,
  bdeg2,
  pord1,
  pord2,
  nseg1,
  nseg2,
  lambda1,
  lambda2,
  ridge_adj,
  wts
)
```

Arguments

family	the response distribution, e.g. "gaussian", "binomial", "poisson", "Gamma" distribution. Quotes are needed.
link	the link function, one of "identity", "log", "sqrt", "logit", "probit", "cloglog", "loglog", "reciprocal"; quotes are needed.
bdeg1	the degree of B-splines.
bdeg2	the degree of B-splines.
pord1	the order of the penalty.
pord2	the order of the penalty.
nseg1	the number of evenly spaced B-spline segments.
nseg2	the number of evenly spaced B-spline segments.
lambda1	the positive tuning parameter for the difference penalty.
lambda2	the positive tuning parameter for the difference penalty.
ridge_adj	the positive tuning parameter for the ridge penalty.
wts	the weight vector, separate from GLM weights.

Value

list same as inputs, with warnings if required.

pspline_checker	<i>P-spline checking algorithm for the GLM.</i>
-----------------	---

Description

pspline_checker checks to see if all the inputs associated for P-splines are properly defined.

Usage

```
pspline_checker(family, link, bdeg, pord, nseg, lambda, ridge_adj, wts)
```

Arguments

family	the response distribution, e.g. "gaussian", "binomial", "poisson", "Gamma" distribution. Quotes are needed.
link	the link function, one of "identity", "log", "sqrt", "logit", "probit", "cloglog", "loglog", "reciprocal";
bdeg	the degree of B-splines.
pord	the order of the penalty.
nseg	the number of evenly-spaced B-spline segments.
lambda	the positive tuning parameter for the difference penalty.
ridge_adj	the positive tuning parameter for the ridge penalty.
wts	the weight vector, separate from GLM weights.

Value

list	same as inputs, with warnings if required.
------	--

pspline_fitter	<i>P-spline fitting algorithm for the GLM.</i>
----------------	--

Description

pspline_fitter applies the method of scoring to a variety of response distributions and link functions within for P-spline fitting within the GLM framework.

Usage

```
pspline_fitter(
  y,
  B,
  family = "gaussian",
  link = "identity",
  P,
  P_ridge = 0 * diag(ncol(B)),
  wts = 0 * y + 1,
  m_binomial = 0 * y + 1,
  r_gamma = 0 * y + 1
)
```

Arguments

y	the glm response vector of length m.
B	The effective P-spline regressors, e.g. B for B-splines, $Q=X \%*\% B$ for PSR.
family	the response distribution, e.g. "gaussian", "binomial", "poisson", "Gamma" distribution; quotes are needed (default family = "gaussian".)
link	the link function, one of "identity", "log", "sqrt", "logit", "probit", "cloglog", "loglog", "reciprocal"; quotes are needed (default link = "identity").
P	P-spline ("half") penalty matrix for data augmentation, such that $P'P = \lambda D'D$.

P_ridge	ridge ("half") penalty for data augmentation, usually $\sqrt{\lambda_r} \cdot I$ (default 0).
wts	the weight vector of $\text{length}(y)$, separate from GLM weights.
m_binomial	a vector of binomial trials having $\text{length}(y)$, when family = "binomial". Default is 1 vector.
r_gamma	a vector of gamma shape parameters, when family = "Gamma". Default is 1 vector.

Value

coef	the estimated P-spline coefficient regressor, using the effective regressors.
w	$\text{wts} \cdot w$, GLM weight vector times input weights of length m.
f	the <code>lsfit</code> object using data augmentation to get P-spline coefficient estimates.
eta	the linear predictor from f.

psPoisson	<i>Smoothing scattered Poisson data using P-splines.</i>
-----------	--

Description

psPoisson is used to smooth scattered Poisson data using P-splines with a log link function.

Usage

