

# Package ‘gps’

April 29, 2023

**Version** 1.1

**Date** 2023-04-29

**Title** General P-Splines

**Author** Zheyuan Li [aut, cre] (<<https://orcid.org/0000-0002-7434-5947>>)

**Maintainer** Zheyuan Li <zheyuan.li@bath.edu>

**Depends** R (>= 4.0.0)

**Imports** stats, splines, Matrix, methods, graphics, grDevices

**Description** General P-splines are non-uniform B-splines penalized by a general difference penalty, proposed by Li and Cao (2022) <[arXiv:2201.06808](https://arxiv.org/abs/2201.06808)>. Constructible on arbitrary knots, they extend the standard P-splines of Eilers and Marx (1996) <[doi:10.1214/ss/1038425655](https://doi.org/10.1214/ss/1038425655)>. They are also related to the O-splines of O'Sullivan (1986) <[doi:10.1214/ss/1177013525](https://doi.org/10.1214/ss/1177013525)> via a sandwich formula that links a general difference penalty to a derivative penalty. The package includes routines for setting up and handling difference and derivative penalties. It also fits P-splines and O-splines to (x, y) data (optionally weighted) for a grid of smoothing parameter values in the automatic search intervals of Li and Cao (2023) <[doi:10.1007/s11222-022-10178-z](https://doi.org/10.1007/s11222-022-10178-z)>. It aims to facilitate other packages to implement P-splines or O-splines as a smoothing tool in their model estimation framework.

**License** GPL-3

**NeedsCompilation** yes

**URL** <https://github.com/ZheyuanLi/gps>

## R topics documented:

DemoBS . . . . .	2
DemoKnots . . . . .	3
DemoNull . . . . .	3
DemoPBS . . . . .	4
DemoSpl . . . . .	5
gps2GS . . . . .	6
GramBS . . . . .	8
MakeGrid . . . . .	10

penalty . . . . .	11
penutils . . . . .	13
periodic . . . . .	15
PlaceKnots . . . . .	16
<b>Index</b>	<b>18</b>

---

DemoBS

---

*Demonstrate the construction of ordinary B-splines*


---

## Description

Demonstrate the construction of 4 ordinary cubic B-splines on 8 knots.

## Usage

```
DemoBS(uniform = TRUE, clamped = FALSE)
```

## Arguments

uniform	if TRUE, place uniform knots; if FALSE, place non-uniform knots.
clamped	if TRUE, place clamped boundary knots when uniform = FALSE. For aesthetic reason, only boundary knots on the left end are clamped. This parameter is ignored when uniform = TRUE.

## Value

This function has no returned values.

## Author(s)

Zheyuan Li <zheyuan.li@bath.edu>

## Examples

```
require(gps)

## uniform B-splines
DemoBS(uniform = TRUE)

## non-uniform B-splines
DemoBS(uniform = FALSE, clamped = FALSE)

## non-uniform & clamped B-splines
DemoBS(uniform = FALSE, clamped = TRUE)
```

---

DemoKnots

---

*Demonstrate ordinary cubic B-splines on three types of knots*


---

**Description**

Demonstrate ordinary cubic B-splines on three types of knots: (a) uniform knots; (b) non-uniform knots; (c) non-uniform knots with clamped boundary knots. The same interior knots are positioned in cases (b) and (c).

**Usage**

```
DemoKnots(aligned = TRUE)
```

**Arguments**

`aligned` if TRUE, interior knots in cases (b) and (c) are aligned for a better display.

**Value**

This function has no returned values.

**Author(s)**

Zheyuan Li <zheyuan.li@bath.edu>

**Examples**

```
require(gps)

DemoKnots(aligned = TRUE)
```

---

DemoNull

---

*Demonstrate the null space of P-splines*


---

**Description**

Cubic P-splines set up with non-uniform B-splines and a 2nd order standard or general difference penalty are fitted to observations simulated from  $y = x$ . Should the resulting standard or general P-splines have the correct null space, the limiting fit at  $\lambda = +\infty$  will be a straight line regardless of knot locations. In this demo, non-uniform knots from different distributions (primarily Beta distributions with varying shape parameters) are attempted. Results show that standard P-splines have an incorrect and unpredictable limiting behavior that is sensitive to knot locations, whereas general P-splines have a correct and consistent limiting behavior.

