

NAG Library Function Document

nag_5d_shep_eval (e01tnc)

1 Purpose

nag_5d_shep_eval (e01tnc) evaluates the five-dimensional interpolating function generated by nag_5d_shep_interp (e01tnc) and its first partial derivatives.

2 Specification

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

void nag_5d_shep_eval (Integer m, const double x[], const double f[],
    const Integer iq[], const double rq[], Integer n, const double xe[],
    double q[], double qx[], NagError *fail)
```

3 Description

nag_5d_shep_eval (e01tnc) takes as input the interpolant $Q(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^5$ of a set of scattered data points (\mathbf{x}_r, f_r) , for $r = 1, 2, \dots, m$, as computed by nag_5d_shep_interp (e01tnc), and evaluates the interpolant and its first partial derivatives at the set of points \mathbf{x}_i , for $i = 1, 2, \dots, n$.

nag_5d_shep_eval (e01tnc) must only be called after a call to nag_5d_shep_interp (e01tnc).

nag_5d_shep_eval (e01tnc) is derived from the new implementation of QS3GRD described by Renka (1988). It uses the modification for five-dimensional interpolation described by Berry and Minser (1999).

4 References

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

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

5 Arguments

- 1: **m** – Integer *Input*
On entry: **must** be the same value supplied for argument **m** in the preceding call to nag_5d_shep_interp (e01tnc).
Constraint: **m** \geq 23.
- 2: **x**[5 \times **m**] – const double *Input*
Note: the (i, j) th element of the matrix X is stored in **x**[($j - 1$) \times 5 + $i - 1$].
On entry: **must** be the same array supplied as argument **x** in the preceding call to nag_5d_shep_interp (e01tnc). It **must** remain unchanged between calls.
- 3: **f**[**m**] – const double *Input*
On entry: **must** be the same array supplied as argument **f** in the preceding call to nag_5d_shep_interp (e01tnc). It **must** remain unchanged between calls.

- 4: **iq**[$2 \times m + 1$] – const Integer *Input*
On entry: **must** be the same array returned as argument **iq** in the preceding call to `nag_5d_shep_interp` (e01tnc). It **must** remain unchanged between calls.
- 5: **rq**[$21 \times m + 11$] – const double *Input*
On entry: **must** be the same array returned as argument **rq** in the preceding call to `nag_5d_shep_interp` (e01tnc). It **must** remain unchanged between calls.
- 6: **n** – Integer *Input*
On entry: *n*, the number of evaluation points.
Constraint: $n \geq 1$.
- 7: **xe**[$5 \times n$] – const double *Input*
Note: the (*i*, *j*)th element of the matrix is stored in `xe[(j - 1) × 5 + i - 1]`.
On entry: `xe[(i - 1) × 5], ..., xe[(i - 1) × 5 + 4]` must be set to the evaluation point \mathbf{x}_i , for $i = 1, 2, \dots, n$.
- 8: **q**[*n*] – double *Output*
On exit: `q[i - 1]` contains the value of the interpolant, at \mathbf{x}_i , for $i = 1, 2, \dots, n$. If any of these evaluation points lie outside the region of definition of the interpolant the corresponding entries in **q** are set to the largest machine representable number (see `nag_real_largest_number` (X02ALC)), and `nag_5d_shep_eval` (e01tnc) returns with **fail.code** = NE_BAD_POINT.
- 9: **qx**[$5 \times n$] – double *Output*
Note: the (*i*, *j*)th element of the matrix is stored in `qx[(j - 1) × 5 + i - 1]`.
On exit: `qx[(i - 1) × 5 + j - 1]` contains the value of the partial derivatives with respect to \mathbf{x}_j of the interpolant $Q(\mathbf{x})$ at \mathbf{x}_i , for $i = 1, 2, \dots, n$, and for each of the five partial derivatives $j = 1, 2, 3, 4, 5$. If any of these evaluation points lie outside the region of definition of the interpolant, the corresponding entries in **qx** are set to the largest machine representable number (see `nag_real_largest_number` (X02ALC)), and `nag_5d_shep_eval` (e01tnc) returns with **fail.code** = NE_BAD_POINT.
- 10: **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.
See Section 3.2.1.2 in the Essential Introduction for further information.

NE_BAD_PARAM

On entry, argument *<value>* had an illegal value.

NE_BAD_POINT

On entry, at least one evaluation point lies outside the region of definition of the interpolant. At all such points the corresponding values in **q** and **qx** have been set to `nag_real_largest_number`:
`nag_real_largest_number = <value>`.

NE_INT

On entry, $\mathbf{m} = \langle value \rangle$.

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

On entry, $\mathbf{n} = \langle value \rangle$.

Constraint: $\mathbf{n} \geq 1$.

NE_INT_ARRAY

On entry, values in \mathbf{iq} appear to be invalid. Check that \mathbf{iq} has not been corrupted between calls to `nag_5d_shep_interp` (e01tmc) and `nag_5d_shep_eval` (e01tnc).

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.

An unexpected error has been triggered by this function. Please contact NAG.

See Section 3.6.6 in the Essential Introduction for further information.

NE_NO_LICENCE

Your licence key may have expired or may not have been installed correctly.

See Section 3.6.5 in the Essential Introduction for further information.

NE_REAL_ARRAY

On entry, values in \mathbf{rq} appear to be invalid. Check that \mathbf{rq} has not been corrupted between calls to `nag_5d_shep_interp` (e01tmc) and `nag_5d_shep_eval` (e01tnc).

7 Accuracy

Computational errors should be negligible in most practical situations.

8 Parallelism and Performance

`nag_5d_shep_eval` (e01tnc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

`nag_5d_shep_eval` (e01tnc) 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 X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this function. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

The time taken for a call to `nag_5d_shep_eval` (e01tnc) will depend in general on the distribution of the data points. If the data points are approximately uniformly distributed, then the time taken should be only $O(n)$. At worst $O(mn)$ time will be required.

10 Example

This program evaluates the function

$$f(\mathbf{x}) = \frac{(1.25 + \cos(5.4x_5)) \cos(6x_1) \cos(6x_2) \cos(6x_3)}{6 + 6(3x_4 - 1)^2}$$

at a set of 30 randomly generated 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 random points.

To reduce the time taken by this example, the number of data points is limited to 30. Increasing this value to the suggested minimum of 4000 improves the interpolation accuracy at the expense of more time.

See also Section 10 in `nag_5d_shep_interp` (e01tmc).

10.1 Program Text