```
psPoisson(
  x,
  y,
  x1 = min(x),
  xr = max(x),
  nseg = 10,
  bdeg = 3,
  pord = 2,
  lambda = 1,
  wts = NULL,
  show = FALSE,
  iter = 100,
  xgrid = 100
)
```

Arguments

x	the vector for the continuous regressor of $\text{length}(y)$ and the abscissae used to build the B-spline basis.
y	the response vector, usually count data.
x1	the number for the min along x (default is $\min(x)$).
xr	the number for the max along x (default is $\max(x)$).
nseg	the number of evenly spaced segments between x1 and xr (default 10).
bdeg	the number of the degree of the basis, usually 1, 2, or 3 (default).

pord	the number of the order of the difference penalty, usually 1, 2 (default), or 3.
lambda	the (positive) number for the tuning parameter for the penalty (default 1).
wts	the vector of general weights, zeros are allowed (default 1).
show	Set to TRUE or FALSE to display iteration history (default FALSE).
iter	a scalar to set the maximum number of iterations, default iter=100.
xgrid	a scalar or a vector that gives the x locations for prediction, useful for plotting. If a scalar (default 100) is used then a uniform grid of this size along (x1, xr).

Value

pcoef	a vector of length n of estimated P-spline coefficients.
muhat	a vector of length m of estimated means.
B	the m by n B-spline basis.
dev	deviance of fit.
effdim	effective dimension of fit.
aic	AIC.
wts	the vector of given prior weights.
nseg	the number of B-spline segments.
bdeg	the degree of the B-spline basis.
pord	the order of the difference penalty.
lambda	the positive tuning parameter.
family	the family of the response ("Poisson").
link	the link function used ("log").
xgrid	gridded x values, useful for plotting.
ygrid	gridded fitted linear predictor values, useful for plotting.
mugrid	gridded (inverse link) fitted mean values, useful for plotting.
se_eta	gridded standard errors for the linear predictor.
dispersion	Dispersion parameter estimated $dev/(m-effdim)$.

Author(s)

Paul Eilers and Brian Marx

References

- Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.
- Eilers, P.H.C., Marx, B.D., and Durban, M. (2015). Twenty years of P-splines, *SORT*, 39(2): 149-186.

Examples

```

library(JOPS)
library(boot)

# Extract the data
Count <- hist(coal$date, breaks = c(1851:1963), plot = FALSE)$counts
Year <- c(1851:1962)
xl <- min(Year)
xr <- max(Year)

# Poisson smoothing
nseg <- 20
bdeg <- 3
fit1 <- psPoisson(Year, Count, xl, xr, nseg, bdeg, pord = 2, lambda = 1)
plot(fit1, xlab = "Year", ylab = "Count", se = 2)

```

psSignal

Smooth signal (multivariate calibration) regression using P-splines.

Description

Smooth signal (multivariate calibration) regression using P-splines.

Usage

```

psSignal(
  y,
  x_signal,
  x_index = c(1:ncol(x_signal)),
  nseg = 10,
  bdeg = 3,
  pord = 3,
  lambda = 1,
  wts = 1 + 0 * y,
  family = "gaussian",
  link = "default",
  m_binomial = 1 + 0 * y,
  r_gamma = wts,
  y_predicted = NULL,
  x_predicted = x_signal,
  ridge_adj = 0,
  int = TRUE
)

```

Arguments

y	a (glm) response vector, usually continuous, binomial or count data.
x_signal	a matrix of continuous regressor with $nrow(x_signal) == length(y)$, often a discrete digitization of a signal or histogram or time series.
x_index	a vector to of length $ncol(x_signal) == p$, associated with the ordering index of the signal. Default is $1:ncol(x_signal)$.

nseg	the number of evenly spaced segments between x1 and xr (default 10).
bdeg	the degree of the basis, usually 1, 2, or 3 (default).
pord	the order of the difference penalty, usually 1, 2, or 3 (default).
lambda	the (positive) tuning parameter for the penalty (default 1).
wts	the weight vector of length(y); default is 1.
family	the response distribution, e.g. "gaussian", "binomial", "poisson", "Gamma" distribution; quotes are needed. Default is "gaussian".
link	the link function, one of "identity", "log", "sqrt", "logit", "probit", "cloglog", "loglog", "reciprocal"; quotes are needed (default "identity").
m_binomial	a vector of binomial trials having length(y); default is 1 vector for family = "binomial", NULL otherwise.
r_gamma	a vector of gamma shape parameters. Default is 1 vector for family = "Gamma", NULL otherwise.
y_predicted	a vector of responses associated with x_predicted which are used to calculate standard error of external prediction. Default is NULL.
x_predicted	a matrix of external signals to yield external prediction.
ridge_adj	A ridge penalty tuning parameter, which can be set to small value, e.g. 1e-8 to stabilize estimation, (default 0).
int	set to TRUE or FALSE to include intercept term in linear predictor (default TRUE).

Details

Support functions needed: pspline_fitter, bbase and pspline_checker.

Value

coef	a vector with length(n) of estimated P-spline coefficients.
mu	a vector with length(m) of estimated means.
eta	a vector of length(m) of estimated linear predictors.
B	the B-spline basis (for the coefficients), with dimension p by n.
deviance	the deviance of fit.
eff_df	the approximate effective dimension of fit.
aic	AIC.
df_resid	approximate df residual.
beta	a vector of length p, containing estimated smooth signal coefficients.
std_beta	a vector of length p, containing standard errors of smooth signal coefficients.
cv	leave-one-out standard error prediction, when family = "gaussian".
cv_predicted	standard error prediction for y_predict, when family = "gaussian", NULL otherwise.
nseg	the number of evenly spaced B-spline segments.
bdeg	the degree of B-splines.
pord	the order of the difference penalty.
lambda	the positive tuning parameter.

family	the family of the response.
link	the link function.
y_intercept	the estimated y-intercept (when int = TRUE.)
int	a logical variable related to use of y-intercept in model.
dispersion_param	estimate of dispersion, Dev/df_resid.
summary_predicted	inverse link prediction vectors, and twice se bands.
eta_predicted	estimated linear predictor of length(y).
press_mu	leave-one-out prediction of mean, when family = "gaussian", NULL otherwise.
bin_percent_correct	percent correct classification based on 0.5 cut-off, when family = binomial, NULL otherwise.
x_index	a vector to of length ncol(x_signal) == p, associated with the ordering of the signal.

Author(s)

Brian Marx

References

- Marx, B.D. and Eilers, P.H.C. (1999). Generalized linear regression for sampled signals and curves: A P-spline approach. *Technometrics*, 41(1): 1-13.
- Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(JOPS)
# Get the data
library(fds)
data(nirc)
iindex <- nirc$x
X <- nirc$y
sel <- 50:650 # 1200 <= x & x<= 2400
X <- X[sel, ]
iindex <- iindex[sel]
dX <- diff(X)
diindex <- iindex[-1]
y <- as.vector(labc[1, 1:40]) # percent fat
oout <- 23
dX <- t(dX[, -oout])
y <- y[-oout]
fit1 <- psSignal(y, dX, diindex, nseg = 25, bdeg = 3, lambda = 0.0001,
pord = 2, family = "gaussian", link = "identity", x_predicted = dX, int = TRUE)
plot(fit1, xlab = "Coefficient Index", ylab = "ps Smooth Coeff")
title(main = "25 B-spline segments with tuning = 0.0001")
names(fit1)
```

