

Package ‘bspline’

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Type Package

Title B-Spline Interpolation and Regression

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Description Build and use B-splines for interpolation and regression.

In case of regression, equality constraints as well as monotonicity and/or positivity of B-spline weights can be imposed. Moreover, knot positions (not only spline weights) can be part of optimized parameters too. For this end, 'bspline' is able to calculate Jacobian of basis vectors as function of knot positions. User is provided with functions calculating spline values at arbitrary points. These functions can be differentiated and integrated to obtain B-splines calculating derivatives/integrals at any point. B-splines of this package can simultaneously operate on a series of curves sharing the same set of knots. 'bspline' is written with concern about computing performance that's why the basis and Jacobian calculation is implemented in C++. The rest is implemented in R but without notable impact on computing speed.

URL <https://github.com/MathsCell/bspline>

BugReports <https://github.com/MathsCell/bspline/issues>

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bsc	<i>Basis matrix and knot Jacobian for B-spline of order 0 (step function) and higher</i>
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Description

This function is analogous but not equivalent to `splines:bs()` and `splines2::bSpline()`. It is also several times faster.

Usage

```
bsc(x, xk, n = 3L, cjac = FALSE)
```

Arguments

x	Numeric vector, abscissa points
xk	Numeric vector, knots
n	Integer scalar, polynomial order (3 by default)
cjac	Logical scalar, if TRUE makes to calculate Jacobian of basis vectors as function of knot positions (FALSE by default)

Details

For $n=0$, step function is defined as constant on each interval $[xk[i]; xk[i+1][$, i.e. closed on the left and open on the right except for the last interval which is closed on the right too. The Jacobian for step function is considered 0 in every x point even if in points where $x=xk$, the derivative is not defined.

For $n=1$, Jacobian is discontinuous in such points so for these points we take the derivative from the right.

Value

Numeric matrix (for `cjac=FALSE`), each column correspond to a B-spline calculated on `x`; or List (for `cjac=TRUE`) with components

mat basis matrix of dimension `nx x nw`, where `nx` is the length of `x` and `nw=nk-n-1` is the number of basis vectors

jac array of dimension `nx x (n+2) x nw` where `n+2` is the number of support knots for each basis vector

See Also

`splines::bs()`, `splines2::bSpline()`

Examples

```
x=seq(0, 5, length.out=101)
# cubic basis matrix
n=3
m=bsc(x, xk=c(rep(0, n+1), 1:4, rep(5, n+1)), n=n)
matplot(x, m, t="l")
stopifnot(all.equal(numeric(c(m), c(splines::bs(x, knots = 1:4, degree = n, intercept = TRUE))))))
```

 bsp

Calculate B-spline values from their coefficients qw and knots xk

Description

Calculate B-spline values from their coefficients `qw` and knots `xk`

Usage

```
bsp(x, xk, qw, n = 3L)
```

Arguments

<code>x</code>	Numeric vector, abscissa points at which B-splines should be calculated. They are supposed to be non decreasing.
<code>xk</code>	Numeric vector, knots of the B-splines. They are supposed to be non decreasing.
<code>qw</code>	Numeric vector or matrix, coefficients of B-splines. <code>NROW(qw)</code> must be equal to <code>length(xk)-n-1</code> where <code>n</code> is the next parameter
<code>n</code>	Integer scalar, polynomial order of B-splines, by default cubic splines are calculated.

Details

This function does nothing else than calculate a dot-product between a B-spline basis matrix calculated by `bsc()` and coefficients `qw`. If `qw` is a matrix, each column corresponds to a separate set of coefficients. For `x` values falling outside of `xk` range, the B-splines values are set to 0. To get a function calculating spline values at arbitrary points from `xk` and `qw`, cf. `par2bsp()`.

Value

Numeric matrix (column number depends on qw dimensions), B-spline values on x.

See Also

bsc, par2bsp

bspline

bspline: build and use B-splines for interpolation and regression.

Description

Build and use B-splines for interpolation and regression. In case of regression, equality constraints as well as monotonicity requirement can be imposed. Moreover, knot positions (not only spline coefficients) can be part of optimized parameters too. User is provided with functions calculating spline values at arbitrary points. This functions can be differentiated to obtain B-splines calculating derivatives at any point. B-splines of this package can simultaneously operate on a series of curves sharing the same set of knots. 'bspline' is written with concern about computing performance that's why the basis calculation is implemented in C++. The rest is implemented in R but without notable impact on computing speed.

bspline functions

- bsc: basis matrix (implemented in C++)
- bsp: values of B-spline from its coefficients
- dbsp: derivative of B-spline
- par2bsp: build B-spline function from parameters
- bsppar: retrieve B-spline parameters from its function
- smbbsp: build smoothing B-spline
- fitsmbbsp: build smoothing B-spline with optimized knot positions
- diffn: finite differences

bsppar

Retrieve parameters of B-splines

Description

Retrieve parameters of B-splines

Usage

bsppar(f)

Arguments

f Function, B-splines such that returned by par3bsp(), smbbsp(), ...

