NAG Library Function Document

nag_5d_shep_interp (e01tmc)

1 Purpose

nag_5d_shep_interp (e01tmc) generates a five-dimensional interpolant to a set of scattered data points, using a modified Shepard method.

2 Specification

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

```
void nag_5d_shep_interp (Integer m, const double x[], const double f[],
     Integer nw, Integer nq, Integer iq[], double rq[], NagError *fail)
```

3 Description

nag_5d_shep_interp (e01tmc) constructs a smooth function $Q(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^5$ which interpolates a set of m scattered data points $(\mathbf{x}_r, f_r)$, for $r = 1, 2, \ldots, m$, using a modification of Shepard's method. The surface is continuous and has continuous first partial derivatives.

The basic Shepard method, which is a generalization of the two-dimensional method described in Shepard (1968), interpolates the input data with the weighted mean

$$Q(\mathbf{x}) = \frac{\sum_{r=1}^{m} w_r(\mathbf{x}) q_r}{\sum_{r=1}^{m} w_r(\mathbf{x})},$$

where $q_r = f_r$, $w_r(\mathbf{x}) = \frac{1}{d_r^2}$ and $d_r^2 = \|\mathbf{x} - \mathbf{x}_r\|_2^2$.

The basic method is global in that the interpolated value at any point depends on all the data, but nag_5d_shep_interp (e01tmc) uses a modification (see Franke and Nielson (1980) and Renka (1988a)), whereby the method becomes local by adjusting each $w_r(\mathbf{x})$ to be zero outside a hypersphere with centre $\mathbf{x}_r$ and some radius R_w. Also, to improve the performance of the basic method, each q_r above is replaced by a function $q_r(\mathbf{x})$, which is a quadratic fitted by weighted least squares to data local to $\mathbf{x}_r$ and forced to interpolate $(\mathbf{x}_r, f_r)$. In this context, a point $\mathbf{x}$ is defined to be local to another point if it lies within some distance R_q of it.

The efficiency of nag_5d_shep_interp (e01tmc) is enhanced by using a cell method for nearest neighbour searching due to Bentley and Friedman (1979) with a cell density of 3.

The radii R_w and R_q are chosen to be just large enough to include N_w and N_q data points, respectively, for user-supplied constants N_w and N_q. Default values of these arguments are provided, and advice on alternatives is given in Section 9.2.

nag_5d_shep_interp (e01tmc) is derived from the new implementation of QSHEP3 described by Renka (1988b). It uses the modification for five-dimensional interpolation described by Berry and Minser (1999).

Values of the interpolant $Q(\mathbf{x})$ generated by nag_5d_shep_interp (e01tmc), and its first partial derivatives, can subsequently be evaluated for points in the domain of the data by a call to nag_5d_shep_eval (e01tnc).

4 References

Bentley J L and Friedman J H (1979) Data structures for range searching *ACM Comput. Surv.* **11** 397–409

Berry M W, Minser K S (1999) Algorithm 798: high-dimensional interpolation using the modified Shepard method *ACM Trans. Math. Software* **25** 353–366

Franke R and Nielson G (1980) Smooth interpolation of large sets of scattered data *Internat. J. Num. Methods Engrg.* **15** 1691–1704

Renka R J (1988a) Multivariate interpolation of large sets of scattered data *ACM Trans. Math. Software* **14** 139–148

Renka R J (1988b) Algorithm 661: QSHEP3D: Quadratic Shepard method for trivariate interpolation of scattered data *ACM Trans. Math. Software* **14** 151–152

Shepard D (1968) A two-dimensional interpolation function for irregularly spaced data *Proc. 23rd Nat. Conf. ACM* 517–523 Brandon/Systems Press Inc., Princeton

5 Arguments

1: **m** – Integer *Input*

On entry: m, the number of data points.

Note: on the basis of experimental results reported in Berry and Minser (1999), it is recommended to use $\mathbf{m} \geq 4000$.

Constraint: $\mathbf{m} \geq 23$.

