

NAG Library Function Document

nag_2d_spline_deriv_rect (e02dhc)

1 Purpose

nag_2d_spline_deriv_rect (e02dhc) computes the partial derivative (of order ν_x, ν_y), of a bicubic spline approximation to a set of data values, from its B-spline representation, at points on a rectangular grid in the x - y plane. This function may be used to calculate derivatives of a bicubic spline given in the form produced by nag_2d_spline_interpolant (e01dac), nag_2d_spline_fit_panel (e02dac), nag_2d_spline_fit_grid (e02dcc) and nag_2d_spline_fit_scatter (e02ddc).

2 Specification

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

void nag_2d_spline_deriv_rect (Integer mx, Integer my, const double x[],
    const double y[], Integer nux, Integer nuy, double z[],
    Nag_2dSpline *spline, NagError *fail)
```

3 Description

nag_2d_spline_deriv_rect (e02dhc) determines the partial derivative $\frac{\partial^{\nu_x+\nu_y}}{\partial x^{\nu_x} \partial y^{\nu_y}}$ of a smooth bicubic spline approximation $s(x, y)$ at the set of data points (x_q, y_r) .

The spline is given in the B-spline representation

$$s(x, y) = \sum_{i=1}^{n_x-4} \sum_{j=1}^{n_y-4} c_{ij} M_i(x) N_j(y), \quad (1)$$

where $M_i(x)$ and $N_j(y)$ denote normalized cubic B-splines, the former defined on the knots λ_i to λ_{i+4} and the latter on the knots μ_j to μ_{j+4} , with n_x and n_y the total numbers of knots of the computed spline with respect to the x and y variables respectively. For further details, see Hayes and Halliday (1974) for bicubic splines and de Boor (1972) for normalized B-splines. This function is suitable for B-spline representations returned by nag_2d_spline_interpolant (e01dac), nag_2d_spline_fit_panel (e02dac), nag_2d_spline_fit_grid (e02dcc) and nag_2d_spline_fit_scatter (e02ddc).

The partial derivatives can be up to order 2 in each direction; thus the highest mixed derivative available is $\frac{\partial^4}{\partial x^2 \partial y^2}$.

The points in the grid are defined by coordinates x_q , for $q = 1, 2, \dots, m_x$, along the x axis, and coordinates y_r , for $r = 1, 2, \dots, m_y$, along the y axis.

4 References

- de Boor C (1972) On calculating with B-splines *J. Approx. Theory* **6** 50–62
- Dierckx P (1981) An improved algorithm for curve fitting with spline functions *Report TW54* Department of Computer Science, Katholieke Universiteit Leuven
- Dierckx P (1982) A fast algorithm for smoothing data on a rectangular grid while using spline functions *SIAM J. Numer. Anal.* **19** 1286–1304
- Hayes J G and Halliday J (1974) The least squares fitting of cubic spline surfaces to general data sets *J. Inst. Math. Appl.* **14** 89–103
- Reinsch C H (1967) Smoothing by spline functions *Numer. Math.* **10** 177–183

5 Arguments

- 1: **mx** – Integer *Input*
On entry: m_x , the number of grid points along the x axis.
Constraint: $\mathbf{mx} \geq 1$.
- 2: **my** – Integer *Input*
On entry: m_y , the number of grid points along the y axis.
Constraint: $\mathbf{my} \geq 1$.
- 3: **x[**mx**]** – const double *Input*
On entry: $\mathbf{x}[q - 1]$ must be set to x_q , the x coordinate of the q th grid point along the x axis, for $q = 1, 2, \dots, m_x$, on which values of the partial derivative are sought.
Constraint: $x_1 < x_2 < \dots < x_{m_x}$.
- 4: **y[**my**]** – const double *Input*
On entry: $\mathbf{y}[r - 1]$ must be set to y_r , the y coordinate of the r th grid point along the y axis, for $r = 1, 2, \dots, m_y$ on which values of the partial derivative are sought.
Constraint: $y_1 < y_2 < \dots < y_{m_y}$.
- 5: **nux** – Integer *Input*