psVCSignal

*Varying-coefficient penalized signal regression using P-splines.***Description**

psVCSignal is used to regress a (glm) response onto a signal such that the signal coefficients can vary over another covariate t . Anisotropic penalization of tensor product B-splines produces a 2D coefficient surface that can be sliced at t .

@details Support functions needed: pspline_fitter, pspline_2dchecker, and bbase.

@import stats

Usage

```
psVCSignal(
  y,
  X,
  x_index,
  t_var,
  Pars = rbind(c(min(x_index), max(x_index), 10, 3, 1, 2), c(min(t_var), max(t_var),
    10, 3, 1, 2)),
  family = "gaussian",
  link = "default",
  m_binomial = 1 + 0 * y,
  wts = 1 + 0 * y,
  r_gamma = 1 + 0 * y,
  X_pred = X,
  t_pred = t_var,
  y_predicted = NULL,
  ridge_adj = 1e-08,
  int = TRUE
)
```

Arguments

y	a glm response vector of length m , usually continuous, binary/binomial or counts.
X	a m by p_1 Signal matrix of regressors.
x_index	p_1 -vector for index of Signal (e.g. wavelength).
t_var	p_2 -vector with other (indexing) variable in coefficient surface (e.g. temperature, depth, time).
$Pars$	a matrix with 2 rows, each with P-spline parameters: min max nseg bdeg lambda pord, for row and columns of tensor product surface; defaults are min and max for x_index and t_var (resp.), nseg = 10, bdeg = 3, lambda = 1, pord = 2.
family	the response distribution, e.g. "gaussian", "binomial", "poisson", "Gamma" distribution; quotes are needed (default "gaussian").
link	the link function, one of "identity", "log", "sqrt", "logit", "probit", "cloglog", "loglog", "reciprocal"); quotes are needed (default "identity").
$m_binomial$	a vector of binomial trials having length(y). Default is 1 vector for family = "binomial", NULL otherwise.

wt	a m vector of weights (default 1).
r_gamma	a vector of gamma shape parameters. Default is 1 vector for family = "Gamma", NULL otherwise.
X_pred	a matrix of signals with ncol(X) columns for prediction, default is X.
t_pred	a vector for the VC indexing variable with length nrow(X_pred), default is t_var.
y_predicted	a vector for the responses associated with X_pred with length nrow(X_pred) useful for CV when family = "binomial", default is NULL.
ridge_adj	a small ridge penalty tuning parameter to regularize estimation (default 1e-8).
int	intercept set to TRUE or FALSE for intercept term.

