NAG Library Function Document

nag_2d_spline_fit_ts_scat (e02jdc)

Note: *this function uses* **optional arguments** *to define choices in the problem specification and in the details of the algorithm. If you wish to use* default *settings for all of the optional arguments, you need only read Sections 1 to 10 of this document. If, however, you wish to reset some or all of the settings please refer to Section 11 for a detailed description of the specification of the optional arguments produced by the function.*

1 Purpose

nag_2d_spline_fit_ts_scat (e02jdc) computes a spline approximation to a set of scattered data using a two-stage approximation method.

The computational complexity of the method grows linearly with the number of data points; hence large datasets are easily accommodated.

2 Specification

```
#include <nag.h>
#include <nage02.h>
void nag_2d_spline_fit_ts_scat (Integer n, const double x[],
     const double y[], const double f[], Integer lsminp, Integer lsmaxp,
     Integer nxcels, Integer nycels, Integer lcoefs, double coefs[],
     Integer iopts[], double opts[], NagError *fail)
```

Before calling nag_2d_spline_fit_ts_scat (e02jdc), nag_fit_opt_set (e02zkc) must be called with **optstr** set to `"Initialize = e02jdc"`. Settings for optional algorithmic arguments may be specified by calling nag_fit_opt_set (e02zkc) before a call to nag_2d_spline_fit_ts_scat (e02jdc).

3 Description

nag_2d_spline_fit_ts_scat (e02jdc) determines a smooth bivariate spline approximation to a set of data points (x_i, y_i, f_i), for $i = 1, 2, \ldots, n$. Here, 'smooth' means C^1.

The approximation domain is the bounding box $[x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}]$, where $x_{\min}$ (respectively $y_{\min}$) and $x_{\max}$ (respectively $y_{\max}$) denote the lowest and highest data values of the (x_i) (respectively (y_i)).

The spline is computed by local approximations on a uniform triangulation of the bounding box. These approximations are extended to a smooth spline representation of the surface over the domain. The local approximation scheme is by least squares polynomials (Davydov and Zeilfelder (2004)).

The two-stage approximation method employed by nag_2d_spline_fit_ts_scat (e02jdc) is derived from the TSFIT package of O. Davydov and F. Zeilfelder.

Values of the computed spline can subsequently be computed by calling nag_2d_spline_ts_eval (e02jec) or nag_2d_spline_ts_eval_rect (e02jfc).

4 References

Davydov O and Zeilfelder F (2004) Scattered data fitting by direct extension of local polynomials to bivariate splines *Advances in Comp. Math.* **21** 223–271

5 Arguments

1: **n** – Integer *Input*

On entry: n, the number of data values to be fitted.

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

2: **x**[**n**] – const double *Input*
3: **y**[**n**] – const double *Input*
4: **f**[**n**] – const double *Input*

On entry: the (x_i, y_i, f_i) data values to be fitted.

Constraint: $\mathbf{x}[j-1] \neq \mathbf{x}[0]$ for some $j = 2, \ldots, n$ and $\mathbf{y}[k-1] \neq \mathbf{y}[0]$ for some $k = 2, \ldots, n$; i.e., there are at least two distinct x and y values.

5: **lsminp** – Integer *Input*
6: **lsmaxp** – Integer *Input*

On entry: are control parameters for the local approximations.

Each local approximation is computed on a local domain containing one of the triangles in the discretization of the bounding box. The size of each local domain will be adaptively chosen such that if it contains fewer than **lsminp** sample points it is expanded, else if it contains greater than **lsmaxp** sample points a thinning method is applied. **lsmaxp** mainly controls computational cost (in that working with a thinned set of points is cheaper and may be appropriate if the input data is densely distributed), while **lsminp** allows handling of different types of scattered data.

Setting **lsmaxp** $<$ **lsminp**, and therefore forcing either expansion or thinning, may be useful for computing initial coarse approximations. In general smaller values for these arguments reduces cost.

A calibration procedure (experimenting with a small subset of the data to be fitted and validating the results) may be needed to choose the most appropriate values for **lsminp** and **lsmaxp**.

Constraints:

$1 \leq \mathbf{lsminp} \leq \mathbf{n}$;
$\mathbf{lsmaxp} \geq 1$.

7: **nxcels** – Integer *Input*
8: **nycels** – Integer *Input*

On entry: **nxcels** (respectively **nycels**) is the number of cells in the x (respectively y) direction that will be used to create the triangulation of the bounding box of the domain of the function to be fitted.

Greater efficiency generally comes when **nxcels** and **nycels** are chosen to be of the same order of magnitude and are such that **n** is $O(\mathbf{nxcels} \times \mathbf{nycels})$. Thus for a 'square' triangulation — when $\mathbf{nxcels} = \mathbf{nycels}$ — the quantities $\sqrt{\mathbf{n}}$ and **nxcels** should be of the same order of magnitude. See also Section 9.

