nag_1d_spline_deriv (e02bcc)

1. Purpose

nag_1d_spline_deriv (e02bcc) evaluates a cubic spline and its first three derivatives from its B-spline representation.

2. Specification

```
#include <nag.h>
#include <nage02.h>

void nag_1d_spline_deriv(Nag_DerivType derivs, double x, double s[4],
            Nag_Spline *spline, NagError *fail)
```

3. Description

This routine evaluates the cubic spline $s(x)$ and its first three derivatives at a prescribed argument x. It is assumed that $s(x)$ is represented in terms of its B-spline coefficients c_i, for $i = 1, 2, \ldots, \bar{n}+3$ and (augmented) ordered knot set λ_i, for $i = 1, 2, \ldots, \bar{n}+7$, (see nag_1d_spline_fit_knots (e02bac)), i.e.

$$s(x) = \sum_{i=1}^{q} c_i N_i(x)$$

Here $q = \bar{n}+3$, $\bar{n}$ is the number of intervals of the spline and $N_i(x)$ denotes the normalised B-spline of degree 3 (order 4) defined upon the knots $\lambda_i, \lambda_{i+1}, \ldots, \lambda_{i+4}$. The prescribed argument x must satisfy $\lambda_4 \le x \le \lambda_{\bar{n}+4}$.

At a simple knot λ_i (i.e., one satisfying $\lambda_{i-1} < \lambda_i < \lambda_{i+1}$), the third derivative of the spline is in general discontinuous. At a multiple knot (i.e., two or more knots with the same value), lower derivatives, and even the spline itself, may be discontinuous. Specifically, at a point $x = u$ where (exactly) r knots coincide (such a point is termed a knot of multiplicity r), the values of the derivatives of order $4-j$, for $j = 1, 2, \ldots, r$, are in general discontinuous. (Here $1 \le r \le 4; r > 4$ is not meaningful.) The user must specify whether the value at such a point is required to be the left- or right-hand derivative.

The method employed is based upon:

(i) carrying out a binary search for the knot interval containing the argument x (see Cox (1978)),

(ii) evaluating the non-zero B-splines of orders 1,2,3 and 4 by recurrence (see Cox (1972) and Cox (1978)),

(iii) computing all derivatives of the B-splines of order 4 by applying a second recurrence to these computed B-spline values (see de Boor (1972)),

(iv) multiplying the 4th-order B-spline values and their derivative by the appropriate B-spline coefficients, and summing, to yield the values of $s(x)$ and its derivatives.

nag_1d_spline_deriv can be used to compute the values and derivatives of cubic spline fits and interpolants produced by nag_1d_spline_fit_knots (e02bac), nag_1d_spline_fit (e02bec) or nag_1d_spline_interpolant (e01bac).

If only values and not derivatives are required, nag_1d_spline_evaluate (e02bbc)may be used instead of nag_1d_spline_deriv, which takes about 50% longer than nag_1d_spline_evaluate (e02bbc).

4. Parameters

derivs

Input: **derivs**, of type Nag_DerivType, specifies whether left- or right-hand values of the spline and its derivatives are to be computed (see Section 3). Left- or right-hand values are formed according to whether **derivs** is equal to **Nag_LeftDerivs** or **Nag_RightDerivs** respectively. If x does not coincide with a knot, the value of **derivs** is immaterial. If $x =$ **spline.lamda**[3], right-hand values are computed, and if $x =$ **spline.lamda**[**spline.n**-4]), left-hand values are formed, regardless of the value of **derivs**.

Constraint: **derivs** = **Nag_LeftDerivs** or **Nag_RightDerivs** .

x

Input: the argument x at which the cubic spline and its derivatives are to be evaluated.
Constraint: **spline.lamda**$[3] \leq$ **x** $\leq$ **spline.lamda**[**spline.n**-4].

s[4]

Output: **s**$[j]$ contains the value of the jth derivative of the spline at the argument x, for $j = 0, 1, 2, 3$. Note that **s**$[0]$ contains the value of the spline.

spline

Input: Pointer to structure of type Nag_Spline with the following members:

n - Integer

Input: $\bar{n}+7$, where $\bar{n}$ is the number of intervals of the spline (which is one greater than the number of interior knots, i.e., the knots strictly within the range λ_4 to $\lambda_{\bar{n}+4}$ over which the spline is defined).
Constraint: **spline.n** ≥ 8.

lamda - double *

Input: a pointer to which memory of size **spline.n** must be allocated. **spline.lamda**$[j-1]$ must be set to the value of the jth member of the complete set of knots, λ_j, for $j = 1, 2, \ldots, \bar{n}+7$.
Constraint: the λ_j must be in non-decreasing order with
spline.lamda[**spline.n**-4] $>$ **spline.lamda**$[3]$.

c - double *

Input: a pointer to which memory of size **spline.n**-4 must be allocated. **spline.c** holds the coefficient c_i of the B-spline $N_i(x)$, for $i = 1, 2, \ldots, \bar{n}+3$.