**Usage**

```
DemoNull(n, k, gps = FALSE)
```

**Arguments**

n                    number of simulated observations from  $y = x$ .  
 k                    number of interior knots to place.  
 gps                  if TRUE, fit general P-splines; if FALSE, fit standard P-splines.

**Value**

This function has no returned values.

**Author(s)**

Zheyuan Li <zheyuan.li@bath.edu>

**Examples**

```
require(gps)

## standard P-splines
DemoNull(n = 100, k = 10, gps = FALSE)

## general P-splines
DemoNull(n = 100, k = 10, gps = TRUE)
```

---

DemoPBS

*Demonstrate the construction of periodic B-splines*

---

**Description**

Demonstrate the construction of 6 periodic cubic B-splines on 7 domain knots.

**Usage**

```
DemoPBS(uniform = TRUE)
```

**Arguments**

uniform              if TRUE, place uniform knots; if FALSE, place non-uniform knots.

**Value**

This function has no returned values.

**Author(s)**

Zheyuan Li <zheyuan.li@bath.edu>

**Examples**

```
require(gps)

## uniform periodic cubic B-splines
DemoPBS(uniform = TRUE)

## non-uniform periodic cubic B-splines
DemoPBS(uniform = FALSE)
```

---

DemoSpl*Demonstrate a polynomial spline and its B-spline representation*

---

**Description**

Demonstrate a cubic spline and its B-spline representation.

**Usage**

```
DemoSpl(uniform = TRUE)
```

**Arguments**

uniform            if TRUE, place uniform knots; if FALSE, place non-uniform knots.

**Value**

A list giving domain knots, B-spline coefficients and piecewise polynomial coefficients of the illustrated cubic spline.

**Author(s)**

Zheyuan Li <zheyuan.li@bath.edu>

**Examples**

```
require(gps)

## a cubic spline with uniform knots
DemoSpl(uniform = TRUE)

## a cubic spline with non-uniform knots
DemoSpl(uniform = FALSE)
```

---

gps2GS	<i>Penalized B-splines estimation with automatic grid search of their smoothing parameter</i>
--------	-----------------------------------------------------------------------------------------------

---

## Description

Fit penalized B-splines (including standard or general P-splines and O-splines) to  $(x, y, w)$  for a grid of smoothing parameter values in the automatic search intervals of Li and Cao (2023). The GCV score and effective degree of freedom of each fit are also returned.

## Usage

```
gps2GS(x, y, w = NULL, xt, d = 4, m = 2, gps = TRUE, periodic = FALSE,
       ng = 20, scalePen = TRUE)
```

```
DemoRhoLim(fit, plot = TRUE)
```

## Arguments

<code>x, y, w</code>	a vector of $x$ -values, $y$ -values and weights.
<code>xt</code>	full knot sequence for ordinary B-splines ( $\text{length}(xt) \geq 2 * d$ ).
<code>d</code>	B-spline order ( $d \geq 2$ ).
<code>m</code>	penalty order ( $1 \leq m \leq d - 1$ ).
<code>gps</code>	if TRUE, use a difference penalty; if FALSE, use a derivative penalty.
<code>periodic</code>	if TRUE, periodic boundary conditions are applied to B-splines and their penalty, so that periodic P-splines are estimated.
<code>ng</code>	number of grid points in the grid search of $\rho$ ; can be set to 0 to set up the grid search only, without actual P-splines estimation.
<code>scalePen</code>	if TRUE, scale the penalty matrix $\mathbf{S}$ (as <b>mgcv</b> does).
<code>fit</code>	fitted P-splines returned by <code>gps2GS</code> .
<code>plot</code>	if TRUE, produce summary plots.

## Details

We smooth  $y_i$  using  $f(x_i) = \mathbf{B}_i \boldsymbol{\beta}$ , where  $\mathbf{B}_i$  is  $i$ -th row of the B-spline design matrix  $\mathbf{B}$  and  $\boldsymbol{\beta}$  is a vector of B-spline coefficients. These coefficients are estimated by minimizing:

$$\|\mathbf{y} - \mathbf{B}\boldsymbol{\beta}\|^2 + \exp(\rho) \cdot \|\mathbf{D}\boldsymbol{\beta}\|^2,$$

where the  $L_2$  penalty  $\|\mathbf{D}\boldsymbol{\beta}\|^2$  is some wiggleness measure for  $f(x)$  and  $\rho \in (-\infty, +\infty)$  is a smoothing parameter.

