NAG Library Function Document

nag_1d_spline_interpolant (e01bac)

1 Purpose

nag_1d_spline_interpolant (e01bac) determines a cubic spline interpolant to a given set of data.

2 Specification

```
#include <nag.h>
#include <nage01.h>
```

```
void nag_1d_spline_interpolant (Integer m, const double x[],
     const double y[], Nag_Spline *spline, NagError *fail)
```

3 Description

nag_1d_spline_interpolant (e01bac) determines a cubic spline $s(x)$, defined in the range $x_1 \leq x \leq x_m$, which interpolates (passes exactly through) the set of data points (x_i, y_i), for $i = 1, 2, \ldots, m$, where $m \geq 4$ and $x_1 < x_2 < \cdots < x_m$. Unlike some other spline interpolation algorithms, derivative end conditions are not imposed. The spline interpolant chosen has $m - 4$ interior knots $\lambda_5, \lambda_6, \ldots, \lambda_m$, which are set to the values of $x_3, x_4, \ldots, x_{m-2}$ respectively. This spline is represented in its B-spline form (see Cox (1975)):

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

where $N_i(x)$ denotes the normalized B-spline of degree 3, defined upon the knots $\lambda_i, \lambda_{i+1}, \ldots, \lambda_{i+4}$, and c_i denotes its coefficient, whose value is to be determined by the function.

The use of B-splines requires eight additional knots λ_1, λ_2, λ_3, λ_4, λ_{m+1}, λ_{m+2}, λ_{m+3} and λ_{m+4} to be specified; the function sets the first four of these to x_1 and the last four to x_m.

The algorithm for determining the coefficients is as described in Cox (1975) except that QR factorization is used instead of LU decomposition. The implementation of the algorithm involves setting up appropriate information for the related function nag_1d_spline_fit_knots (e02bac) followed by a call of that function. (For further details of nag_1d_spline_fit_knots (e02bac), see the function document.)

Values of the spline interpolant, or of its derivatives or definite integral, can subsequently be computed as detailed in Section 9.

4 References

Cox M G (1975) An algorithm for spline interpolation *J. Inst. Math. Appl.* **15** 95–108

Cox M G (1977) A survey of numerical methods for data and function approximation *The State of the Art in Numerical Analysis* (ed D A H Jacobs) 627–668 Academic Press

5 Arguments

1: **m** – Integer *Input*

On entry: m, the number of data points.

Constraint: **m** ≥ 4.

2: **x**[**m**] – const double *Input*

On entry: **x**$[i-1]$ must be set to x_i, the ith data value of the independent variable x, for $i = 1, 2, \ldots, m$.

Constraint: **x**$[i] <$ **x**$[i+1]$, for $i = 0, 1, \ldots, m-2$.

3: **y**[**m**] – const double *Input*

On entry: **y**$[i-1]$ must be set to y_i, the ith data value of the dependent variable y, for $i = 1, 2, \ldots, m$.

4: **spline** – Nag_Spline *

Pointer to structure of type Nag_Spline with the following members:

n – Integer *Output*

On exit: the size of the storage internally allocated to **lamda**. This is set to **m** $+ 4$.

lamda – double * *Output*

On exit: the pointer to which storage of size **n** is internally allocated. **lamda**$[i-1]$ contains the ith knot, for $i = 1, 2, \ldots, m+4$.

c – double * *Output*

On exit: the pointer to which storage of size **n** $- 4$ is internally allocated. **c**$[i-1]$ contains the coefficient c_i of the B-spline $N_i(x)$, for $i = 1, 2, \ldots, m$.

Note that when the information contained in the pointers **lamda** and **c** is no longer of use, or before a new call to nag_1d_spline_interpolant (e01bac) with the same **spline**, you should free this storage using the NAG macro `NAG_FREE`. This storage will not have been allocated if this function returns with **fail.code** $\neq$ NE_NOERROR.

5: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_INT_ARG_LT

On entry, **m** $= \langle value \rangle$.
Constraint: **m** ≥ 4.

NE_NOT_STRICTLY_INCREASING

The sequence **x** is not strictly increasing: **x**$[\langle value \rangle] = \langle value \rangle$, **x**$[\langle value \rangle] = \langle value \rangle$.

7 Accuracy

The rounding errors incurred are such that the computed spline is an exact interpolant for a slightly perturbed set of ordinates $y_i + \delta y_i$. The ratio of the root-mean-square value of the δy_i to that of the y_i is no greater than a small multiple of the relative ***machine precision***.

8 Parallelism and Performance

Not applicable.

9 Further Comments

The time taken by nag_1d_spline_interpolant (e01bac) is approximately proportional to m.

All the x_i are used as knot positions except x_2 and x_{m-1}. This choice of knots (see Cox (1977)) means that $s(x)$ is composed of $m-3$ cubic arcs as follows. If $m=4$, there is just a single arc space spanning the whole interval x_1 to x_4. If $m \geq 5$, the first and last arcs span the intervals x_1 to x_3 and x_{m-2} to x_m respectively. Additionally if $m \geq 6$, the ith arc, for $i = 2, 3, \ldots, m-4$, spans the interval x_{i+1} to x_{i+2}.

After the call

```
e01bac(m, x, y, &spline, &fail)
```

the following operations may be carried out on the interpolant $s(x)$.