Constraints:

$\mathbf{nxcels} \geq 1$;
$\mathbf{nycels} \geq 1$.

9: **lcoefs** – Integer *Input*
10: **coefs**[**lcoefs**] – double *Output*

On exit: if **fail.code** = NE_NOERROR on exit, **coefs** contains the computed spline coefficients.

Constraint: $\mathbf{lcoefs} \geq (((\mathbf{nxcels}+2) \times (\mathbf{nycels}+2)+1)/2) \times 10 + 1$.

11: **iopts**[dim] – Integer *Communication Array*

Note: the dimension, dim, of this array is dictated by the requirements of associated functions that must have been previously called. This array MUST be the same array passed as argument **iopts** in the previous call to nag_fit_opt_set (e02zkc).

On entry: the contents of **iopts** MUST NOT be modified in any way either directly or indirectly, by further calls to nag_fit_opt_set (e02zkc), before calling either or both of the evaluation routines nag_2d_spline_ts_eval (e02jec) and nag_2d_spline_ts_eval_rect (e02jfc).

12: **opts**[dim] – double *Communication Array*

Note: the dimension, dim, of this array is dictated by the requirements of associated functions that must have been previously called. This array MUST be the same array passed as argument **opts** in the previous call to nag_fit_opt_set (e02zkc).

On entry: the contents of **opts** MUST NOT be modified in any way either directly or indirectly, by further calls to nag_fit_opt_set (e02zkc), before calling either or both of the evaluation routines nag_2d_spline_ts_eval (e02jec) and nag_2d_spline_ts_eval_rect (e02jfc).

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

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

6 Error Indicators and Warnings

NE_ALL_ELEMENTS_EQUAL

On entry, all elements of **x** or of **y** are equal.

NE_ALLOC_FAIL

Dynamic memory allocation failed.

NE_BAD_PARAM

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

NE_INITIALIZATION

Option arrays are not initialized or are corrupted.

NE_INT

On entry, **lcoefs** = ⟨*value*⟩.
Constraint: **lcoefs** $\geq (((\mathbf{nxcels}+2)\times(\mathbf{nycels}+2)+1)/2)\times 10+1$.

On entry, **lsmaxp** = ⟨*value*⟩.
Constraint: **lsmaxp** ≥ 1.

On entry, **n** = ⟨*value*⟩.
Constraint: **n** > 1.

On entry, **nxcels** = ⟨*value*⟩.
Constraint: **nxcels** ≥ 1.

On entry, **nycels** = ⟨*value*⟩.
Constraint: **nycels** ≥ 1.

NE_INT_2

On entry, **lsminp** = ⟨*value*⟩ and **n** = ⟨*value*⟩.
Constraint: $1 \leq$ **lsminp** $\leq$ **n**.

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 algorithmic failure was encountered. Please contact NAG.

NE_INVALID_OPTION

The value of optional argument **Polynomial Starting Degree** was invalid.

7 Accuracy

Technical results on error bounds can be found in Davydov and Zeilfelder (2004).

Local approximation by polynomials of degree d for n data points has optimal approximation order $n^{-(d+1)/2}$.

The approximation error for C^1 global smoothing is $O(n^{-2})$.

Whether maximal accuracy is achieved depends on the distribution of the input data and the choices of the algorithmic parameters. The reference above contains extensive numerical tests and further technical discussions of how best to configure the method.

8 Parallelism and Performance

nag_2d_spline_fit_ts_scat (e02jdc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_2d_spline_fit_ts_scat (e02jdc) 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

n-linear complexity and memory usage can be attained for sufficiently dense input data if the triangulation parameters **nxcels** and **nycels** are chosen as recommended in their descriptions above. For sparse input data on such triangulations, if many expansion steps are required (see **lsminp**) the complexity may rise to be loglinear.

10 Example

The Franke function

$$\begin{aligned} f(x,y) \quad = \quad & 0.75\exp\Big(-\Big((9x-2)^2+(9y-2)^2\Big)/4\Big)+ \\ & 0.75\exp\Big(-(9x+1)^2/49-(9y+1)/10\Big)+ \\ & 0.5\exp\Big(-\Big((9x-7)^2+(9y-3)^2\Big)/4\Big)- \\ & 0.2\exp\Big(-(9x-4)^2-(9y-7)^2\Big) \end{aligned}$$

is widely used for testing surface-fitting methods. The example program randomly generates a number of points on this surface. From these a spline is computed and then evaluated at a vector of points and on a mesh.