2: $\mathbf{x}[\mathbf{5} \times \mathbf{m}]$ – const double *Input*

Note: the (i, j)th element of the matrix X is stored in $\mathbf{x}[(j-1) \times 5 + i - 1]$.

On entry: $\mathbf{x}[(r-1) \times 5], \dots, \mathbf{x}[(r-1) \times 5 + 4]$ must be set to the Cartesian coordinates of the data point $\mathbf{x}_r$, for $r = 1, 2, \dots, m$.

Constraint: these coordinates must be distinct, and must not all lie on the same four-dimensional hypersurface.

3: $\mathbf{f}[\mathbf{m}]$ – const double *Input*

On entry: $\mathbf{f}[r-1]$ must be set to the data value f_r, for $r = 1, 2, \dots, m$.

4: **nw** – Integer *Input*

On entry: the number N_w of data points that determines each radius of influence R_w, appearing in the definition of each of the weights w_r, for $r = 1, 2, \dots, m$ (see Section 3). Note that R_w is different for each weight. If $\mathbf{nw} \leq 0$ the default value $\mathbf{nw} = \min(32, \mathbf{m} - 1)$ is used instead.

Constraint: $\mathbf{nw} \leq \min(50, \mathbf{m} - 1)$.

5: **nq** – Integer *Input*

On entry: the number N_q of data points to be used in the least squares fit for coefficients defining the quadratic functions $q_r(\mathbf{x})$ (see Section 3). If $\mathbf{nq} \leq 0$ the default value $\mathbf{nq} = \min(50, \mathbf{m} - 1)$ is used instead.

Constraint: $\mathbf{nq} \leq 0$ or $20 \leq \mathbf{nq} \leq \min(70, \mathbf{m} - 1)$.

6: $\mathbf{iq}[\mathbf{2} \times \mathbf{m} + \mathbf{1}]$ – Integer *Output*

On exit: integer data defining the interpolant $Q(\mathbf{x})$.

7: **rq**[**21** × **m** + **11**] – double *Output*

On exit: real data defining the interpolant $Q(\mathbf{x})$.

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

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

6 Error Indicators and Warnings

NE_BAD_PARAM

On entry, argument ⟨*value*⟩ had an illegal value.

NE_DATA_HYPERSURFACE

On entry, all the data points lie on the same four-dimensional hypersurface. No unique solution exists.

NE_DUPLICATE_NODE

There are duplicate nodes in the dataset. $\mathbf{x}[(k-1)\times 5+i-1]=\mathbf{x}[(k-1)\times 5+j-1]$, for $i=\langle value\rangle$, $j=\langle value\rangle$ and $k=1,2,\ldots,5$. The interpolant cannot be derived.

NE_INT

On entry, $\mathbf{m}=\langle value\rangle$.
Constraint: $\mathbf{m}\geq 23$.

On entry, $\mathbf{nq}=\langle value\rangle$.
Constraint: $\mathbf{nq}\leq 0$ or $\mathbf{nq}\geq 20$.

NE_INT_2

On entry, $\mathbf{nq}=\langle value\rangle$ and $\mathbf{m}=\langle value\rangle$.
Constraint: $\mathbf{nq}\leq\min(70,\mathbf{m}-1)$.

On entry, $\mathbf{nw}=\langle value\rangle$ and $\mathbf{m}=\langle value\rangle$.
Constraint: $\mathbf{nw}\leq\min(50,\mathbf{m}-1)$.

NE_INTERNAL_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

7 Accuracy

On successful exit, the function generated interpolates the input data exactly and has quadratic precision. Overall accuracy of the interpolant is affected by the choice of arguments **nw** and **nq** as well as the smoothness of the function represented by the input data. Berry and Minser (1999) report on the results obtained for a set of test functions.

8 Parallelism and Performance

nag_5d_shep_interp (e01tmc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_5d_shep_interp (e01tmc) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

9.1 Timing

The time taken for a call to nag_5d_shep_interp (e01tmc) will depend in general on the distribution of the data points and on the choice of N_w and N_q parameters. If the data points are uniformly randomly distributed, then the time taken should be $O(m)$. At worst $O(m^2)$ time will be required.