On entry: specifies the order, ν_x of the partial derivative in the x -direction.
Constraint: $0 \leq \mathbf{nux} \leq 2$.
- 6: **nuy** – Integer *Input*
On entry: specifies the order, ν_y of the partial derivative in the y -direction.
Constraint: $0 \leq \mathbf{nuy} \leq 2$.
- 7: **z[**mx** × **my**]** – double *Output*
On exit: $\mathbf{z}[m_y \times (q - 1) + r - 1]$ contains the derivative $\frac{\partial^{\nu_x + \nu_y}}{\partial x^{\nu_x} \partial y^{\nu_y}} s(x_q, y_r)$, for $q = 1, 2, \dots, m_x$ and $r = 1, 2, \dots, m_y$.
- 8: **spline** – Nag_2dSpline * *Input*
 Pointer to structure of type Nag_2dSpline describing the bicubic spline approximation to be differentiated.
 In normal usage, the call to nag_2d_spline_deriv_rect (e02dhc) follows a call to nag_2d_spline_interpolant (e01dac), nag_2d_spline_fit_panel (e02dac), nag_2d_spline_fit_grid (e02dcc) or nag_2d_spline_fit_scatter (e02ddc), in which case, members of the structure **spline** will have been set up correctly for input to nag_2d_spline_deriv_rect (e02dhc).
- 9: **fail** – NagError * *Input/Output*
 The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.

See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

NE_BAD_PARAM

On entry, argument $\langle value \rangle$ had an illegal value.

NE_INT

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

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

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

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

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

Constraint: $0 \leq \mathbf{nux} \leq 2$.

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

Constraint: $0 \leq \mathbf{nuy} \leq 2$.

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 2.7.6 in How to Use the NAG Library and its Documentation for further information.

NE_NO_LICENCE

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

See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

NE_NOT_STRICTLY_INCREASING

On entry, for $i = \langle value \rangle$, $\mathbf{x}[i - 2] = \langle value \rangle$ and $\mathbf{x}[i - 1] = \langle value \rangle$.

Constraint: $\mathbf{x}[i - 2] \leq \mathbf{x}[i - 1]$, for $i = 2, 3, \dots, \mathbf{mx}$.

On entry, for $i = \langle value \rangle$, $\mathbf{y}[i - 2] = \langle value \rangle$ and $\mathbf{y}[i - 1] = \langle value \rangle$.

Constraint: $\mathbf{y}[i - 2] \leq \mathbf{y}[i - 1]$, for $i = 2, 3, \dots, \mathbf{my}$.

7 Accuracy

On successful exit, the partial derivatives on the given mesh are accurate to *machine precision* with respect to the supplied bicubic spline. Please refer to Section 7 in nag_2d_spline_interpolant (e01dac), nag_2d_spline_fit_panel (e02dac), nag_2d_spline_fit_grid (e02dcc) and nag_2d_spline_fit_scatter (e02ddc) of the function document for the respective function which calculated the spline approximant for details on the accuracy of that approximation.

8 Parallelism and Performance

nag_2d_spline_deriv_rect (e02dhc) is not threaded in any implementation.

9 Further Comments

None.

10 Example

This example reads in values of m_x , m_y , x_q , for $q = 1, 2, \dots, m_x$, and y_r , for $r = 1, 2, \dots, m_y$, followed by values of the ordinates $f_{q,r}$ defined at the grid points (x_q, y_r) . It then calls `nag_2d_spline_fit_grid` (e02dcc) to compute a bicubic spline approximation for one specified value of S . Finally it evaluates the spline and its first x derivative at a small sample of points on a rectangular grid by calling `nag_2d_spline_deriv_rect` (e02dhc).

10.1 Program Text

