Package: JOPS (via r-universe)

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Type Package

Title Practical Smoothing with P-Splines

Version 0.1.19

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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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Depends R ($>= 3.1.0$), SpATS ($>= 1.0-13$)

Imports colorspace, MASS, boot, fds, rpart, ggplot2, fields, spam, SemiPar, stats, graphics, grDevices

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Repository https://pauleilers.r-universe.dev

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bbase *Compute a B-spline basis matrix*

Description

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

Usage

bbase(x, $x1 = min(x)$, $xr = max(x)$, $nseg = 10$, $bdeg = 3$)

Arguments

Details

If x1 is larger than $min(x)$, it will be adjusted to $min(x)$ and a warning wil be given. If xr is smaller than $max(x)$, it will be adjusted to $max(x)$ and a warning wil 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 $length(x)$ rows and n seg + 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 *Translated number vector to bin index.*

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

bone_data 5

Value

A list with components:

References

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

bone_data *Spinal bone relative mineral density*

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.

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

Usage

 $\text{chase}(x, x1 = \text{min}(x), xr = \text{max}(x), nseg = 10, bdeg = 3)$

Arguments

Details

If x1 is larger than $min(x)$, it wil be adjusted to $min(x)$ and a warning wil be given. If xr is smaller than $max(x)$, it wil be adjusted to $max(x)$ and a warning wil be given.

The design parameters x , $x1$, xr , ndeg, 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 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.

cdiff $\overline{7}$

Examples

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

Compute a second order circular differencing matrix

Description

Compute difference matrix used for circular penalities.

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.

```
# Compare standard and circular differencing matrix
n = 8D1 = diff(diag(n), diff = 2)D2 = \text{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

Complaints 9

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) * 0.2B = bbase(x)nb = ncol(B)D = diff(diag(nb), diff = 2)lambda = 1a = 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')
```


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

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.

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_{\text{gamma}} = 0 \times y + 1)
```
Arguments

Value

A list with two fields:

dev the estimated deviance.

dispersion_parm

the ML estimated dispersion parameter.

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.

fitample to the contract of th

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 coeffcients 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

Details

The expectile bundle model determines a set of expectile curves for a point cloud with data vectors x and y, as $\psi_i x_i = a_i g(x_i)$. Here a_i 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 alternatingly. 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 explict 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.

```
# Get the data
data(bone_data)
x = bone_data$age
y = bone_data$spnbmd
m \leftarrow 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 < -5x1 < -30ndx <- 20
bdeg <-3pord <-2# Compute bases
B \le - bbase(x, x0, x1, ndx, bdeg)
xg \le -\text{seq}(\text{from } = \text{min}(x), \text{ to } = \text{max}(x), \text{ length } = 100)Bg <- clone_base(B, xg)
```
fitasy 15

```
n \leftarrow \text{ncol}(B)lambda = 1alpha \leq rep(1,n)
a = pfor (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 = anewcat(it, da, '\n')
     if (da < 1e-6) break
}
# Compute bundle on grid
ampl <- Bg %*% alpha
Z \leftarrow \text{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

Details

The expectile bundle model determines a set of expectile curves for a point cloud with data vectors x and y, as $\psi_i x_i = a_i g(x_i)$. Here a_i 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 alternatingly. 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 explict 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.

```
# Get the data
data(bone_data)
x = bone_data$age
y = bone_data$spnbmd
m \leftarrow 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
```
 $G519C18$ 17

```
x0 < -5x1 < -30ndx <- 20
bdeg <-3pord <-2# Compute bases
B <- bbase(x, x0, x1, ndx, bdeg)
xg \le -\text{seq}(\text{from} = \text{min}(x), \text{to} = \text{max}(x), \text{length} = 100)Bg <- clone_base(B, xg)
n \leftarrow \text{ncol}(B)lambda = 1alpha \leq rep(1,n)
a = pfor (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 \leftarrow 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.

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 *Compute a 2D histogram*

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

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:

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,
```


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```
dx = 3,
 dy = dx,
 Mu = Y + 0.01,
 kappa = 1e-04,
 tol = 1e-05)
```
Arguments

Value

A list with elements:

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 *An X-ray diffractogram.*

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 Diffractometry, which is no longer available from CRAN in binary form.

Source

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

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


Inverse link function, used for GLM fitting.

Usage

inverse_link(x, link)

Arguments

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.

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 *Themeing functions used to unify ggplot features*

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.

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

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:

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.