The value of $s(x)$ at $x =$ **xval** can be provided in the variable **sval** by calling the function

```
e02bbc(xval, &sval, &spline, &fail)
```

The values of $s(x)$ and its first three derivatives at $x =$ **xval** can be provided in the array **sdif** of dimension 4, by the call

```
e02bcc(derivs, xval, sdif, &spline, &fail)
```

Here **derivs** must specify whether the left- or right-hand value of the third derivative is required (see nag_1d_spline_deriv (e02bcc) for details). The value of the integral of $s(x)$ over the range x_1 to x_m can be provided in the variable **sint** by

```
e02bdc(&spline, &sint, &fail)
```

10 Example

The following example program sets up data from 7 values of the exponential function in the interval 0 to 1. nag_1d_spline_interpolant (e01bac) is then called to compute a spline interpolant to these data.

The spline is evaluated by nag_1d_spline_evaluate (e02bbc), at the data points and at points halfway between each adjacent pair of data points, and the spline values and the values of e^x are printed out.

10.1 Program Text

```
/* nag_1d_spline_interpolant (e01bac) Example Program.
 *
 * Copyright 1991 Numerical Algorithms Group.
 *
 * Mark 2, 1991.
 *
 * Mark 6 revised, 2000.
 * Mark 8 revised, 2004.
 */

#include <nag.h>
#include <stdio.h>
#include <math.h>
#include <nag_stdlib.h>
#include <nage01.h>
#include <nage02.h>

#define MMAX 7

int main(void)
{
  Integer    exit_status = 0, i, j, m = MMAX;
  NagError   fail;
  Nag_Spline spline;
  double     fit, *x = 0, xarg, *y = 0;

  INIT_FAIL(fail);

  /* Initialise spline */
  spline.lamda = 0;
```

```
spline.c = 0;

printf(
       "nag_1d_spline_interpolant (e01bac) Example Program Results\n");

if (m >= 1)
  {
    if (!(y = NAG_ALLOC(m, double)) ||
        !(x = NAG_ALLOC(m, double)))
      {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
      }
  }
else
  {
    exit_status = 1;
    return exit_status;
  }

x[0] = 0.0; x[1] = 0.2; x[2] = 0.4;
x[3] = 0.6; x[4] = 0.75; x[5] = 0.9; x[6] = 1.0;

for (i = 0; i < m; ++i)
  y[i] = exp(x[i]);
/* nag_1d_spline_interpolant (e01bac).
 * Interpolating function, cubic spline interpolant, one
 * variable
 */
nag_1d_spline_interpolant(m, x, y, &spline, &fail);
if (fail.code != NE_NOERROR)
  {
    printf("Error from nag_1d_spline_interpolant (e01bac).\n%s\n",
            fail.message);
    exit_status = 1;
    goto END;
  }

printf("\nNumber of distinct knots = %ld\n\n", m-2);
printf("Distinct knots located at \n\n");
for (j = 3; j < m+1; j++)
  printf("%8.4f%s", spline.lamda[j], (j-3)%5 == 4 || j == m?"\n":" ");
printf("\n\n    J    B-spline coeff c\n\n");
for (j = 0;  j < m; ++j)
  printf("    %ld  %13.4f\n", j+1, spline.c[j]);
printf(
       "\n    J       Abscissa            Ordinate            Spline\n\n");
for (j = 0; j < m; ++j)
  {
    /* nag_1d_spline_evaluate (e02bbc).
     * Evaluation of fitted cubic spline, function only
     */
    nag_1d_spline_evaluate(x[j], &fit, &spline, &fail);
    if (fail.code != NE_NOERROR)
      {
        printf("Error from nag_1d_spline_evaluate (e02bbc).\n%s\n",
                fail.message);
        exit_status = 1;
        goto END;
      }

    printf("    %ld %13.4f      %13.4f       %13.4f\n",
            j+1, x[j], y[j], fit);
    if (j < m-1)
      {
        xarg = (x[j] + x[j+1]) * 0.5;
        /* nag_1d_spline_evaluate (e02bbc), see above. */
        nag_1d_spline_evaluate(xarg, &fit, &spline, &fail);
        if (fail.code != NE_NOERROR)
          {
```

```
            printf(
                    "Error from nag_1d_spline_evaluate (e02bbc).\n%s\n",
                    fail.message);
            exit_status = 1;
            goto END;
          }
        printf("      %13.4f                         %13.4f\n",
                xarg, fit);
      }
    }
  /* Free memory allocated by nag_1d_spline_interpolant (e01bac) */
 END:
  NAG_FREE(y);
  NAG_FREE(x);
  NAG_FREE(spline.lamda);
  NAG_FREE(spline.c);
  return exit_status;
}
```

10.2 Program Data

None.

10.3 Program Results

```
nag_1d_spline_interpolant (e01bac) Example Program Results

Number of distinct knots = 5

Distinct knots located at

  0.0000   0.4000   0.6000   0.7500   1.0000


    J    B-spline coeff c

    1         1.0000
    2         1.1336
    3         1.3726
    4         1.7827
    5         2.1744
    6         2.4918
    7         2.7183

    J       Abscissa            Ordinate            Spline

    1        0.0000             1.0000              1.0000
             0.1000                                 1.1052
    2        0.2000             1.2214              1.2214
             0.3000                                 1.3498
    3        0.4000             1.4918              1.4918
             0.5000                                 1.6487
    4        0.6000             1.8221              1.8221
             0.6750                                 1.9640
    5        0.7500             2.1170              2.1170
             0.8250                                 2.2819
    6        0.9000             2.4596              2.4596
             0.9500                                 2.5857
    7        1.0000             2.7183              2.7183
```