```

/* nag_2d_spline_deriv_rect (e02dhc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#include <math.h>
#include <string.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nage02.h>
#include <nagx04.h>

#ifdef __cplusplus
extern "C"
{
#endif

    static void NAG_CALL print_spline(Integer *ngx, double *gridx, Integer *ngy,
                                      double *gridy, double *z, double *zder,
                                      Integer *exit_status);

#ifdef __cplusplus
}
#endif

#define F(I, J) f[my*(I)+(J)]

int main(void)
{
    /* Scalars */
    Integer exit_status = 0;
    Integer i, j, mx, my, ngx, ngy, nux, nuy, nxest, nyest;
    double delta, fp, s, xhi, xlo, yhi, ylo;
    /* Arrays */
    double *f = 0, *gridx = 0, *gridy = 0, *x = 0, *y = 0, *z = 0, *zder = 0;
    /* NAG types */
    Nag_2dSpline spline;
    Nag_Comm warmstartinf;
    Nag_Start startc;
    NagError fail;

    INIT_FAIL(fail);

    printf("nag_2d_spline_deriv_rect (e02dhc) Example Program Results\n");
    fflush(stdout);

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

    /* Input the number of X, Y co-ordinates MX, MY. */
#ifdef _WIN32

```

```

scanf_s("%" NAG_IFMT " %" NAG_IFMT "%*[\n]", &mx, &my);
#else
scanf("%" NAG_IFMT " %" NAG_IFMT "%*[\n]", &mx, &my);
#endif
nxest = mx + 4;
nyest = my + 4;
spline.nx = 4;
spline.ny = 4;

/* Allocations for spline fitting */
if (!(x = NAG_ALLOC((mx), double)) ||
    !(y = NAG_ALLOC((my), double)) || !(f = NAG_ALLOC((mx * my), double))
    )
{
printf("Allocation failure\n");
exit_status = -1;
goto END;
}

#ifdef _WIN32
for (i = 0; i < mx; i++)
scanf_s("%lf", &x[i]);
#else
for (i = 0; i < mx; i++)
scanf("%lf", &x[i]);
#endif
#ifdef _WIN32
scanf_s("%*[\n]");
#else
scanf("%*[\n]");
#endif
#ifdef _WIN32
for (i = 0; i < my; i++)
scanf_s("%lf", &y[i]);
#else
for (i = 0; i < my; i++)
scanf("%lf", &y[i]);
#endif
#ifdef _WIN32
scanf_s("%*[\n]");
#else
scanf("%*[\n]");
#endif

/* Input the MX*MY function values F at grid points and smoothing factor. */
for (i = 0; i < mx; i++)
for (j = 0; j < my; j++)
#ifdef _WIN32
scanf_s("%lf", &F(i, j));
#else
scanf("%lf", &F(i, j));
#endif

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

/* nag_2d_spline_fit_grid (e02dcc).
* Least squares bicubic spline fit with automatic knot placement,
* two variables (rectangular grid)
*/
startc = Nag_Cold;
nag_2d_spline_fit_grid(startc, mx, x, my, y, f, s, nxest, nyest, &fp,
&swarmstartinf, &spline, &fail);

```

```

if (fail.code != NE_NOERROR) {
    printf("Error from nag_2d_spline_fit_grid (e02dcc)\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

printf("\nSpline fit used smoothing factor s = %13.4e.\n", s);
printf("Number of knots in each direction = %5" NAG_IFMT ",%5" NAG_IFMT
       ".\n\n", spline.nx, spline.ny);
printf("Sum of squared residuals          = %13.4e.\n", fp);
fflush(stdout);

/* Spline and its derivative to be evaluated on rectangular grid with
 * ngx*ngy points on the domain [xlo,xhi] by [ylo,yhi].
 */
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "%lf%lf%*[\n]", &ngx, &xlo, &xhi);
#else
    scanf("%" NAG_IFMT "%lf%lf%*[\n]", &ngx, &xlo, &xhi);
#endif
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "%lf%lf%*[\n]", &ngy, &ylo, &yhi);
#else
    scanf("%" NAG_IFMT "%lf%lf%*[\n]", &ngy, &ylo, &yhi);
#endif

/* Allocations for spline evaluation. */
if (!(gridx = NAG_ALLOC((ngx), double)) ||
    !(gridy = NAG_ALLOC((ngy), double)) ||
    !(z = NAG_ALLOC((ngx * ngy), double)) ||
    !(zder = NAG_ALLOC((ngx * ngy), double))
    )
{
    printf("Allocation failure\n");
    exit_status = -2;
    goto END;
}

delta = (xhi - xlo) / (double) (ngx - 1);
gridx[0] = xlo;
for (i = 1; i < ngx - 1; i++)
    gridx[i] = gridx[i - 1] + delta;
gridx[ngx - 1] = xhi;

delta = (yhi - ylo) / (double) (ngy - 1);
gridy[0] = ylo;
for (i = 1; i < ngy - 1; i++)
    gridy[i] = gridy[i - 1] + delta;
gridy[ngy - 1] = yhi;

/* Evaluate spline (nux=nuy=0) using
 * nag_2d_spline_deriv_rect (e02dhc).
 * Evaluation of spline surface at mesh of points with derivatives
 */
nux = 0;
nuy = 0;
nag_2d_spline_deriv_rect(ngx, ngy, gridx, gridy, nux, nuy, z, &spline,
                          &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_2d_spline_deriv_rect (e02dhc)\n%s\n",
          fail.message);
    exit_status = 2;
    goto END;
}