Under normal usage, the call to nag_1d_spline_deriv will follow a call to nag_1d_spline_fit_knots (e02bac), nag_1d_spline_fit_knots (e02bac)or nag_1d_spline_fit (e02bec). In that case, the structure **spline** will have been set up correctly for input to nag_1d_spline_deriv.

fail

The NAG error parameter, see the Essential Introduction to the NAG C Library.

5. Error Indications and Warnings

NE_INT_ARG_LT

On entry, **spline.n** must not be less than 8: **spline.n** $= \langle$*value*$\rangle$.

NE_BAD_PARAM

On entry, parameter **derivs** had an illegal value.

NE_ABSCI_OUTSIDE_KNOT_INTVL

On entry, **x** must satisfy **spline.lamda**$[3] \leq$ **x** $\leq$ **spline.lamda**[**spline.n**-4]:
spline.lamda$[3] = \langle$*value*$\rangle$, **x** $= \langle$*value*$\rangle$, **spline.lamda**$[\langle$*value*$\rangle] = \langle$*value*$\rangle$.

NE_SPLINE_RANGE_INVALID

On entry, the cubic spline range is invalid:
spline.lamda$[3] = \langle$*value*$\rangle$ while **spline.lamda**[**spline.n**-4] $= \langle$*value*$\rangle$.
These must satisfy **spline.lamda**$[3] <$ **spline.lamda**[**spline.n**-4].

6. Further Comments

The time taken by this function is approximately linear in $\log(\bar{n}+7)$.

Note: the function does not test all the conditions on the knots given in the description of **spline.lamda** in Section 4, since to do this would result in a computation time approximately linear in $\bar{n}+7$ instead of $\log(\bar{n}+7)$. All the conditions are tested in nag_1d_spline_fit_knots (e02bac), however, and the knots returned by nag_1d_spline_interpolant (e01bac) or nag_1d_spline_fit (e02bec) will satisfy the conditions.

6.1. Accuracy

The computed value of $s(x)$ has negligible error in most practical situations. Specifically, this value has an absolute error bounded in modulus by $18 \times c_{max} \times$ ***machine precision***, where c_{max} is the largest in modulus of c_j, c_{j+1}, c_{j+2} and c_{j+3}, and j is an integer such that $\lambda_{j+3} \leq x \leq \lambda_{j+4}$. If c_j, c_{j+1}, c_{j+2} and c_{j+3} are all of the same sign, then the computed value of $s(x)$ has relative error bounded by $20\times$ ***machine precision***. For full details see Cox (1978).

No complete error analysis is available for the computation of the derivatives of $s(x)$. However, for most practical purposes the absolute errors in the computed derivatives should be small.

6.2. References

Cox M G (1972) The Numerical Evaluation of B-splines *J. Inst. Math. Appl.* **10** 134–149.

Cox M G (1978) The Numerical Evaluation of a Spline from its B-spline Representation *J. Inst. Math. Appl.* **21** 135–143.

De Boor C (1972) On Calculating with B-splines *J. Approx. Theory* **6** 50–62.

7. See Also

nag_1d_spline_interpolant (e01bac)
nag_1d_spline_fit_knots (e02bac)
nag_1d_spline_evaluate (e02bbc)
nag_1d_spline_fit (e02bec)

8. Example

Compute, at the 7 arguments $x = 0, 1, 2, 3, 4, 5, 6$, the left- and right-hand values and first 3 derivatives of the cubic spline defined over the interval $0 \leq x \leq 6$ having the 6 interior knots $x = 1, 3, 3, 3, 4, 4$, the 8 additional knots 0, 0, 0, 0, 6, 6, 6, 6, and the 10 B-spline coefficients 10, 12, 13, 15, 22, 26, 24, 18, 14, 12.

The input data items (using the notation of Section 4) comprise the following values in the order indicated:

$\bar{n}$	m
spline.lamda$[j]$,	for $j = 0, 1, \ldots, \bar{n} + 6$
spline.c$[j]$,	for $j = 0, 1, \ldots, \bar{n} + 2$
x	m values of **x**

The example program is written in a general form that will enable the values and derivatives of a cubic spline having an arbitrary number of knots to be evaluated at a set of arbitrary points. Any number of data sets may be supplied.