```
# Smoothing a histogram of Old Faithful eruption durations
data(faithful)
durations = faithful[, 1] # Eruption length
# Histogram with narrow bin widths
bw = 0.05hst = hist(durations, breaks = seq(1, 6, by = bw), plot = TRUE)
```
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```
x = hst$mids
y = hst$counts
# B-spline basis matrices, for fitting and plotting
nseg = 30B = \text{bbase}(x, \text{nseg} = \text{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, flat2, col = "blue", lw = 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 mixure 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 wavelengths 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 Intellegent 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.

ova *Ovarian cancer data*

Description

Ovarian cancer data

Usage

data(ova)

Format

A dataframe with five columns:

Diameter

FIGO

Karnofsky

time

death death

Source

tba

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

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:

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 \leq 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 \leq -\max(ce)C \leftarrow matrix(0, m, n)for (i in 1:m) C[i, cb[i]:ce[i]] <- 1
mids = (cb + ce) / 2 - 0.5widths = ce - cb + 1dens = y / widths / sum(y)
x = (1:n) - 0.5B = 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) smooothing (using ps2DGLM with class ps2dglm).

Usage

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

Arguments

Value

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 \le -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 *Plotting function for* ps2DNormal

Description

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

Usage

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

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.

```
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")
```


Plotting function for 2D P-spline signal regression coefficients (using ps2DSignal with class ps2dsignal). Although standard error surface bands can be comuputed they are intentially 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

Value

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.

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

```
# Inputs for two-dimensional signal regression
nseg <- c(7, 37)
pord \leq 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 = 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", peh = 1)
```
Arguments

plot.pspfit 35

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.

```
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(boot::coal$date, breaks=c(1851:1963), plot = FALSE)$counts
Year = c(1851:1962)
x1 = min(Year)xr = max(Year)
# Poisson smoothing
nseg = 20bdeg = 3fit1=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 *Plotting function for* psSignal

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

Value

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.
plot.psvcsignal 37

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])
out = 23dX=t(dX[,-oout])
y=y[-oout]
fit2 = psSignal(y, dX, d/index, 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-coefficent signal regression P-spline smooth coefficients (using psVCSignal with class psvcsignal). Although se surface bands can be comuputed they are intentially 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

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 Intellegent 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 \leftarrow diff(X)diindex <- iindex[-1]
y \le - as.vector(labc[1, 1:40]) # percent fat
t_var <- as.vector(labc[4, 1:40]) # percent flour
oout <- 23
dX \leftarrow t(dX[, -\text{count}]y \leftarrow y[-\text{out}]t_var = t_var[-count]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).

plot.simpsr 39

Usage

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

Arguments

Value

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 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.

```
library(JOPS)
# Get the data
library(fds)
data(nirc)
iindex <- nirc$x
X <- nirc$y
sel <- 50:650 # 1200 <= x & x<= 2400
X \leftarrow X[\text{sel}, \ ]iindex <- iindex[sel]
dX \leftarrow diff(X)diindex <- iindex[-1]
y <- as.vector(labc[1, 1:40])
oout <- 23
dX <- t(dX[, -oout])
y \leftarrow y[-count]pords \leq c(2, 2)nsegs \leq c(27, 7)bdegs = c(3, 3)
```

```
lambdas \leq 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 product Psplines (using sim_vcpsr with class simvcpsr).

Usage

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

Arguments

Value

```
Plot a plot of the estimated 2D P-spline signal coefficient surface along with the com-
                  panion 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 Intellegent Laboratory Systems*, 143, 111–121.

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

plot.simvcpsr 41

```
# Load libraries
library(fields) # Needed for plotting
# Get the data
Dat <- Mixture
# Dimensions: observations, temperature index, signal
m < -34p1 < -401p2 <- 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$wl
# Select response and replicated for the 12 temps
# Column 1: water; 2: ethanediol; 3: amino-1-propanol
y <- as.vector(y_mixture[, 2])
y \leq -rep(y, each = p2)bdegs = c(3, 3, 3, 3)pords \leq -c(2, 2, 2, 2)nsegs \le 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 \leftarrow seq(from = 701, to = 1100, by = 1) # for dXt_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

Value

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.

predict.ps2dnormal 43

Examples

```
library(fields)
library(JOPS)
# Extract data
library(rpart)
Kyphosis <- kyphosis$Kyphosis
Age <- kyphosis$Age
Start <- kyphosis$Start
y \le -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

Value

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 < -0.5vhi <- 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 \leq ps2DNormal(cbind(x, y, z), Pars = Pars1)
predict(fit, XY = child(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

Value

pred the estimated mean (inverse link function) or the linear predictor prediction with type = "eta", for arbitary 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$X
x0 \leq x0 - apply(x0, 1, mean) # center Signal
y <- as.vector(Sugar$y[, 3]) # Response is Ash
# Inputs for two-dimensional signal regression
nseg < -c(7, 37)pord \leq c(3, 3)min_ <- c(230, 275)
max_ - < -c(340, 560)M1_index <- rev(c(340, 325, 305, 290, 255, 240, 230))
M2_index \le - 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])
\lambdafit <- 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")

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

Value

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.