**Value**

gps2GS returns a large list with the following components:

- eqn
- eigen
- rho.lim
- E
- pwls

**Author(s)**

Zheyuan Li <zheyuan.li@bath.edu>

**References**

Zheyuan Li and Jiguo Cao (2023). Automatic search intervals for the smoothing parameter in penalized splines, *Statistics and Computing*, doi:10.1007/s1122202210178z

**Examples**

```
require(gps)

x <- rnorm(100)
xt <- PlaceKnots(x, d = 4, k = 10)

## set ng = 0 to set up grid search only
## here the y-values does not matter; we simply use the x-values
setup <- gps2GS(x, x, xt = xt, d = 4, m = 2, ng = 0)

## compute exact eigenvalues
DemoResult <- DemoRhoLim(setup)

## simulate 100 (x, y) data from g(x) = sin(2 * pi * x) on [0, 1]
## x-values are not equidistant but at quantiles of Beta(2, 2)
## note that g(x) is a periodic function
x <- qbeta(seq.int(0, 1, length.out = 100), 2, 2)
gx <- sin(2 * pi * x)
y <- rnorm(length(x), gx, sd = 0.1)

## place quantile knots with clamped boundary knots
xt <- PlaceKnots(x, d = 4, k = 10)

## fit a general P-spline with different boundary constraints
ordinary <- gps2GS(x, y, xt = xt, d = 4, m = 2)
periodic <- gps2GS(x, y, xt = xt, d = 4, m = 2, periodic = TRUE)

## identify the optimal fit minimizing GCV score
opt.ordinary <- which.min(ordinary$pwls$gcv)
opt.periodic <- which.min(periodic$pwls$gcv)
```

```

## inspect grid search result
## column 1: ordinary cubic spline
## column 2: periodic cubic spline
op <- par(mfcol = c(2, 2), mar = c(2, 2, 1.5, 0.5))
## ordinary spline
with(ordinary$pwls, plot(rho, edf, ann = FALSE))
title("edf v.s. log(lambda)")
with(ordinary$pwls, plot(rho, gcv, ann = FALSE))
with(ordinary$pwls, points(rho[opt.ordinary], gcv[opt.ordinary], pch = 19))
title("GCV v.s. log(lambda)")
## periodic spline
with(periodic$pwls, plot(rho, edf, ann = FALSE))
title("edf v.s. log(lambda)")
with(periodic$pwls, plot(rho, gcv, ann = FALSE))
with(periodic$pwls, points(rho[opt.periodic], gcv[opt.periodic], pch = 19))
title("GCV v.s. log(lambda)")
par(op)

## inspect fitted splines
yhat.ordinary <- with(ordinary, eqn$B %*% pwls$beta)
yhat.periodic <- with(periodic, eqn$B %*% pwls$beta)
op <- par(mfrow = c(1, 2), mar = c(2, 2, 1.5, 0.5))
## ordinary spline
matplot(x, yhat.ordinary, type = "l", lty = 1, ann = FALSE)
title("ordinary")
## periodic spline
matplot(x, yhat.periodic, type = "l", lty = 1, ann = FALSE)
title("periodic")
par(op)

## pick and plot the optimal fit minimizing GCV score
best.ordinary <- yhat.ordinary[, opt.ordinary]
best.periodic <- yhat.periodic[, opt.periodic]
op <- par(mfrow = c(1, 2), mar = c(2, 2, 1.5, 0.5))
## ordinary spline
plot(x, y, ann = FALSE)
lines(x, gx, lwd = 2, col = 2)
lines(x, best.ordinary, lwd = 2)
title("ordinary")
## periodic spline
plot(x, y, ann = FALSE)
lines(x, gx, lwd = 2, col = 2)
lines(x, best.periodic, lwd = 2)
title("periodic")
par(op)

```



**Description**

Compute the Gram matrix  $G$ , i.e., the matrix of inner products between B-splines  $b_1(x), b_2(x), \dots$ . Precisely, its element is  $G_{uv} = \int b_u(x)b_v(x)dx$ . Such matrix is useful for estimating functional linear models.

