Package 'bspline'

October 12, 2022

Type Package

Title B-Spline Interpolation and Regression

Version 2.1

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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

License GPL-2 Encoding UTF-8 Imports Rcpp (>= 1.0.7), nlsic (>= 1.0.2), arrApply LinkingTo Rcpp, RcppArmadillo RoxygenNote 7.2.1 Suggests RUnit Copyright INRAE/INSA/CNRS NeedsCompilation yes Repository CRAN

Date/Publication 2022-09-28 23:10:02 UTC

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bsc

Basis matrix and knot Jacobian for B-spline of order 0 (step function) and higher

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

| х | 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="1")
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

| x | Numeric vector, abscissa points at which B-splines should be calculated. They are supposed to be non decreasing. |
|----|---|
| xk | Numeric vector, knots of the B-splines. They are supposed to be non decreasing. |
| qw | Numeric vector or matrix, coefficients of B-splines. NROW(qw) must be equal to $length(xk)-n-1$ where n is the next parameter |
| n | 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
- smbsp: build smoothing B-spline
- fitsmbsp: 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)

dbsp

Arguments

f

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

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, same_xk = FALSE)

Arguments

| f | Function, B-spline such as returned by smbsp() or par2bsp() |
|---------|---|
| nderiv | Integer scalar >= 0, order of derivative to calculate (1 by default) |
| same_xk | Logical scalar, if TRUE, indicates to calculate derivative on the same knot grid as original function. In this case, coefficient number will be incremented by 2. Otherwise, extreme knots are removed on each side of the grid and coefficient number is maintained (FALSE by default). |

Value

Function calculating requested derivative

Examples

```
x=seq(0., 1., length.out=11L)
y=sin(2*pi*x)
f=smbsp(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

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

| d | ma | t |
|---|----|---|
| | | |

Differentiation matrix

Description

Calculate matrix for obtaining coefficients of first-derivative B-spline. They can be calculated as dqw=Md %*% qw. Here, dqw are coefficients of the first derivative, Md is the matrix returned by this function, and qw are the coefficients of differentiated B-spline.

Usage

dmat(nqw = NULL, xk = NULL, n = NULL, f = NULL, same_xk = FALSE)

Arguments

| nqw | Integer scalar, row number of qw matrix (i.e. degree of freedom of a B-spline) |
|---------|--|
| xk | Numeric vector, knot positions |
| n | Integer scalar, B-spline polynomial order |
| f | Function from which previous parameters can be retrieved. If both f and any of previous parameters are given then explicitly set parameters take precedence over those retrieved from f. |
| same_xk | Logical scalar, the same meaning as in dbsp |

Value

Numeric matrix of size nqw-1 x nqw

ibsp

Description

Indefinite integral of B-spline

Usage

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

Arguments

| f | Function, B-spline such as returned by smbsp() 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

Estimate internal knot positions equalizing jumps in n-th derivative

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)smbsp() and a priori has no interest to be called directly by user.

Usage

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

Arguments

| х | Numeric vector |
|-----|---|
| У | 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

| ipk | Intervals of points in knot intervals | |
|-----|---------------------------------------|--|
|-----|---------------------------------------|--|

Description

Find first and last+1 indexes iip s.t. x[iip] belongs to interval starting at xk[iik]

Usage

ipk(x, xk)

Arguments

| х | Numeric vector, abscissa points (must be non decreasing) |
|----|--|
| xk | Numeric vector, knots (must be non decreasing) |

Value

Integer matrix of size (2 x length(xk)-1). Indexes are 0-based

| • | | |
|-----|-----|--|
| - 1 | acw | |
| J | acw | |

Knot Jacobian of B-spline with weights

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. |

par2bsp

Value

Numeric array of size nx x ncol(qw) x nk, where nx=dim(jac)[1] and nk 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, covqw = NULL, sdy = NULL, sdqw = NULL)

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 |
| covqw | Numeric Matrix, covariance matrix of qw (can be estimated in smbsp). |
| sdy | Numeric vector, SD of each y column (can be estimated in smbsp). |
| sdqw | Numeric Matrix, SD of qw thus having the same dimension as qw (can be estimated in smbsp). |

Value

Function, calculating B-splines at arbitrary points and having interface f(x, 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.

smbsp

Description

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

Usage

```
smbsp(
 х,
 у,
 n = 3L,
 xki = NULL,
 nki = 1L,
 lieq = NULL,
 monotone = 0,
 positive = 0,
 mat = NULL,
 estSD = FALSE,
  tol = 1e-10
)
fitsmbsp(
 х,
 у,
 n = 3L,
 xki = NULL,
 nki = 1L,
 lieq = NULL,
 monotone = 0,
 positive = 0,
 control = list(),
 estSD = FALSE,
  tol = 1e-10
)
```

Arguments

| х | Numeric vector, abscissa points |
|-----|---|
| У | 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 iknots(). |

| | 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 nki==0, it corresponds to polynomial regression. If xki 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 (xe, ye) where for each xe, an ye value is imposed. If a list item is NULL, no constraint is imposed on corresponding y column. |
| monotone | Numeric scalar or vector, if monotone > 0 , resulting B-spline weights must be increasing; if monotone < 0 , B-spline weights must be decreasing; if monotone == 0 (default), no constraint on monotonicity is imposed. If 'monotone' is a vector it must be of length ncol(y), in which case each component indicates the constraint for corresponding column of y. |
| positive | Numeric scalar, if $positive > 0$, resulting B-spline weights must be $>= 0$; if $positive < 0$, B-spline weights must be decreasing; if $positive == 0$ (default), no constraint on positivity is imposed. If 'positive' is a vector it must be of length $ncol(y)$, 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 bsc(). If pro- vided, it is the responsibility of the user to ensure that this matrix be adequate to xki vector. |
| estSD | Logical scalar, if TRUE, indicates to calculate: SD of each y column, covariance matrix and SD of spline coefficients. All these values can be retrieved with bsppar() call (FALSE by default). These estimations are made under assumption that all y points have uncorrelated noise. Optional constraints are not taken into account of SD. |
| tol | Numerical scalar, relative tolerance for small singular values that should be con- sidered as 0 if s[i] <= tol*s[1]. This parameter is ignored if estSD=FALSE (1.e-10 by default). |
| control | List, passed through to nlsic() 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 $nki \ge length(x)-n-1$ (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=smbsp(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=fitsmbsp(x, y, n=1, nki=2)
lines(x, f(x))
```

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