Value

pcoef	a vector of length (Pars[1,3]+Pars[1,4])*(Pars[2,3]+Pars[2,4]) of estimated P-spline coefficients for tensor surface.
summary_predicted	inverse link prediction vectors, and twice se bands.
dev	the deviance of fit.
eff_dim	the approximate effective dimension of fit.
family	the family of the response.
link	the link function.
aic	AIC.
df_resid	approximate df residual.
cv	leave-one-out standard error prediction when family = "gaussian", NULL otherwise.
cv_predicted	standard error prediction for y_predict when family = "gaussian", NULL otherwise.
Pars	design and tuning parameters; see arguments above.
dispersion_parm	estimate of dispersion, Dev/df_resid.
summary_predicted	inverse link prediction vectors, and twice se bands.
eta_predicted	estimated linear predictor of length(y).
press_mu	leave-one-out prediction of mean when family = "gaussian", NULL otherwise.
bin_percent_correct	percent correct classification based on 0.5 cut-off when family = "binomial", NULL otherwise.
Bx	B-spline basis matrix of dimension p1 by n1, along x_index.
By	B-spline basis matrix of dimension p2 by n2, along t_var.
Q	Modified tensor basis (m by (n1*n2)) for VC signal regression.
yint	the estimated y-intercept (when int = TRUE.)
int	a logical variable related to use of y-intercept in model.

Author(s)

Paul Eilers and Brian Marx

References

Eilers, P.H.C. and Marx, B.D. (2003). Multivariate calibration with temperature interaction using two-dimensional penalized signal regression. *Chemometrics and Intelligent Laboratory Systems*, 66, 159–174.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(fds)
data(nirc)
iindex <- nirc$x
X <- nirc$y
sel <- 50:650 # 1200 <= x & x<= 2400
X <- X[sel, ]
iindex <- iindex[sel]
dX <- diff(X)
diindex <- iindex[-1]
y <- as.vector(labc[1, 1:40]) # percent fat
t_var <- as.vector(labc[4, 1:40]) # percent flour
oout <- 23
dX <- t(dX[, -oout])
y <- y[-oout]
t_var = t_var[-oout]
Pars = rbind(c(min(diindex), max(diindex), 25, 3, 1e-7, 2),
c(min(t_var), max(t_var), 20, 3, 0.0001, 2))
fit1 <- psVCSignal(y, dX, diindex, t_var, Pars = Pars,
family = "gaussian", link = "identity", int = TRUE)
plot(fit1, xlab = "Coefficient Index", ylab = "VC: % Flour")
names(fit1)
```

rdw

Observations on the widths of red blood cell distributions (RDW).

Description

Observations on the widths of red blood cell distributions (RDW).

Usage

```
data(rdw)
```

Format

A vector.

Source

Erasmus University Medical Centre, Rotterdam, The Netherlands

Examples

```
data(rdw)
hist(rdw, breaks = 20)
```

rowtens	<i>Compute the row tensor product of two matrices</i>
---------	---

Description

Compute the row tensor product of two matrices with identical numbers of rows.

Usage

```
rowtens(X, Y = X)
```

Arguments

X a numeric matrix.
Y a numeric matrix (if missing, Y = X).

Details

The input matrices must have the same number of rows, say m . If their numbers of columns are n_1 and n_2 , the result is a matrix with m rows and $n_1 * n_2$ columns. Each row of the result is the Kronecker product of the corresponding rows of X and Y.

Value

The row-wise tensor product of the two matrices.

Author(s)

Paul Eilers

References

Eilers, P. H. C. and Currie, I. D. and Durban, M. (2006) Fast and compact smoothing on large multidimensional grids *CSDA* 50, 61–76.

save_PDF	<i>Save a plot as a PDF file.</i>
----------	-----------------------------------

Description

Save a plot as a PDF file in a (default) folder. The present default is determined by the folder structure for the production of the book.

Usage

```
save_PDF(  
  fname = "scratch",  
  folder = "../..../Graphs",  
  show = T,  
  width = 6,  
  height = 4.5  
)
```

Arguments

fname	the file name without the extension PDF (default: scratch).
folder	the folder for saving PDF plots (default .././Graphs).
show	a logical parameter; if TRUE the full file name will be displayed.
width	figure width in inches (default = 6).
height	figure height in inches (default = 4.5).

Value

save a plot as a PDF file.

Author(s)

Paul Eilers

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

set_panels

Prepare graphics layout for multiple panels

Description

Adapt margins and axes layout for multiple panels.

Usage

```
set_panels(rows = 1, cols = 1)
```

Arguments

rows	number of rows.
cols	number of columns.

Value

Prepare graphics layout for multiple panels

Author(s)

Paul Eilers

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

set_window	<i>Open a graphics window.</i>
------------	--------------------------------

Description

Open a a window for graphics, with specified width and height.

Usage

```
set_window(width = 6, height = 4.5, kill = TRUE, noRStudioGD = TRUE)
```

Arguments

width	figure width in inches (default = 6).
height	figure height in inches (default = 4.5).
kill	if TRUE (default) closes all graphics windows. Works only for Windows.
noRStudioGD	if TRUE: do not use the RStudio device (which does not accept width and height).

Value

open a graphics window.

Note

Currently only works for Windows!

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

sim_psr	<i>Single-Index signal regression using P-splines</i>
---------	---

Description

sim_psr is a single-index signal regression model that estimates both the signal coefficients vector and the unknown link function using P-splines.

Usage