The Gram matrix of differentiated B-splines gives the derivative penalty matrix  $S$  for O-splines. Precisely, its element is  $S_{uv} = \int b_u^{(m)}(x)b_v^{(m)}(x)dx$ . Such matrix is straightforward to compute using the results of [SparseD](#); see Examples.

**Usage**

```
GramBS(xt, d)
```

**Arguments**

xt	full knot sequence for ordinary B-splines ( $\text{length}(\text{xt}) \geq 2 * d$ ).
d	B-spline order ( $d \geq 2$ ).

**Value**

A sparse matrix of "dsCMatrix" class.

**Author(s)**

Zheyuan Li <zheyuan.li@bath.edu>

**Examples**

```
require(gps)
require(Matrix)

## 11 domain knots at equal quantiles of Beta(3, 3) distribution
xd <- qbeta(seq.int(0, 1, by = 0.1), 3, 3)
## full knots (with clamped boundary knots) for constructing cubic B-splines
xt <- c(0, 0, 0, xd, 1, 1, 1)
## compute Gram matrix of B-splines
G <- GramBS(xt, d = 4)
round(G, digits = 3)

## Gram matrix of differentiated B-splines, i.e., a derivative penalty matrix
## compute derivative penalty matrices of all orders (m = NULL in SparseD)
D <- SparseD(xt, d = 4, gps = FALSE)
S <- lapply(D, crossprod)
lapply(S, round, digits = 1)
```

---

MakeGrid

---

*Make a grid of  $x$ -values between domain knots*


---

### Description

Place equidistant grid points on each knot span to produce a grid of  $x$ -values between domain knots, suitable for evaluating B-splines.

### Usage

```
MakeGrid(xd, n, rm.dup = FALSE)
```

### Arguments

xd	domain knot sequence.
n	number of equidistant grid points on each knot span.
rm.dup	if FALSE, interior knots will appear twice on the grid; if TRUE, they will appear only once.

### Details

Denote the domain knot sequence by  $s_0, s_1, s_2, \dots, s_k, s_{k+1}$ , where  $(s_j)_1^k$  are interior knots and  $s_0 = a, s_{k+1} = b$  are domain endpoints. A knot span is the interval between two successive knots, i.e.,  $[s_j, s_{j+1}]$ .

To make a suitable grid on  $[a, b]$  for evaluating B-splines, we can place  $n$  equidistant grid points on each knot span, ending up with  $n(k + 1)$  grid points in total. Interior knots will show up twice in this grid. To keep only one instance, set `rm.dup = TRUE`.

### Value

A vector of grid points.

### Author(s)

Zheyuan Li <zheyuan.li@bath.edu>

### Examples

```
require(gps)

## 4 domain knots: two interior knots 0.5 and 1.5 in domain [0, 3]
xd <- c(0, 0.5, 1.5, 3)

## interior knots will appear twice
MakeGrid(xd, 5, rm.dup = FALSE)

## interior knots only appear once
MakeGrid(xd, 5, rm.dup = TRUE)
```

penalty

*Wigginess penalties for penalized B-splines***Description**

For penalized B-splines (including standard or general P-splines and O-splines), (1) construct matrix  $D$  in the wigginess penalty  $\|D\beta\|^2$ ; (2) sample B-spline coefficients from their prior distribution  $N(\mathbf{0}, (D'D)^-)$ ; (3) compute the Moore-Penrose generalized inverse matrix  $(D'D)^-$ .

**Usage**

```
SparseD(xt, d, m = NULL, gps = TRUE)
```

```
PriorCoef(n, D)
```

```
MPinv(D, only.diag = FALSE)
```

**Arguments**

xt	full knot sequence for ordinary B-splines ( $\text{length}(\text{xt}) \geq 2 * d$ ).
d	B-spline order ( $d \geq 2$ ).
m	penalty order ( $1 \leq m \leq d - 1$ ). Can be a vector of multiple values for SparseD.
gps	if TRUE, return $D_{\text{gps}}$ ; if FALSE, return $D_{\text{os}}$ .
n	number of samples to draw from the prior distribution.
D	matrix $D_{\text{gps}}$ or $D_{\text{os}}$ .
only.diag	if TRUE, only diagonal elements are computed.