Value

List having components: n - polynomial order, qw - coefficients, xk - knots

dbsp *Derivative of B-spline*

Description

Derivative of B-spline

Usage

```
dbsp(f, nderiv = 1L)
```

Arguments

f Function, B-spline such as returned by smbbsp() or par2bsp()
 nderiv Integer scalar ≥ 0 , order of derivative to calculate (1 by default)

Value

Function calculating requested derivative

Examples

```
x=seq(0., 1., length.out=11L)
y=sin(2*pi*x)
f=smbbsp(x, y, nki=2L)
d_f=dbsp(f)
xf=seq(0., 1., length.out=101) # fine grid for plotting
plot(xf, d_f(xf)) # derivative estimated by B-splines
lines(xf, 2.*pi*cos(2*pi*xf), col="blue") # true derivative
xk=bsppar(d_f)$xk
points(xk, d_f(xk), pch="x", col="red") # knot positions
```

diffn *Finite differences*

Description

Calculate dy/dx where x,y are first and second columns of the entry matrix 'm'

Usage

diffn(m, ndiff = 1L)

Arguments

m 2- or more-column numeric matrix
 ndiff Integer scalar, order of finite difference (1 by default)

Value

Numeric matrix, first column is midpoints of x , the second and following are dy/dx

ibsp *Indefinite integral of B-spline*

Description

Indefinite integral of B-spline

Usage

ibsp(f, const = 0, nint = 1L)

Arguments

f Function, B-spline such as returned by `smbasp()` or `par2bsp()`
 const Numeric scalar or vector of length `ncol(qw)` where `qw` is weight matrix of `f`.
 Defines starting value of weights for indefinite integral (0 by default).
 nint Integer scalar ≥ 0 , defines how many times to take integral (1 by default)

Details

If `f` is B-spline, then following identity is held: `dbsp(ibsp(f))` is identical to `f`. Generally, it does not work in the other sens: `ibsp(dbsp(f))` is not `f` but not very far. If we can get an appropriate constant `C=f(min(x))` then we can assert that `ibsp(dbsp(f), const=C)` is the same as `f`.

Value

Function calculating requested integral

iknots	<i>Estimate internal knot positions equalizing jumps in n-th derivative</i>
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Description

Normalized total variation of n-th finite differences is calculated for each column in y then averaged. These averaged values are fitted by a linear spline to find knot positions that equalize the jumps of n-th derivative.

NB. This function is used internally in (fit)smbasp() and a priori has no interest to be called directly by user.

Usage

```
iknots(x, y, nki = 1L, n = 3L)
```

Arguments

x	Numeric vector
y	Numeric vector or matrix
nki	Integer scalar, number of internal knots to estimate (1 by default)
n	Integer scalar, polynomial order of B-spline (3 by default)

Value

Numeric vector, estimated knot positions

jacw	<i>Knot Jacobian of B-spline with weights</i>
------	---

Description

Knot Jacobian of B-spline with weights

Usage

```
jacw(jac, qws)
```

Arguments

jac	Numeric array, such as returned by bsc(..., cjac=TRUE)
qws	Numeric matrix, each column is a set of weights forming a B-spline. If qws is a vector, it is coerced to 1-column matrix.

Value

Numeric array of size $n_x \times n_{col}(q_w) \times n_k$, where $n_x = \dim(jac)[1]$ and n_k is the number of knots $\dim(jac)[3] + n + 1$ (n being polynomial order).

par2bsp *Convert parameters to B-spline function*

Description

Convert parameters to B-spline function

Usage

```
par2bsp(n, qw, xk)
```

Arguments

n	Integer scalar, polynomial order of B-splines
qw	Numeric vector or matrix, coefficients of B-splines, one set per column in case of matrix
xk	Numeric vector, knots

Value

Function, calculating B-splines at arbitrary points and having interface $f(x, \text{select})$ where x is a vector of abscissa points. Parameter `select` is passed to `qw[,select,drop=FALSE]` and can be missing. This function will return a matrix of size `length(x) x ncol(qw)` if `select` is missing. Elsewhere, a number of column will depend on `select` parameter. Column names in the result matrix will be inherited from `qw`.

smbbsp *Smoothing B-spline of order $n \geq 0$*

Description

Optimize smoothing B-spline coefficients (`smbbsp`) and knot positions (`fitsmbbsp`) such that residual squared sum is minimized for all y columns.