```
sim_psr(
  y,
  X,
  x_index = c(1:ncol(X)),
  nsegs = rep(10, 2),
  bdegs = rep(3, 3),
  lambdas = rep(1, 2),
  pords = rep(2, 2),
  max_iter = 100
)
```

Arguments

<code>y</code>	a response vector of length m , usually continuous.
<code>X</code>	The signal regressors with dimension m by p .
<code>x_index</code>	an index of length p for columns of signal matrix; default is simple sequence, <code>c(1: ncol(X))</code> .
<code>nsegs</code>	a vector of length 2 containing the number of evenly spaced segments between min and max, for each the coefficient vector and the (unknown) link function, resp. (default <code>c(10, 10)</code>).
<code>bdegs</code>	a vector of length 2 containing the degree of B-splines, for the coefficient vector and the (unknown) link function, resp. (default cubic or <code>c(3, 3)</code>).
<code>lambdas</code>	a vector of length 2 containing the positive tuning parameters, for each the coefficient vector and the (unknown) link function, resp. (default <code>c(1, 1)</code>).
<code>pords</code>	a vector of length 2 containing the difference penalty order, for each the coefficient vector and the (unknown) link function, resp. (default <code>c(2, 2)</code>).
<code>max_iter</code>	a scalar for the maximum number of iterations (default 100).

Value

<code>y</code>	the response vector of length m .
<code>alpha</code>	the P-spline coefficient vector of length $(nsegs[1]+bdeg[1])$.
<code>iter</code>	the number of iterations used for the single-index fit.
<code>yint</code>	the estimated y-intercept for the single-index model.
<code>B</code>	the B-spline matrix built along the signal index, using <code>nsegs[1]</code> , used for the coefficient vector.
<code>Q</code>	the effective regressors from the <code>psVCSignal</code> portion of the single-index fit with dimension m by <code>length(alpha)</code> .
<code>nsegs</code>	a vector of length 2 containing the number of evenly spaced segments between min and max, for each the coefficient vector and the link function, resp.
<code>bdegs</code>	a vector of length 2 containing the degree of B-splines, for each the coefficient vector and the link function, resp.
<code>lambdas</code>	a vector of length 2 containing the positive tuning parameters, for each the coefficient vector and the link function, resp.
<code>pords</code>	a vector of length 2 containing the difference penalty order, for each the coefficient vector and the link function, resp.
<code>eta</code>	the estimated linear predictor for the single-index fit.
<code>cv</code>	the leave-one-out cross-validation statistic or the standard error of prediction for the single-index fit.
<code>delta_alpha</code>	change measure in signal-coefficient parameters at convergence.
<code>x_index</code>	the index of length p for columns of signal matrix.
<code>f_fit</code>	the <code>psNormal</code> object, fitting link function $f(\eta)$.
<code>f_eta</code>	the predicted values of the link function estimated with <code>f_fit</code> or estimated $f(\eta)$, at $x = \eta$.

Author(s)

Paul Eilers, Brian Marx, and Bin Li

References

Eilers, P.H.C., B. Li, B.D. Marx (2009). Multivariate calibration with single-index signal regression, *Chemometrics and Intelligent Laboratory Systems*, 96(2), 196-202.

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(JOPS)
# Get the data
library(fds)
data(nirc)
iindex <- nirc$x
X <- nirc$y
sel <- 50:650 # 1200 <= x & x<= 2400
X <- X[sel, ]
iindex <- iindex[sel]
dX <- diff(X)
diindex <- iindex[-1]
y <- as.vector(labc[1, 1:40])
oout <- 23
dX <- t(dX[, -oout])
y <- y[-oout]

pords <- c(2, 2)
nsegs <- c(27, 7)
bdegs = c(3, 3)
lambdas <- c(1e-6, .1)
max_iter <- 100

# Single-index model
fit <- sim_psr(y, dX, diindex, nsegs, bdegs, lambdas, pords,
              max_iter)

plot(fit, xlab = "Wavelength (nm)", ylab = " ")
```

sim_vcpsr

Varying-coefficient single-index signal regression using tensor P-splines.

Description

sim_vcpsr is a varying-coefficient single-index signal regression approach that allows both the signal coefficients and the unknown link function to vary with an indexing variable t , e.g. temperature. Two surfaces are estimated (coefficient and link) that can be sliced at arbitrary t . Anisotropic penalization with P-splines is used on both.