**Details****General Difference Penalty for General P-Splines:**

A general P-spline is characterized by an order- $m$  general difference matrix  $D_{\text{gps}}$ , which can be computed by `SparseD(..., gps = TRUE)`. For interpretation, the differenced coefficients  $D_{\text{gps}}\beta$  are in fact  $f^{(m)}(x)$ 's B-spline coefficients, so the penalty is their squared  $L_2$  norm.

**Derivative Penalty for O-Splines:**

An O-spline is characterized by  $D_{\text{os}}$  such that  $\|D_{\text{os}}\beta\|^2 = \int_a^b f^{(m)}(x)^2 dx$ . Since  $f^{(m)}(x)$  has B-spline coefficients  $D_{\text{gps}}\beta$ , the integral can be shown to be  $\beta'D'_{\text{gps}}\bar{S}D_{\text{gps}}\beta$ , where  $\bar{S}$  is the Gram matrix of those B-splines representing  $f^{(m)}(x)$ . Following the Cholesky factorization  $\bar{S} = U'U$ , the quadratic form becomes  $\|UD_{\text{gps}}\beta\|^2$ , so that  $D_{\text{os}} = UD_{\text{gps}}$ . This matrix can be computed by `SparseD(..., gps = FALSE)`, with  $\bar{S}$  and  $D_{\text{gps}}$  also returned in a "sandwich" attribute.

**Penalty Matrix:**

We can express the  $L_2$  penalty  $\|D\beta\|^2$  as quadratic form  $\beta'S\beta$ , where  $S = D'D$  is called a penalty matrix. It is trivial to compute  $S$  (using function `crossprod`) once  $D$  is available, so we don't feel the need to provide a function for this. Note that the link between  $D_{\text{os}}$  and  $D_{\text{gps}}$  implies a sandwich formula  $S_{\text{os}} = D'_{\text{gps}}\bar{S}D_{\text{gps}}$ , whereas  $S_{\text{gps}} = D'_{\text{gps}}D_{\text{gps}}$ .

### The Bayesian View:

In the Bayesian view, the penalty  $\beta' S \beta$  is a Gaussian prior for B-spline coefficients  $\beta$ . But it is an improper one because  $S$  has a null space where an unpenalized order- $m$  polynomial lies. Let's decompose  $\beta = \xi + \theta$ , where  $\xi$  (the projection of  $\beta$  on this null space) is the coefficients of this order- $m$  polynomial, and  $\theta$  (orthogonal to  $\xi$ ) is the component that can be shrunk to zero by the penalty. As a result,  $\xi \propto \mathbf{1}$  is not proper, but  $\theta \sim N(\mathbf{0}, S^-)$  is. Function `PriorCoef` samples this distribution, and the resulting B-spline coefficients can be used to create random spline curves. The algorithm behind `PriorCoef` bypasses the Moore-Penrose generalized inverse and is very efficient. We don't recommend forming this inverse matrix because it, being completely dense, is expensive to compute and store. But if we need it anyway, it can be computed using function `MPinv`.

### Value

`SparseD` returns a list of sparse matrices (of "dgCMatrix" class), giving  $D_{\text{gps}}$  or  $D_{\text{os}}$  of order `m[1]`, `m[2]`, ..., `m[length(m)]`. In the latter case,  $\bar{S}$  (sparse matrices of "dsCMatrix" or "ddiMatrix" class) and  $D_{\text{gps}}$  for computing  $D_{\text{os}}$  are also returned in a "sandwich" attribute.

`PriorCoef` returns a vector of B-spline coefficients when `n = 1`. If `n > 1`, it returns a matrix of `n` columns, where each column is an independent sample.

`MPinv` returns  $(D'D)^-$  as a dense matrix.

### Author(s)

Zheyuan Li <zheyuan.li@bath.edu>

### References

Zheyuan Li and Jiguo Cao (2022). General P-splines for non-uniform splines, [doi:10.48550/arXiv.2201.06808](https://doi.org/10.48550/arXiv.2201.06808)