/* Evaluate spline partial derivative of order (nux,nuy) */
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "%" NAG_IFMT "%*[\n]", &nux, &nuy);
#else
    scanf("%" NAG_IFMT "%" NAG_IFMT "%*[\n]", &nux, &nuy);
#endif

```

```

printf("\nDerivative of spline has order nux, nuy =%5" NAG_IFMT " , %5"
      NAG_IFMT ".\n", nux, nuy);
fflush(stdout);
/* nag_2d_spline_deriv_rect (e02dhc).
 * Evaluation of spline surface at mesh of points with derivatives
 */
nag_2d_spline_deriv_rect(ngx, ngy, gridx, gridy, nux, nuy, zder, &spline,
                        &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_2d_spline_deriv_rect (e02dhc)\n%s\n",
          fail.message);
    exit_status = 3;
    goto END;
}
fflush(stdout);

/* Print tabulated spline and derivative evaluations. */
print_spline(&ngx, gridx, &ngy, gridy, z, zder, &exit_status);

END:
NAG_FREE(f);
NAG_FREE(gridx);
NAG_FREE(gridy);
NAG_FREE(x);
NAG_FREE(y);
NAG_FREE(z);
NAG_FREE(zder);
NAG_FREE(spline.lamda);
NAG_FREE(spline.mu);
NAG_FREE(spline.c);
NAG_FREE(warmstartinf.nag_w);
NAG_FREE(warmstartinf.nag_iw);
return exit_status;
}

static void NAG_CALL print_spline(Integer *ngx, double *gridx, Integer *ngy,
                                  double *gridy, double *z, double *zder,
                                  Integer *exit_status)
{
    /* Print spline function and spline derivative evaluation */
    Integer indent = 0, ncols = 80;
    char formc[] = "%8.3f";
    Integer i;
    char title[49];
    char *outfile = 0;
    char **clabsc = 0, **rlabsc = 0;
    Nag_OrderType order;
    Nag_MatrixType matrixc;
    Nag_DiagType diagc;
    Nag_LabelType chlabelc;
    NagError fail;

    INIT_FAIL(fail);

    /* Allocate for row and column label */
    if (!(clabsc = NAG_ALLOC(*ngx, char *)) ||
        !(rlabsc = NAG_ALLOC(*ngy, char *)))
    {
        printf("Allocation failure\n");
        *exit_status = -3;
        goto END;
    }

    /* Allocate memory to clabsc and rlabsc elements and generate
     * column and row labels to print the results with.
     */
    for (i = 0; i < *ngx; i++) {
        clabsc[i] = NAG_ALLOC(11, char);
#ifdef _WIN32
        sprintf_s(clabsc[i], 11, "%5.2f%5s", gridx[i], "");

```

```

#else
    sprintf(clabsc[i], "%5.2f%5s", gridx[i], "");
#endif
}
for (i = 0; i < *ngy; i++) {
    rlabsc[i] = NAG_ALLOC(11, char);
#ifdef _WIN32
    sprintf_s(rlabsc[i], 11, "%5.2f%5s", gridy[i], "");
#else
    sprintf(rlabsc[i], "%5.2f%5s", gridy[i], "");
#endif
}

order = Nag_ColMajor;
matrixc = Nag_GeneralMatrix;
diagc = Nag_NonUnitDiag;
chlabelc = Nag_CharacterLabels;

/* Print the spline evaluations, z. */
#ifdef _WIN32
    strcpy_s(title, (unsigned)_countof(title),
             "Spline evaluated on X-Y grid (X across, Y down):");
#else
    strcpy(title, "Spline evaluated on X-Y grid (X across, Y down):");
#endif
printf("\n");
fflush(stdout);

/* nag_gen_real_mat_print_comp (x04cbc).
 * Print real general matrix (comprehensive)
 */
nag_gen_real_mat_print_comp(order, matrixc, diagc, *ngy, *ngx, z, *ngy,
                             formc, title, chlabelc, (const char **) rlabsc,
                             chlabelc, (const char **) clabsc, ncols,
                             indent, outfile, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_real_mat_print_comp (x04cbc)\n%s\n",
          fail.message);
    *exit_status = 4;
    goto END;
}