Usage

```
smbbsp(
  x,
  y,
  n = 3L,
  xki = NULL,
  nki = 1L,
  lieq = NULL,
  monotone = 0,
  positive = 0,
```



```

    mat = NULL
  )

fitsmbsp(
  x,
  y,
  n = 3L,
  xki = NULL,
  nki = 1L,
  lieq = NULL,
  monotone = 0,
  positive = 0,
  control = list()
)

```

Arguments

x	Numeric vector, abscissa points
y	Numeric vector or matrix or data.frame, ordinate values to be smoothed (one set per column in case of matrix or data.frame)
n	Integer scalar, polynomial order of B-splines (3 by default)
xki	Numeric vector, strictly internal B-spline knots, i.e. lying strictly inside of x bounds. If NULL (by default), they are estimated with the help of <code>iknots()</code> . This vector is used as initial approximation during optimization process. Must be non decreasing if not NULL.
nki	Integer scalar, internal knot number (1 by default). When <code>nki==0</code> , it corresponds to polynomial regression. If <code>xki</code> is not NULL, this parameter is ignored.
lieq	List, equality constraints to respect by the smoothing spline, one list item per y column. By default (NULL), no constraint is imposed. Constraints are given as a 2-column matrix (<code>xe, ye</code>) where for each <code>xe</code> , an <code>ye</code> value is imposed. If a list item is NULL, no constraint is imposed on corresponding y column.
monotone	Numeric scalar or vector, if <code>monotone > 0</code> , resulting B-spline weights must be increasing; if <code>monotone < 0</code> , B-spline weights must be decreasing; if <code>monotone == 0</code> (default), no constraint on monotonicity is imposed. If 'monotone' is a vector it must be of length <code>ncol(y)</code> , in which case each component indicates the constraint for corresponding column of y.
positive	Numeric scalar, if <code>positive > 0</code> , resulting B-spline weights must be ≥ 0 ; if <code>positive < 0</code> , B-spline weights must be decreasing; if <code>positive == 0</code> (default), no constraint on positivity is imposed. If 'positive' is a vector it must be of length <code>ncol(y)</code> , in which case each component indicates the constraint for corresponding column of y.
mat	Numeric matrix of basis vectors, if NULL it is recalculated by <code>bsc()</code> . If provided, it is the responsibility of the user to ensure that this matrix be adequate to <code>xki</code> vector.
control	List, passed through to <code>nlsic()</code> call

Details

If constraints are set, we use `nlsic::lsie_ln()` to solve a least squares problem with equality constraints in least norm sens for each y column. Otherwise, `nlsic::ls_ln_svd()` is used for the whole y matrix. The solution of least squares problem is a vector of B-splines coefficients `qw`, one vector per y column. These vectors are used to define B-spline function which is returned as the result.

NB. When `nki >= length(x)-n-1` (be it from direct setting or calculated from `length(xki)`), it corresponds to spline interpolation, i.e. the resulting spline will pass exactly by (x,y) points (well, up to numerical precision).

Border and external knots are fixed, only strictly internal knots can move during optimization. The optimization process is constrained to respect a minimal distance between knots as well as to bound them to x range. This is done to avoid knots getting unsorted during iterations and/or going outside of a meaningful range.

Value

Function, smoothing B-splines respecting optional constraints (generated by `par2bsp()`).

See Also

`bsppar` for retrieving parameters of B-spline functions; `par2bsp` for generating B-spline function; `iknots` for estimation of knot positions

Examples

```
x=seq(0, 1, length.out=11)
y=sin(pi*x)+rnorm(x, sd=0.1)
# constraint B-spline to be 0 at the interval ends
fsm=smbbsp(x, y, nki=1, lieq=list(rbind(c(0, 0), c(1, 0))))
# check parameters of found B-splines
bsppar(fsm)
plot(x, y) # original "measurements"
# fine grained x
xfine=seq(0, 1, length.out=101)
lines(xfine, fsm(xfine)) # fitted B-splines
lines(xfine, sin(pi*xfine), col="blue") # original function
# visualize knot positions
xk=bsppar(fsm)$xk
points(xk, fsm(xk), pch="x", col="red")
# fit broken line with linear B-splines
x1=seq(0, 1, length.out=11)
x2=seq(1, 3, length.out=21)
x3=seq(3, 4, length.out=11)
y1=x1+rnorm(x1, sd=0.1)
y2=-2+3*x2+rnorm(x2, sd=0.1)
y3=4+x3+rnorm(x3, sd=0.1)
x=c(x1, x2, x3)
y=c(y1, y2, y3)
plot(x, y)
```

```
f=fitsmb(x, y, n=1, nki=2)
lines(x, f(x))
```

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