### Examples

```
require(Matrix)
require(gps)

## 11 domain knots at equal quantiles of Beta(3, 3) distribution
xd <- qbeta(seq.int(0, 1, by = 0.1), 3, 3)
## full knots (with clamped boundary knots) for constructing cubic B-splines
xt <- c(0, 0, 0, xd, 1, 1, 1)

## compute D matrices of order 1 to 3 for O-splines
D.os <- SparseD(xt, d = 4, gps = FALSE)
D1.os <- D.os[[1]]; D2.os <- D.os[[2]]; D3.os <- D.os[[3]]

## get D matrices of order 1 to 3 for general P-splines
## we can of course compute them with D.gps <- SparseD(xt, d = 4, gps = TRUE)
## but they are readily stored in the "sandwich" attribute of 'D.os'
D.gps <- attr(D.os, "sandwich")$D
D1.gps <- D.gps[[1]]; D2.gps <- D.gps[[2]]; D3.gps <- D.gps[[3]]

## we can compute the penalty matrix S = D'D
```

```

S.gps <- lapply(D.gps, crossprod)
S1.gps <- S.gps[[1]]; S2.gps <- S.gps[[2]]; S3.gps <- S.gps[[3]]
S.os <- lapply(D.os, crossprod)
S1.os <- S.os[[1]]; S2.os <- S.os[[2]]; S3.os <- S.os[[3]]

## if we want to verify the sandwich formula for 0-splines
## extract 'Sbar' matrices stored in the "sandwich" attribute
## and compute the relative error between S and t(D) %%% Sbar %%% D
Sbar <- attr(D.os, "sandwich")$Sbar
Sbar1 <- Sbar[[1]]; Sbar2 <- Sbar[[2]]; Sbar3 <- Sbar[[3]]
range(S1.os - t(D1.gps) %%% Sbar1 %%% D1.gps) / max(abs(S1.os))
range(S2.os - t(D2.gps) %%% Sbar2 %%% D2.gps) / max(abs(S2.os))
range(S3.os - t(D3.gps) %%% Sbar3 %%% D3.gps) / max(abs(S3.os))

## sample B-spline coefficients from their prior distribution
b.gps <- PriorCoef(n = 5, D2.gps)
b.os <- PriorCoef(n = 5, D2.os)
op <- par(mfrow = c(1, 2), mar = c(2, 2, 1.5, 0.5), oma = c(0, 0, 1, 0))
## prior B-spline coefficients with a general difference penalty
matplot(b.gps, type = "l", lty = 1, ann = FALSE)
title("general difference penalty")
## prior B-spline coefficients with a derivative penalty
matplot(b.os, type = "l", lty = 1, ann = FALSE)
title("derivative penalty")
title("random B-spline coefficients from their prior", outer = TRUE)
par(op)

## plot the corresponding cubic splines with these B-spline coefficients
x <- MakeGrid(xd, n = 11)
B <- splines::splineDesign(xt, x, ord = 4, sparse = TRUE)
y.gps <- B %%% b.gps
y.os <- B %%% b.os
op <- par(mfrow = c(1, 2), mar = c(2, 2, 1.5, 0.5), oma = c(0, 0, 1, 0))
matplot(x, y.gps, type = "l", lty = 1, ann = FALSE)
title("general difference penalty")
matplot(x, y.os, type = "l", lty = 1, ann = FALSE)
title("derivative penalty")
title("random cubic splines with prior B-spline coefficients", outer = TRUE)
par(op)

```

## Description

Evaluate  $\|D\beta\|^2$  without using  $D$ .

## Usage

```
DiffCoef(b, xt, d, m)
```

```
btSb(b, xt, d, m)
```

### Arguments

b	a vector of B-spline coefficients ( $\text{length}(b) == \text{length}(xt) - d$ ).
xt	full knot sequence for ordinary B-splines ( $\text{length}(xt) \geq 2 * d$ ).
d	B-spline order ( $d \geq 2$ ).
m	penalty order ( $1 \leq m \leq d - 1$ ).

### Details

#### Implicit Evaluation of the Penalty:

Sometimes we want to evaluate the penalty  $\|D\beta\|^2$  for some  $\beta$ . The obvious way is to do the matrix-vector multiplication  $D\beta$  then compute its  $L_2$  norm, however, implicit evaluation without using  $D$  is possible. For general P-splines, we can calculate  $D_{\text{gps}}\beta$  by taking order- $m$  general differences between elements of  $\beta$ , and function `DiffCoef` does this. For O-splines, the evaluation can be more refined. Denote domain knots by  $s_0, s_1, s_2, \dots, s_k, s_{k+1}$ , where  $(s_j)_1^k$  are interior knots and  $s_0 = a, s_{k+1} = b$  are domain endpoints. The derivative penalty adds up local wiggleness measure on each interval:  $\int_a^b f^{(m)}(x)^2 dx = \sum_{j=0}^k \int_{s_j}^{s_{j+1}} f^{(m)}(x)^2 dx$ . Function `btSb` calculates each integral in the summation and returns those additive components in a vector.