9.2 Choice of N_w and N_q

Default values of the arguments N_w and N_q may be selected by calling nag_5d_shep_interp (e01tmc) with $\mathbf{nw} \leq 0$ and $\mathbf{nq} \leq 0$. These default values may well be satisfactory for many applications.

If non-default values are required they must be supplied to nag_5d_shep_interp (e01tmc) through positive values of **nw** and **nq**. Increasing these argument values makes the method less local. This may increase the accuracy of the resulting interpolant at the expense of increased computational cost. The default values $\mathbf{nw} = \min(32, \mathbf{m} - 1)$ and $\mathbf{nq} = \min(50, \mathbf{m} - 1)$ have been chosen on the basis of experimental results reported in Berry and Minser (1999). In these experiments the error norm was found to increase with the decrease of N_q, but to be little affected by the choice of N_w. The choice of both, directly affected the time taken by the function. For further advice on the choice of these arguments see Berry and Minser (1999).

10 Example

This program reads in a set of 30 data points and calls nag_5d_shep_interp (e01tmc) to construct an interpolating function $Q(\mathbf{x})$. It then calls nag_5d_shep_eval (e01tnc) to evaluate the interpolant at a set of points.

Note that this example is not typical of a realistic problem: the number of data points would normally be larger.

See also Section 10 in nag_5d_shep_eval (e01tnc).

10.1 Program Text

```
/* nag_5d_shep_interp (e01tmc) Example Program.
 *
 * Copyright 2011 Numerical Algorithms Group.
 *
 * Mark 23, 2010.
 */

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

#define X(I, J) x[I *5 + J]
#define XE(I, J) xe[I *5 + J]

int main(void)
{
  /* Scalars */
  Integer  exit_status, i, j, m, n, nq, nw, liq, lrq;
  NagError fail;

  /* Arrays */
  double   *f = 0, *q = 0, *qx = 0, *rq = 0, *xe = 0, *x = 0;
  Integer  *iq = 0;

  exit_status = 0;

  INIT_FAIL(fail);

  printf("nag_5d_shep_interp (e01tmc) Example Program Results\n");
```

```
  /* Skip heading in data file */
  scanf("%*[^\n] ");

  /* Input the number of nodes. */
  scanf("%ld%*[^\n] ", &m);

  /* Allocate memory */
  lrq = 21 * m + 11;
  liq = 2 * m + 1;
  if (!(f = NAG_ALLOC(m, double)) ||
      !(x = NAG_ALLOC(m*5, double)) ||
      !(rq = NAG_ALLOC(lrq, double)) ||
      !(iq = NAG_ALLOC(liq, Integer)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }

  /* Input the data points X and F. */
  for (i = 0; i < m; ++i) {
    for (j = 0; j < 5; ++j) {
      scanf("%lf", &X(i, j));
    }
    scanf("%lf%*[^\n] ", &f[i]);
  }

  /* Generate the interpolant. */
  nq = 0;
  nw = 0;

  /* nag_5d_shep_interp (e01tmc).
   * Interpolating functions, modified Shepard's method, five
   * variables
   */
  nag_5d_shep_interp(m, x, f, nw, nq, iq, rq, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_5d_shep_interp (e01tmc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  /* Input the number of evaluation points. */
  scanf("%ld%*[^\n] ", &n);

  /* Allocate memory for nag_5d_shep_eval (e01tnc) */
  if (!(q = NAG_ALLOC(n, double)) ||
      !(qx = NAG_ALLOC(n*5, double)) ||
      !(xe = NAG_ALLOC(n*5, double)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }

  /* Input the evaluation points. */
  for (i = 0; i < n; ++i) {
    for (j = 0; j < 5; ++j) {
      scanf("%lf", &XE(i, j));
    }
    scanf("%*[^\n] ");
  }

  /* nag_5d_shep_eval (e01tnc).
   * Evaluate interpolant and first derivatives computed by
   * nag_5d_shep_interp (e01tmc).
   */
  fail.print = Nag_TRUE;
  nag_5d_shep_eval(m, x, f, iq, rq, n, xe, q, qx, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_5d_shep_eval (e01tnc).\n%s\n", fail.message);
```

```
    exit_status = 1;
    goto END;
  }

  printf("\n Evaluation of interpolant at various (5D) points\n");
  printf("\n%6s%30s%17s\n"," pt.no.","point coordinates","value");
  for (i = 0; i < n; ++i)
    printf("%5ld%8.2f%8.2f%8.2f%8.2f%8.2f%10.4f\n", i, XE(i,0),
            XE(i,1), XE(i,2), XE(i,3), XE(i,4), q[i]);

 END:
  NAG_FREE(f);
  NAG_FREE(q);
  NAG_FREE(qx);
  NAG_FREE(rq);
  NAG_FREE(xe);
  NAG_FREE(x);
  NAG_FREE(iq);

  return exit_status;
}
```