/* Print the spline derivative evaluations, zder. */
#ifdef _WIN32
    strcpy_s(title, (unsigned)_countof(title),
             "Spline derivative evaluated on X-Y grid:");
#else
    strcpy(title, "Spline derivative evaluated on X-Y grid:");
#endif
printf("\n");
fflush(stdout);

nag_gen_real_mat_print_comp(order, matrixc, diagc, *ngy, *ngx, zder, *ngy,
                             formc, title, chlabelc, (const char **) rlabsc,
                             chlabelc, (const char **) clabsc, ncols, indent,
                             outfile, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_real_mat_print_comp (x04cbc)\n%s\n",
          fail.message);
    *exit_status = 5;
    goto END;
}

END:
for (i = 0; i < *ngy; i++)
    NAG_FREE(rlabsc[i]);
NAG_FREE(rlabsc);
for (i = 0; i < *ngx; i++)
    NAG_FREE(clabsc[i]);
NAG_FREE(clabsc);
}

```


10.2 Program Data

```
nag_2d_spline_deriv_rect (e02dhc) Example Program Data
 11      9
 0.0      0.5      1.0      1.5      2.0      : mx, my
 2.5      3.0      3.5      4.0      4.5
 5.0
 0.0      0.5      1.0      1.5      2.0      : x
 2.5      3.0      3.5      4.0
 1.0000    0.88758    0.54030    0.070737   -0.41515
-0.80114  -0.97999   -0.93446   -0.65664   -0.62422
 1.5000    1.3564    0.82045    0.10611   -0.62422
-1.2317   -1.4850   -1.3047   -0.98547
 2.0600    1.7552    1.0806    0.15147   -0.83229
-1.6023   -1.9700   -1.8729   -1.4073
 2.5700    2.1240    1.3508    0.17684   -1.0404
-2.0029   -2.4750   -2.3511   -1.6741
 3.0000    2.6427    1.6309    0.21221   -1.2484
-2.2034   -2.9700   -2.8094   -1.9809
 3.5000    3.1715    1.8611    0.24458   -1.4565
-2.8640   -3.2650   -3.2776   -2.2878
 4.0400    3.5103    2.0612    0.28595   -1.6946
-3.2046   -3.9600   -3.7958   -2.6146
 4.5000    3.9391    2.4314    0.31632   -1.8627
-3.6351   -4.4550   -4.2141   -2.9314
 5.0400    4.3879    2.7515    0.35369   -2.0707
-4.0057   -4.9700   -4.6823   -3.2382
 5.5050    4.8367    2.9717    0.38505   -2.2888
-4.4033   -5.4450   -5.1405   -3.5950
 6.0000    5.2755    3.2418    0.42442   -2.4769
-4.8169   -5.9300   -5.6387   -3.9319
 0.1
 6          0.0          5.0          : f(x,y)
 5          0.0          4.0          : s
 1          0          : ngx, xlo, xhi
          : ngy, ylo, yhi
          : nux, nuy
```

10.3 Program Results

```
nag_2d_spline_deriv_rect (e02dhc) Example Program Results
```

```
Spline fit used smoothing factor s = 1.0000e-01.
Number of knots in each direction = 10, 13.

Sum of squared residuals = 1.0004e-01.

Derivative of spline has order nux, nuy = 1, 0.
```

```
Spline evaluated on X-Y grid (X across, Y down):
 0.00    1.00    2.00    3.00    4.00    5.00
0.00    0.992    2.043    3.029    4.014    5.021    5.997
1.00    0.541    1.088    1.607    2.142    2.705    3.239
2.00   -0.417   -0.829   -1.241   -1.665   -2.083   -2.485
3.00   -0.978   -1.975   -2.914   -3.913   -4.965   -5.924
4.00   -0.648   -1.363   -1.991   -2.606   -3.251   -3.933
```

```
Spline derivative evaluated on X-Y grid:
 0.00    1.00    2.00    3.00    4.00    5.00
0.00    1.093    1.013    0.970    1.004    1.001    0.939
1.00    0.565    0.531    0.515    0.558    0.559    0.499
2.00   -0.429   -0.404   -0.421   -0.423   -0.412   -0.389
3.00   -1.060   -0.951   -0.949   -1.048   -1.031   -0.861
4.00   -0.779   -0.661   -0.608   -0.628   -0.663   -0.701
```
