

# NAG Library Function Document

## nag\_2d\_spline\_deriv\_rect (e02dhc)

### 1 Purpose

nag\_2d\_spline\_deriv\_rect (e02dhc) computes the partial derivative (of order  $\nu_x, \nu_y$ ), 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  $\lambda_i$  to  $\lambda_{i+4}$  and the latter on the knots  $\mu_j$  to  $\mu_{j+4}$ , 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,  $\nu_x$  of the partial derivative in the  $x$ -direction.  
*Constraint:*  $0 \leq \mathbf{nux} \leq 2$ .
  
- 6: **nuy** – Integer *Input*  
*On entry:* specifies the order,  $\nu_y$  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                                     : mx, my
0.0      0.5      1.0      1.5      2.0
2.5      3.0      3.5      4.0      4.5
5.0                                     : x
0.0      0.5      1.0      1.5      2.0
2.5      3.0      3.5      4.0                                     : y
1.0000    0.88758    0.54030    0.070737   -0.41515
-0.80114   -0.97999   -0.93446   -0.65664
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                                     : f(x,y)
6                                     : s
5      0.0      5.0                                     : ngx, xlo, xhi
1      0.0      4.0                                     : ngy, ylo, yhi
1      0                                     : 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