Usage

```
sim_vcpsr(
  y,
  X,
```

```

    t_var,
    x_index = c(1:ncol(X)),
    nsegs = rep(10, 4),
    bdeg = rep(3, 4),
    lambdas = rep(1, 4),
    pords = rep(2, 4),
    max_iter = 100,
    mins = c(min(x_index), min(t_var)),
    maxs = c(max(x_index), max(t_var))
)

```

Arguments

y	a response vector of length m, usually continuous.
X	the signal regressors with dimension m by p1.
t_var	the varying coefficient indexing variable of length m.
x_index	an index of length p for columns of signal matrix; default is simple sequence.
nsegs	a vector of length 4 containing the number of evenly spaced segments between min and max, for each the coefficient surface (row and col) and link surface (row and col), resp. (default rep(10, 4)).
bdeg	a vector of length 4 containing the degree of B-splines, for each the coefficient surface (row and col) and link surface (row and col), resp. (default cubic rep(3, 4)).
lambdas	a vector of length 4 containing the positive tuning parameters, for each the coefficient surface (row and col) and link surface (row and col), resp. (default rep(1, 4)).
pords	a vector of length 4 containing the difference penalty order, for each the coefficient surface (row and col) and link surface (row and col), resp. (default rep(2, 4)).
max_iter	a scalar for the maximum number of iterations (default 100)
mins	A vector length 2, containing min for signal index and t_var, default associated with x_index and t_var minimums; default is respective minimums.
maxs	A vector length 2, containing max for signal index and t_var, default associated with x_index and t_var maximums; default is respective maximums.

Value

y	the response vector of length m.
alpha	the P-spline coefficient vector (unfolded) of length (nsegs[1]+bdeg[1])*(nsegs[2]+bdeg[2]).
iter	the number of iterations used for the single-index fit.
yint	the estimated y-intercept for the single-index model.
Bx	the B-spline matrix built along the signal index, using nsegs[1], used for the coefficient surface.
By	the B-spline matrix built along the t_var index, using nsegs[2], used for the coefficient surface.
Q	the effective regressors from the psVCSignal portion of the single-index fit with dimension m by length(alpha).
t_var	the VC indexing variable of length m.

nsegs	a vector of length 4 containing the number of evenly spaced segments between min and max, for each the coefficient surface (row and col) and link surface (row and col).
bdegs	a vector of length 4 containing the degree of B-splines, for each the coefficient surface (row and col) and link surface (row and col).
lambdas	a vector of length 4 containing the positive tuning parameters, for each the coefficient surface (row and col) and link surface (row and col).
por ds	a vector of length 4 containing the difference penalty order, for each the coefficient surface (row and col) and link surface (row and col).
mins	a vector length 2, containing min for signal index and t_var.
maxs	a vector length 2, containing max for signal index and t_var.
eta	the estimated linear predictor for the single-index fit.
Pars	a matrix of 2 rows associated with the signal coefficient surface design parameters, each row: c(min, max, nseg, bdeg, lambda, pord) for linear predictor x_index and t_var, resp.
pPars	a matrix of 2 rows associated with the link function design parameters, each row: c(min, max, nseg, bdeg, lambda, pord) for linear predictor eta and t_var, resp.
cv	the leave-one-out cross-validation statistic or the standard error of prediction for the single-index fit.
delta_alpha	change measure in signal-coefficient parameters at convergence.
fit2D	ps2DNormal object, fitting f(eta, t_var).

Author(s)

Paul Eilers and Brian Marx

References

- Marx, B. D. (2015). Varying-coefficient single-index signal regression. *Chemometrics and Intelligent Laboratory Systems*, 143, 111–121.
- Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
# Load libraries
library(fields) # Needed for plotting

# Get the data
Dat <- Mixture

# Dimensions: observations, temperature index, signal
m <- 34
p1 <- 401
p2 <- 12

# Stacking mixture data, each mixture has 12 signals stacked
# The first differenced spectra are also computed.
mixture_data <- matrix(0, nrow = p2 * m, ncol = p1)
for (ii in 1:m)
{
```

```

mixture_data[((ii - 1) * p2 + 1):(ii * p2), 1:p1] <-
  t(as.matrix(Dat$xspectra[ii, , ]))
d_mixture_data <- t(diff(t(mixture_data)))
}

# Response (typo fixed) and index for signal
y_mixture <- Dat$fractions
y_mixture[17, 3] <- 0.1501
index_mixture <- Dat$w1

# Select response and replicated for the 12 temps
# Column 1: water; 2: ethanediol; 3: amino-1-propanol
y <- as.vector(y_mixture[, 2])
y <- rep(y, each = p2)

bdegs = c(3, 3, 3, 3)
pords <- c(2, 2, 2, 2)
nsegs <- c(12, 5, 5, 5) # Set to c(27, 7, 7, 7) for given lambdas
mins <- c(700, 30)
maxs <- c(1100, 70)
lambdas <- c(1e-11, 100, 0.5, 1) # based on svcm search
x_index <- seq(from = 701, to = 1100, by = 1) # for dX
t_var_sub <- c(30, 35, 37.5, 40, 45, 47.5, 50, 55, 60, 62.5, 65, 70)
t_var <- rep(t_var_sub, m)
max_iter <- 2 # Set higher in practice, e.g. 100
int <- TRUE