### Value

`DiffCoef` (for general P-splines only) returns  $D_{\text{gps}}\beta$  as a vector.

`btSb` (for O-splines only) returns a vector with element  $\int_{s_j}^{s_{j+1}} f^{(m)}(x)^2 dx$ .

### Examples

```
require(Matrix)
require(gps)

## 11 domain knots at equal quantiles of Beta(3, 3) distribution
xd <- qbeta(seq.int(0, 1, by = 0.1), 3, 3)
## full knots (with clamped boundary knots) for constructing cubic B-splines
xt <- c(0, 0, 0, xd, 1, 1, 1)

## compute 2nd order D matrix for O-splines
D.os <- SparseD(xt, d = 4, m = 2, gps = FALSE)
D2.os <- D.os$order.2

## get 2nd order D matrix for general P-splines
## we can of course compute it with D.gps <- SparseD(xt, d = 4, m = 2, gps = TRUE)
## but it is readily stored in the "sandwich" attribute of 'D.os'
D.gps <- attr(D.os, "sandwich")$D
D2.gps <- D.gps$order.2

## random B-spline coefficients
b <- rnorm(ncol(D2.gps))
```

```
## two ways to evaluate a difference penalty
diff.b1 <- DiffCoef(b, xt, d = 4, m = 2) ## implicit
diff.b2 <- as.numeric(D2.gps %*% b)      ## explicit
range(diff.b1 - diff.b2) / max(abs(diff.b1))

## several ways to evaluate a derivative penalty
sum(btSb(b, xt, d = 4, m = 2)) ## recommended
sum(as.numeric(D2.os %*% b) ^ 2)
S2.os <- crossprod(D2.os); sum(b * as.numeric(S2.os %*% b))
```

periodic

*Design matrix and general difference matrices for periodic B-splines***Description**

For order- $d$  periodic B-splines, `pbsDesign` evaluates B-splines or their derivatives at given  $x$ -values, and `SparsePD` computes general difference matrices of order 1 to  $d - 1$ .

**Usage**

```
pbsDesign(x, xd, d, nDeriv = 0, sparse = FALSE, wrap = TRUE)
```

```
SparsePD(xd, d, wrap = TRUE)
```

**Arguments**

<code>x</code>	$x$ -values where periodic B-splines are to be evaluated.
<code>xd</code>	domain knot sequence for periodic B-splines ( $\text{length}(xd) \geq d + 1$ ).
<code>d</code>	B-spline order ( $d \geq 2$ ).
<code>nDeriv</code>	derivative order.
<code>sparse</code>	if TRUE, create a sparse design matrix of "dgCMatrix" class.
<code>wrap</code>	if TRUE, the knots wrapping strategy is used; if FALSE, the linear constraint strategy is used.

**Details**

These functions perform type-2 construction, by transforming design matrix and general difference matrices for ordinary B-splines to satisfy periodic boundary constraints (see Details). By contrast, `pbsDesign` and `SparsePD` in **gps** perform type-1 construction by basis wrapping.

A spline  $f(x)$  on domain  $[a, b]$  can be constructed to satisfy periodic boundary constraints, that is,  $f^{(q)}(a) = f^{(q)}(b)$ ,  $q = 0, 1, \dots$ , degree - 1. These are actually linear equality constraints

Unlike ordinary B-splines, period B-splines do not require explicit auxiliary boundary knots for their construction. The magic is that auxiliary boundary knots will be automatically positioned by periodic extension of interior knots.

Denote the domain knot sequence by  $s_0, s_1, s_2, \dots, s_k, s_{k+1}$ , where  $(s_j)_1^k$  are interior knots and  $s_0 = a, s_{k+1} = b$  are domain endpoints. For order- $d$  B-splines, we replicate the first  $d - 1$  interior knots (after adding  $b - a$ ) to the right of  $[a, b]$  for an augmented set of  $K = k + d + 1$  knots, which spawns  $p = K - d = k + 1$  ordinary B-splines. It turns out that periodic B-splines can be obtained by wrapping segments of those ordinary B-splines that stretch beyond  $[a, b]$  to the start of the domain (a demo is offered by [DemoPBS](#)).