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

Value

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, dilinear, 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

Value


```
predict.simpsr 49
```
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 Intellegent 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 \leftarrow X[\text{sel}, \ ]iindex <- iindex[sel]
dX \leftarrow 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 \leftarrow y[-oout]
t_var = t_var[-count]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_lar[1:5])
```
predict.simpsr *Predict function for* sim_psr

Description

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

Usage

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

Arguments

Value

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 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.

```
library(JOPS)
# Get the data
library(fds)
data(nirc)
iindex <- nirc$x
X <- nirc$y
sel <- 50:650 # 1200 <= x & x<= 2400
X \leftarrow X[\text{sel}, \ ]iindex <- iindex[sel]
dX \leftarrow diff(X)diindex <- iindex[-1]
y <- as.vector(labc[1, 1:40])
oout <- 23
dX <- t(dX[, -oout])
y \leftarrow y[-count]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 *Predict function for* sim_vcpsr

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

Value

Author(s)

Paul Eilers and Brian Marx

References

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

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

```
# Load libraries
library(fields) # Needed for plotting
# Get the data
Dat <- Mixture
# Dimensions: observations, temperature index, signal
m < -34
```

```
p1 < -401p2 < -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$wl
# Select response and replicated for the 12 temps
# Column 1: water; 2: ethanediol; 3: amino-1-propanol
y <- as.vector(y_mixture[, 2])
y \leftarrow rep(y, each = p2)bdegs = c(3, 3, 3, 3)pords <- c(2, 2, 2, 2)
nsegs \le 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 \leftarrow seq(from = 701, to = 1100, by = 1) # for dXt_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 *Two-dimensional smoothing of scattered normal or non-normal (GLM) responses using tensor product P-splines.*

ps2DGLM 53

Description

ps2DGLM is used to smooth scattered normal or non-normal responses, with aniosotripic 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))
```

```
\mathcal{L}
```
Arguments

Support functions needed: pspline_fitter, bbase, and pspline_2dchecker.

Value

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

ps2DNormal 55

Examples

```
library(fields)
library(JOPS)
# Extract data
library(rpart)
Kyphosis <- kyphosis$Kyphosis
Age <- kyphosis$Age
Start <- kyphosis$Start
y \le -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 aniosotripic 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])
\mathcal{L}
```
Arguments

Details

Support functions needed: pspline_fitter, bbase, and pspline_2dchecker.

Value

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

```
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 \leftarrow 7xhi \leq 19ylo <- 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 \leq 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 aniosotripic 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_{\text{gamma}} = 1 + 0 \times y,
  int = TRUE,se\_pred = 2)
```
Arguments

Details

Support functions needed: pspline_fitter, bbase, and pspline_2dchecker.

Value

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.

```
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 \leftarrow c(3, 3)
min_ <- c(230, 275)
max_ - < -c(340, 560)M1_index <- rev(c(340, 325, 305, 290, 255, 240, 230))
M2_index \le 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 *Partial derivative two-dimensional smoothing scattered (normal) data using P-splines.*

Description

ps2D_PartialDeriv provides the partial derivative P-spline surface along x, with aniosotripic 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

Details

This is support function for sim_vcpsr.

Value

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.

Description

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

Usage

```
psBinomial(
 x,
 y,
 x1 = 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

psBinomial 63

Value

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.

```
library(JOPS)
# Extract data
library(rpart)
Kyphosis <- kyphosis$Kyphosis
Age <- kyphosis$Age
```

```
y \le -1 * (Kyphosis == "present") # make y 0/1
fit1 <- psBinomial(Age, y,
 x1 = min(Age), xr = max(Age), nseg = 20,
 bdeg = 3, pord = 2, lambda = 10\mathcal{L}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,
 x1 = min(x),
 xr = max(x),
 nseg = 10,bdeg = 3,
 pord = 2,
 lambda = 1,
 wts = NULL,xgrid = 100)
```
Arguments

psNormal 65

Value

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.

```
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")
```
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\mathcal{E}
```
Arguments

Details

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

Value

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

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

Value

Description

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

Usage

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

Arguments

Value

list same as inputs, with warnings if required.

pspline_fitter *P-spline fitting algorithm for the GLM.*

Description

pspline_fitter appies 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_{\text{middle}} = 0 \times \text{diag}(\text{ncol}(B)),wts = 0 * y + 1,m_binomial = 0 * y + 1,
  r_{\text{gamma}} = 0 \times y + 1\mathcal{L}
```
Arguments