# Defining x as first differenced spectra, number of channels.
x <- d_mixture_data

# Single-index VC model using optimal tuning
fit <- sim_vcpsr(y, x, t_var, x_index, nsegs, bdegs, lambdas, pords,
  max_iter = max_iter, mins = mins, maxs = maxs)

plot(fit, xlab = "Wavelength (nm)", ylab = "Temp C")

```

SpATS.nogeno

Two-dimensional P-spline smoothing

Description

Two-dimensional smoothing of scattered data points with tensor product P-splines.

Usage

```

SpATS.nogeno(
  response,
  spatial,
  fixed = NULL,
  random = NULL,
  data,
  family = gaussian(),
  offset = 0,

```

```

weights = NULL,
control = list(maxit = 100)
)

```

Arguments

response	a character string with the name of the variable that contains the response variable of interest.
spatial	a right hand formula object specifying the spatial P-Spline model. See SAP and PSANOVA for more details about how to specify the spatial trend.
fixed	an optional right hand formula object specifying the fixed effects.
random	an optional right hand formula object specifying the random effects. Currently, only sets of independent and identically distributed random effects can be incorporated.
data	a data frame containing the variables.
family	object of class family specifying the distribution and link function.
offset	an optional numerical vector containing an a priori known component to be included in the linear predictor during fitting.
weights	an optional numerical vector of weights to be used in the fitting process. By default, the weights are considered to be one.
control	a list of control values.

Details

This function is a modified version of the function [SpATS](#) in the package SpATS. The difference is that genotypes have been removed.

Value

A list with the following components:

call	the matched call.
data	the original supplied data argument with a new column with the weights used during the fitting process.
model	a list with the model components: response, spatial, fixed and/or random.
fitted	a numeric vector with the fitted values.
residuals	a numeric vector with deviance residuals.
psi	a two-length vector with the values of the dispersion parameters at convergence. For Gaussian responses both elements coincide, being the (REML) estimate of dispersion parameter. For non-Gaussian responses, the result depends on the argument <code>update.psi</code> of the controlSpATS function. If this argument was specified to FALSE (the default), the first component of the vector corresponds to the default value used for the dispersion parameter (usually 1). The second element, correspond to the (REML) estimate of the dispersion parameter at convergence. If the argument <code>update.psi</code> was specified to TRUE, both components coincide (as in the Gaussian case).
var.comp	a numeric vector with the (REML) variance component estimates. This vector contains the variance components associated with the spatial trend, as well as those related with the random model terms.

eff.dim	a numeric vector with the estimated effective dimension (or effective degrees of freedom) for each model component (spatial, fixed and/or random).
dim	a numeric vector with the (model) dimension of each model component (spatial, fixed and/or random). This value corresponds to the number of parameters to be estimated.
dim.nom	a numeric vector with the (nominal) dimension of each component (spatial, fixed and/or random). For the random terms of the model, this value corresponds to upper bound for the effective dimension (i.e., the maximum effective dimension a random term can achieve). This nominal dimension is $rank[X, Z_k] - rank[X]$, where Z_k is the design matrix of the k th random factor and X is the design matrix of the fixed part of the model. In most cases (but not always), the nominal dimension corresponds to the model dimension minus one, "lost" due to the implicit constraint that ensures the mean of the random effects to be zero.
nobs	number of observations used to fit the model.
niterations	number of iterations EM-algorithm.
deviance	the (REML) deviance at convergence (i.e., -2 times the restricted log-likelihood).
coeff	a numeric vector with the estimated fixed and random effect coefficients.
terms	a list with the model terms: response, spatial, fixed and/or random. The information provided here is useful for printing and prediction purposes.
vcov	inverse of the coefficient matrix of the mixed models equations. The inverse is needed for the computation of standard errors. For computational issues, the inverse is returned as a list: C22_inv corresponds to the coefficient matrix associated with the spatial, the fixed and the random components.

Author(s)

Maria-Xose Rodriguez-Alvarez and Paul Eilers

References

Rodriguez-Alvarez, M.X, Boer, M.P., van Eeuwijk, F.A., and Eilers, P.H.C. (2018). Correcting for spatial heterogeneity in plant breeding experiments with P-splines. *Spatial Statistics*, 23, 52 - 71. <https://doi.org/10.1016/j.spasta.2017.10.003>.

Examples

```
# Get the data
library(SemiPar)
data(ethanol)

# Fit the PS-ANOVA model
ps2d <- SpATS.nogeno(response = "NOx",
                    spatial = ~PSANOVA(E, C, nseg = c(20, 20), nest.div = c(2, 2)),
                    data = ethanol,
                    control = list(maxit = 100, tolerance = 1e-05,
                                   monitoring = 0, update.psi = FALSE))