Note that we must have at least  $d - 1$  interior knots to do such periodic extension. This means that  $d + 1$  domain knots are required at a minimum for construction of periodic B-splines.

### Value

`pbsDesign` returns a design matrix with `length(x)` rows and `length(xd) - 1` columns. `SparsePD` returns a list of sparse matrices (of "dgCMatrix" class), giving general difference matrices of order 1 to  $d - 1$ .

### Author(s)

Zheyuan Li <zheyuan.li@bath.edu>

### Examples

```
require(gps)

## 5 domain knots: three interior knots 0.5, 1.5 and 1.8 in domain [0, 3]
xd <- c(0, 0.5, 1.5, 1.8, 3)

## make a grid
x <- MakeGrid(xd, n = 10)

## construct periodic cubic B-splines
PB1 <- pbsDesign(x, xd, d = 4, wrap = TRUE)
PB2 <- pbsDesign(x, xd, d = 4, wrap = FALSE)

## construct general difference matrices of order 1 to 3
SparsePD(xd, d = 4, wrap = TRUE)
SparsePD(xd, d = 4, wrap = FALSE)
```

---

PlaceKnots

*Automatically place knots according to data*


---

### Description

Place knots for ordinary B-splines or periodic B-splines using automatic strategies.

### Usage

```
PlaceKnots(x, d, k, domain = NULL, uniform = FALSE, periodic = FALSE)
```



**Arguments**

x	observed $x$ -values.
d	B-spline order.
k	number of interior knots.
domain	a vector of two values giving domain interval $[a, b]$ . Will use $\min(x)$ and $\max(x)$ if not specified.
uniform	if TRUE, place equidistant knots; if FALSE, place quantile knots with clamped boundary knots.
periodic	if TRUE, return the domain knot sequence that is sufficient for constructing periodic B-splines (see <a href="#">pbsDesign</a> ); if FALSE, return the full knot sequence that is required for constructing ordinary B-splines.

**Value**

A vector of  $K = k + 2d$  knots for ordinary B-splines, or  $k + 2$  knots for periodic B-splines.

**Author(s)**

Zheyuan Li <zheyuan.li@bath.edu>

**Examples**

```
require(gps)

x <- rnorm(50)

## uniform knots for uniform cubic B-splines
xt1 <- PlaceKnots(x, d = 4, k = 5, uniform = TRUE)
B1 <- splines::splineDesign(xt1, x, ord = 4)

## clamped quantile knots for clamped non-uniform cubic B-splines
xt2 <- PlaceKnots(x, d = 4, k = 5, uniform = FALSE)
B2 <- splines::splineDesign(xt2, x, ord = 4)

## uniform knots for uniform periodic cubic B-splines
xd1 <- PlaceKnots(x, d = 4, k = 5, uniform = TRUE, periodic = TRUE)
PB1 <- pbsDesign(x, xd1, d = 4)

## quantile knots for non-uniform periodic cubic B-splines
xd2 <- PlaceKnots(x, d = 4, k = 5, uniform = FALSE, periodic = TRUE)
PB2 <- pbsDesign(x, xd2, d = 4)
```

# Index

btSb (penutils), [13](#)

DemoBS, [2](#)

DemoKnots, [3](#)

DemoNull, [3](#)

DemoPBS, [4](#), [16](#)

DemoRhoLim (gps2GS), [6](#)

DemoSpl, [5](#)

DiffCoef (penutils), [13](#)

gps2GS, [6](#)

GramBS, [8](#)

MakeGrid, [10](#)

MPinv (penalty), [11](#)

pbsDesign, [17](#)

pbsDesign (periodic), [15](#)

penalties (penalty), [11](#)

penalty, [11](#)

penalty.utilities (penutils), [13](#)

penalty.utils (penutils), [13](#)

penutils, [13](#)

periodic, [15](#)

PlaceKnots, [16](#)

PriorCoef (penalty), [11](#)

SparseD, [9](#)

SparseD (penalty), [11](#)

SparsePD (periodic), [15](#)