```

/* nag_5d_shep_eval (e01tnc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 23, 2010.
 */

#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nage01.h>
#include <nagg05.h>
#include <math.h>

#ifdef __cplusplus
extern "C" {
#endif
static double NAG_CALL funct(double x[]);
#ifdef __cplusplus
}
#endif

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

int main(void)
{
    /* Scalars */
    Integer    exit_status, i, m, n, nq, nw, liq, lrq, lstate, subid;
    Integer    lseed = 1;
    double     fun;
    Nag_BaseRNG genid;
    NagError   fail;
    /* Arrays */
    double     *f = 0, *q = 0, *qx = 0, *rq = 0, *xe = 0, *x = 0;
    Integer     *iq = 0, *state = 0;
    Integer     seed[1], seed2[1];

    exit_status = 0;

    INIT_FAIL(fail);

    printf("nag_5d_shep_eval (e01tnc) Example Program Results\n");

    /* Skip heading in data file */
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endif

    /* Input the seeds. */
#ifdef _WIN32
    scanf_s("%"NAG_IFMT%"NAG_IFMT"%*[\n] ", &seed[0], &seed2[0]);
#else
    scanf("%"NAG_IFMT%"NAG_IFMT"%*[\n] ", &seed[0], &seed2[0]);
#endif

    /* Choose the base generator */

```

```

genid = Nag_Basic;
subid = 0;

/* Get the length of the state array */
lstate = -1;
nag_rand_init_repeatabe(genid, subid, seed, lseed, state, &lstate, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_rand_init_repeatabe (g05kfc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Input the number of nodes. */
#ifdef _WIN32
    scanf_s("%NAG_IFMT"%"^\\n] ", &m);
#else
    scanf("%NAG_IFMT"%"^\\n] ", &m);
#endif

/* 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)) ||
    !(state = NAG_ALLOC(lstate, Integer)))
{
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
}

/* Initialise the generator to a repeatable sequence */
nag_rand_init_repeatabe(genid, subid, seed, lseed, state, &lstate, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_rand_init_repeatabe (g05kfc).\n%s\n",
        fail.message);
    exit_status = 1;
    goto END;
}

/* Generate the data points X */
nag_rand_basic(m*5, state, x, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_rand_basic (g05sac).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Evaluate F */
for (i = 0; i < m; ++i) {
    f[i] = funct(&X(i,0));
}

/* 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. */

```

```

#ifdef _WIN32
    scanf_s("%"NAG_IFMT"%*[\n] ", &n);
#else
    scanf("%"NAG_IFMT"%*[\n] ", &n);
#endif

/* 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;
}

/* Generate repeatable evaluation points. */
nag_rand_init_repeatable(genid, subid, seed2, lseed, state, &lstate, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_rand_init_repeatable (g05kfc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}
nag_rand_basic(n*5, state, xe, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_rand_basic (g05sac).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* 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      i      f(x)      q(x)      |f(x)-Q(x)|\n");
for (i = 0; i < n; ++i) {
    fun = funct(&XE(i,0));
    printf("%6"NAG_IFMT"%10.4f%10.4f%10.4f\n", i, fun, q[i],
          fabs(fun-q[i]));
}

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

return exit_status;
}

static double NAG_CALL funct(double x[])
{
    /* Scalars */
    double ret_val;

    ret_val = ((1.25+cos(5.4*x[4]))*cos(6.0*x[0])*cos(6.0*x[1])
              *cos(6.0*x[2]))/(6.0+6.0*pow((3.0*x[3]-1.0),2.0));
    return ret_val;
}

```

10.2 Program Data

```
nag_5d_shep_eval (e01tnc) Example Program Data
1762543 43331      : random seeds
30          : m the number of data points
8          : n the number of evaluation points
```

10.3 Program Results

```
nag_5d_shep_eval (e01tnc) Example Program Results
```

i	f(x)	q(x)	f(x)-Q(x)
0	0.0058	0.0464	0.0407
1	0.0034	0.4855	0.4821
2	-0.1096	0.0724	0.1820
3	0.0875	0.0320	0.0555
4	0.0015	0.0373	0.0358
5	-0.0158	-0.1170	0.1012
6	0.0046	-0.0484	0.0530
7	-0.0090	-0.0134	0.0043