8.1. Program Text

```
/* nag_1d_spline_deriv(e02bcc) Example Program
 *
 * Copyright 1991 Numerical Algorithms Group.
 *
 * Mark 2, 1991.
 *
 * Mark 3 revised, 1994.
 */

#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nage02.h>


main()
{
  Integer i, j, l, m, ncap, ncap7;
  double s[4], x;
  Nag_Spline spline;
  Nag_DerivType derivs;
```

```
  Vprintf("e02bcc Example Program Results\n");
  Vscanf("%*[^\n]"); /* Skip heading in data file */
  while(scanf("%ld%ld",&ncap,&m) != EOF)
    {
      if (m>0)
        {
          if (ncap>0)
            {
              ncap7 = ncap+7;
              spline.n = ncap7;
              spline.c = NAG_ALLOC(ncap7, double);
              spline.lamda = NAG_ALLOC(ncap7, double);
              if (spline.c != (double *)0 && spline.lamda != (double *)0)
                {
                  for (j=0; j<ncap7; j++)
                    Vscanf("%lf",&(spline.lamda[j]));
                  for (j=0; j<ncap+3; j++)
                    Vscanf("%lf",&(spline.c[j]));
                  Vprintf("        x             Spline    1st deriv  \
2nd deriv   3rd deriv");
                  for (i=1; i<=m; i++)
                    {
                      Vscanf("%lf",&x);
                      derivs = Nag_LeftDerivs;
                      for (j=1; j<=2; j++)
                        {
                          e02bcc(derivs, x, s, &spline, NAGERR_DEFAULT);
                          if (derivs ==Nag_LeftDerivs)
                            {
                              Vprintf("\n\n%11.4f   Left",x);
                              for (l=0; l<4; l++)
                                Vprintf("%11.4f",s[l]);
                            }
                          else
                            {
                              Vprintf("\n%11.4f  Right",x);
                              for (l=0; l<4; l++)
                                Vprintf("%11.4f",s[l]);
                            }
                          derivs = Nag_RightDerivs;
                        }
                    }
                  Vprintf("\n");
                  NAG_FREE(spline.c);
                  NAG_FREE(spline.lamda);
                }
              else
                {
                  Vfprintf(stderr,"Storage allocation failed. Reduce the \
size of spline.n\n");
                  exit(EXIT_FAILURE);
                }
            }
          else
            {
              Vfprintf(stderr,"ncap is negative or zero : ncap = %ld\n",ncap);
              exit(EXIT_FAILURE);
            }
        }
      else
        {
          Vfprintf(stderr,"m is negative or zero : m = %ld\n",m);
          exit(EXIT_FAILURE);
        }
    }
  exit(EXIT_SUCCESS);
}
```

8.2. Program Data

```
e02bcc Example Program Data
  7   7
  0.0      0.0      0.0      0.0      1.0      3.0      3.0      3.0
  4.0      4.0      6.0      6.0      6.0      6.0
 10.0     12.0     13.0     15.0     22.0     26.0     24.0     18.0
 14.0     12.0
  0.0
  1.0
  2.0
  3.0
  4.0
  5.0
  6.0
```

8.3. Program Results

```
e02bcc Example Program Results
        x            Spline    1st deriv  2nd deriv   3rd deriv

     0.0000   Left    10.0000     6.0000   -10.0000    10.6667
     0.0000  Right    10.0000     6.0000   -10.0000    10.6667

     1.0000   Left    12.7778     1.3333     0.6667    10.6667
     1.0000  Right    12.7778     1.3333     0.6667     3.9167

     2.0000   Left    15.0972     3.9583     4.5833     3.9167
     2.0000  Right    15.0972     3.9583     4.5833     3.9167

     3.0000   Left    22.0000    10.5000     8.5000     3.9167
     3.0000  Right    22.0000    12.0000   -36.0000    36.0000

     4.0000   Left    22.0000    -6.0000     0.0000    36.0000
     4.0000  Right    22.0000    -6.0000     0.0000     1.5000

     5.0000   Left    16.2500    -5.2500     1.5000     1.5000
     5.0000  Right    16.2500    -5.2500     1.5000     1.5000

     6.0000   Left    12.0000    -3.0000     3.0000     1.5000
     6.0000  Right    12.0000    -3.0000     3.0000     1.5000
```