Value

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

)

Value

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.

```
library(JOPS)
library(boot)
# Extract the data
Count <- hist(boot::coal$date, breaks = c(1851:1963), plot = FALSE)$counts
Year <- c(1851:1962)
xl <- min(Year)
xr <- max(Year)
# Poisson smoothing
nseg <- 20
```
psSignal 73

```
bdeg <-3fit1 <- 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

Details

Support functions needed: pspline_fitter, bbase and pspline_checker.

Value

psSignal 75

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 \leftarrow X[\text{sel}, 1]iindex <- iindex[sel]
dX \leftarrow diff(X)diindex <- iindex[-1]
y \le - as.vector(labc[1, 1:40]) # percent fat
oout <- 23
dX \leftarrow t(dX[, -\text{count}]y \leftarrow y[-count]fit1 <- psSignal(y, dX, dindex, 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)
```
Description

psVCSignal is used to regress a (glm) response onto a signal such that the signal coefficients can vary over another covariate t. Anisotripic 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_{\text{gamma}} = 1 + 0 \times y,
  X_pred = X,
  t<sub>-</sub>pred = t<sub>-</sub>var,
  y_predicted = NULL,
  ridge\_adj = 1e-08,int = TRUE)
```
Arguments

ps VCSignal 77

Value

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 Intellegent 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 \leftarrow X[\text{sel}, \ ]iindex <- iindex[sel]
dX \leftarrow diff(X)diindex <- iindex[-1]
y \le - as.vector(labc[1, 1:40]) # percent fat
t_var <- as.vector(labc[4, 1:40]) # percent flour
oout <- 23
dX \leq t(dX[, -\text{count}]y \leftarrow y[-oout]
t_v = t_v = r_cPars = 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).

rowtens **79**

Usage

data(rdw)

Format

A vector.

Source

Erasmus University Medical Centre, Rotterdam, The Netherlands

Examples

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

rowtens *Compute the row tensor product of two matrices*

Description

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

Usage

rowtens($X, Y = X$)

Arguments

Details

The input matrices must have the same number of rows, say m. If their numbers of columns are n1 and n2, the result is a matrix with m rows and $n1 \times n2$ 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 *Save a plot as a PDF file.*

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

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.

Description

Adapt margins and axes layout for multiple panels.

Usage

set_panels(rows = 1, cols = 1)

Arguments

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 *Open a graphics window.*

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

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 *Single-Index signal regression using P-splines*

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

sim_psr 83

Value

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 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.

Examples

```
library(JOPS)
# Get the data
library(fds)
data(nirc)
iindex <- nirc$x
X <- nirc$y
sel <- 50:650 # 1200 <= x & x<= 2400
X \leftarrow X[\text{sel}, \ ]iindex <- iindex[sel]
dX \leftarrow diff(X)diindex <- iindex[-1]
y <- as.vector(labc[1, 1:40])
oout <- 23
dX \leq t(dX[, -\text{count}]y \leftarrow y[-oout]
pords \leq c(2, 2)nsegs <-c(27, 7)bdegs = c(3, 3)lambdas \leq 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 Psplines.*

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 (coefficent and link) that can be sliced at arbitary t. Anisotripic 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),
```


sim_vcpsr 85

```
bdegs = 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))\mathcal{L}
```
Arguments

Value

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 < -34p1 < -401
```
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 $p2 < -12$

```
# 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$wl
# Select response and replicated for the 12 temps
# Column 1: water; 2: ethanediol; 3: amino-1-propanol
y <- as.vector(y_mixture[, 2])
y \leftarrow 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 \leftarrow seq(from = 701, to = 1100, by = 1) # for dXt_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)\mathcal{L}
```
Arguments

Details

This function is a modified version of the function [SpATS](#page-0-0) in the package SpATS. The difference is that genotypes have been removed.

Value

A list with the following components:

SpATS.nogeno 89

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 = \simPSANOVA(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.spatial trend(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

 $sphase(x, x1 = min(x), xr = max(x), nseg = 10, bdeg = 3)$

Arguments

Value

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

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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 = sphase(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 fluoresence 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)

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time readmetime Lname LabNumber ProcNumber Proc DimLab DimProc

Source

<https://ucphchemometrics.com/sugar-process-data/>

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.

Description

Compute a truncated power function.

Usage

tpower(x, knot, p)

Arguments

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 = 0:3Y = outer(x, knots, topower, 1)matplot(x, Y, type ='l', lwd = 2, xlab = 'x', ylab = '',
main ='Linear TPF basis')
```


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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