# Report effective dimensions, if desired
# print(summary(ps2d))

# Compute component surface and their sum on a fine grid
Tr = obtain.spatialtrend(ps2d, grid = c(100, 100))
```

```
# Plot surface and contours
image(Tr$row.p, Tr$col.p, Tr$fit, col = terrain.colors(100), xlab = 'C', ylab = 'E')
contour(Tr$row.p, Tr$col.p, Tr$fit, add = TRUE, col = 'blue')
points(ethanol$C, ethanol$E, pch = '+')
```

spbase

Compute a sparse B-spline basis on evenly spaced knots

Description

Constructs a sparse B-spline basis on evenly spaced knots.

Usage

```
spbase(x, xl = min(x), xr = max(x), nseg = 10, bdeg = 3)
```

Arguments

x	a vector of argument values, at which the B-spline basis functions are to be evaluated.
xl	the lower limit of the domain of x (default min(x)).
xr	the upper limit of the domain of x (default max(x)).
nseg	the number of evenly spaced segments between xl and xr (default 10).
bdeg	the degree of the basis, usually 1, 2, or 3 (default).

Value

A sparse matrix (in spam format) with length(x) of rows= and nseg + bdeg columns.

Author(s)

Paul Eilers

References

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

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(JOPS)
# Basis on grid
x = seq(0, 4, length = 1000)
B = spbase(x, 0, 4, nseg = 50, bdeg = 3)
nb1 = ncol(B)
matplot(x, B, type = 'l', lty = 1, lwd = 1, xlab = 'x', ylab = '')
cat('Dimensions of B:', nrow(B), 'by', ncol(B), 'with', length(B@entries), 'non-zero elements' )
```

Sugar

Sugar Processing Data

Description

Sugar was sampled continuously during eight hours to make a mean sample representative for one "shift" (eight hour period). Samples were taken during the three months of operation (the so-called campaign) in late autumn from a sugar plant in Scandinavia giving a total of 268 samples. The sugar was sampled directly from the final unit operation (centrifuge) of the process.

Usage

`data(Sugar)`

Format

A list consisting of the following:

`y` a 268 x 3 matrix of quality parameters: date, color, ash*1000

`X` fluorescence array, 268 (observations) x [571 (emission channels) x 7 (excitation channels)]

`Lab` Lab information

`DimX` array dimension for `X`

`Yidx` names (id) for `y`

`EmAx` Emmission levels for axis (nm)

`ExAx` Excitation levels for axis (nm)

`time`

`readmetime`

`Lname`

`LabNumber`

`ProcNumber`

`Proc`

`DimLab`

`DimProc`

Source

http://www.models.kvl.dk/Sugar_Process

References

R. Bro, Exploratory study of sugar production using fluorescence spectroscopy and multi-way analysis, *Chemom. Intell. Lab. Syst.*, 1999, (46), 133-147.

Suicide

Suicide Data Set

Description

The dataset comprises lengths (in days) of psychiatric treatment spells for patients used as controls in a study of suicide risks.

Usage

```
data(Suicide)
```

Format

A dataframe with one column: y.

Source

Silverman, B. (1986). Density Estimation for Statistics and Data Analysis. Chapman & Hall.

References

Silverman, B. (1986). Density Estimation for Statistics and Data Analysis. Chapman & Hall.

tpower

Compute a truncated power function.

Description

Compute a truncated power function.

Usage

```
tpower(x, knot, p)
```

Arguments

x a vector on which the basis is calculated.
knot a scalar giving the truncation point.
p a scalar power for the basis, e.g. $p = 3$ for cubic TPF.

Value

a vector with the truncated power function.

Author(s)

Paul Eilers

References

Eilers, P.H.C. and Marx, B.D. (2021). *Practical Smoothing, The Joys of P-splines*. Cambridge University Press.

Examples

```
library(JOPS)
# Basis on grid
x = seq(0, 4, length = 500)
knots = 0:3
Y = outer(x, knots, tpower, 1)
matplot(x, Y, type = 'l', lwd = 2, xlab = 'x', ylab = '',
main = 'Linear TPF basis')
```

Varstar

Brightness of a variable star.

Description

Brightness of a variable star.

Usage

```
data(Varstar)
```

Format

A dataframe with eleven columns (V1-V11):

V1 day index

V2 brightness

V3-V11 Paul Eilers, personal communication.

References

Paul Eilers (personal communication).

Woodsurf

Profile of a sanded piece of wood.

Description

Profile of a sanded piece of wood.

Usage

```
data(Woodsurf)
```

Format

A data frame with one column: y .

Source

Pandit, S.M. and Wu, S.M. (1993). *Time Series and System Analysis with Applications*. Krieger Publishing Company.

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