10.2 Program Data

```
nag_5d_shep_interp (e01tmc) Example Program Data
30                                      : number of data points
 0.81  0.15  0.44  0.83  0.21  6.39 : x and f(x)
 0.91  0.96  0.00  0.09  0.98  2.50
 0.13  0.88  0.22  0.21  0.73  9.34
 0.91  0.49  0.39  0.79  0.47  7.52
 0.63  0.41  0.72  0.68  0.65  6.91
 0.10  0.13  0.77  0.47  0.22  4.68
 0.28  0.93  0.24  0.90  0.96 45.40
 0.55  0.01  0.04  0.41  0.26  5.48
 0.96  0.19  0.95  0.66  0.99  2.75
 0.96  0.32  0.53  0.96  0.84  7.43
 0.16  0.05  0.16  0.30  0.58  6.05
 0.97  0.14  0.36  0.72  0.78  5.77
 0.96  0.73  0.28  0.75  0.28  8.68
 0.49  0.48  0.58  0.19  0.25  2.38
 0.80  0.34  0.64  0.57  0.08  3.70
 0.14  0.24  0.12  0.06  0.63  1.34
 0.42  0.45  0.03  0.68  0.66 15.18
 0.92  0.19  0.48  0.67  0.28  4.35
 0.79  0.32  0.15  0.13  0.40  1.50
 0.96  0.26  0.93  0.89  0.61  3.43
 0.66  0.83  0.41  0.17  0.09  3.10
 0.04  0.70  0.40  0.54  0.37 14.33
 0.85  0.33  0.15  0.03  0.36  0.35
 0.93  0.58  0.88  0.81  0.40  4.30
 0.68  0.29  0.88  0.60  0.47  3.77
 0.76  0.26  0.09  0.41  0.14  4.16
 0.74  0.26  0.33  0.64  0.36  6.75
 0.39  0.68  0.69  0.37  0.12  5.22
 0.66  0.52  0.17  1.00  0.43 16.23
 0.17  0.08  0.35  0.71  0.17 10.62 : End of data points
6                                       : number of evaluation points
 0.10  0.10  0.10  0.10  0.10       : evaluation point ordinates
 0.20  0.20  0.20  0.20  0.20
 0.30  0.30  0.30  0.30  0.30
 0.40  0.40  0.40  0.40  0.40
 0.50  0.50  0.50  0.50  0.50
 0.60  0.60  0.60  0.60  0.60       : End of evaluation points
```

10.3 Program Results

```
nag_5d_shep_interp (e01tmc) Example Program Results

 Evaluation of interpolant at various (5D) points

 pt.no.             point coordinates             value
    0     0.10    0.10    0.10    0.10    0.10    3.2313
    1     0.20    0.20    0.20    0.20    0.20    4.2476
    2     0.30    0.30    0.30    0.30    0.30    5.2695
    3     0.40    0.40    0.40    0.40    0.40    6.3838
    4     0.50    0.50    0.50    0.50    0.50    7.6837
    5     0.60    0.60    0.60    0.60    0.60    9.3885
```