10.1 Program Text

```
/* nag_2d_spline_fit_ts_scat (e02jdc) Example Program.
 *
 * Copyright 2013 Numerical Algorithms Group.
 *
 * Mark 24, 2013.
 */

#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nage02.h>
#include <nagf16.h>
#include <nagg05.h>
#include <string.h>

static Integer generate_data(Integer *n, double **x, double **y, double **f,
                             Integer *lsminp, Integer *lsmaxp,
                             Integer *nxcels, Integer *nycels,
                             Integer *lcoefs, double **coefs);
static Integer handle_options(Integer iopts[], const Integer liopts,
                              double opts[], const Integer lopts);
static Integer evaluate_at_vector(const double coefs[], const Integer iopts[],
                                  const double opts[], const double pmin[],
                                  const double pmax[]);
static Integer evaluate_on_mesh(const double coefs[], const Integer iopts[],
                                const double opts[], const double pmin[],
                                const double pmax[]);

int main(void)
{
  /* Scalars */
  Integer   exit_status = 0;
  Integer   liopts = 100, lopts = 100;
  Integer   i, lcoefs, lsmaxp, lsminp, n, nxcels, nycels;
  /* Arrays */
  double    *coefs = 0, *f = 0, *x = 0, *y = 0;
  double    opts[100], pmax[2], pmin[2];
  Integer   iopts[100];
  /* Nag Types */
  NagError  fail;

  INIT_FAIL(fail);

  printf("nag_2d_spline_fit_ts_scat (e02jdc) Example Program Results\n");

  /* Generate the data to fit. */
  exit_status = generate_data(&n, &x, &y, &f, &lsminp, &lsmaxp, &nxcels,
                              &nycels, &lcoefs, &coefs);
  if (exit_status != 0) goto END;

  /* Initialize the options arrays and set/get some options. */
  exit_status = handle_options(iopts, liopts, opts, lopts);
  if (exit_status != 0) goto END;

  /* Compute the spline coefficients using
   * nag_2d_spline_fit_ts_scat (e02jdc).
   */
  nag_2d_spline_fit_ts_scat(n, x, y, f, lsminp, lsmaxp, nxcels, nycels, lcoefs,
                            coefs, iopts, opts, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_2d_spline_fit_ts_scat (e02jdc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }

  /* pmin and pmax form the bounding box of the spline. We must not attempt to
   * evaluate the spline outside this box. Use nag_dmin_val (f16jpc) and
   * nag_dmax_val (f16jnc) to obtain the mi and max values.
```

```
   */
  nag_dmin_val(n, x, 1, &i, &pmin[0], &fail);
  if (fail.code == NE_NOERROR)
    nag_dmin_val(n, y, 1, &i, &pmin[1], &fail);
  if (fail.code == NE_NOERROR)
    nag_dmax_val(n, x, 1, &i, &pmax[0], &fail);
  if (fail.code == NE_NOERROR)
    nag_dmax_val(n, y, 1, &i, &pmax[1], &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_dmin_val (f16jpc) or nag_dmax_val (f16jnc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }

  NAG_FREE(x);
  NAG_FREE(y);
  NAG_FREE(f);

  /* Evaluate the approximation at a vector of values. */
  exit_status = evaluate_at_vector(coefs, iopts, opts, pmin, pmax);
  if (exit_status != 0) goto END;

  /* Evaluate the approximation on a mesh. */
  exit_status = evaluate_on_mesh(coefs, iopts, opts, pmin, pmax);
  if (exit_status != 0) goto END;

 END:

  NAG_FREE(coefs);

  return exit_status;
}

static Integer generate_data(Integer *n, double **x, double **y, double **f,
                             Integer *lsminp, Integer *lsmaxp, Integer *nxcels,
                             Integer *nycels, Integer *lcoefs, double **coefs)
{
  /* Reads n from a data file and then generates an x and a y vector of n
   * pseudorandom uniformly distributed values on (0,1]. These are passed
   * to the bivariate function of R. Franke to create the data set to fit.
   * The remaining input data for the fitter are set to suitable values for
   * this problem, as discussed by Davydov and Zeilfelder.
   */

  /* Scalars */
  Integer   exit_status = 0;
  Integer   lseed = 4, mstate = 21;
  Integer   i, lstate, subid;
  /* Arrays */
  Integer   seed[4], state[21];
  /* Nag Types */
  NagError  fail;

  INIT_FAIL(fail);

  /* Read the size of the data set to be generated and fitted.
   * (Skip the heading in the data file.)
   */
  scanf("%*[^\n]");
  scanf("%ld%*[^\n] ", n);

  if (!(*x = NAG_ALLOC(*n, double)) ||
      !(*y = NAG_ALLOC(*n, double)) ||
      !(*f = NAG_ALLOC(*n, double)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }
```

```
  /* Initialize the random number generator using
   * nag_rand_init_repeatable (g05kfc) and then generate the data using
   * nag_rand_basic (g05sac).
   */
  subid = 53;
  seed[0] = 32958;
  seed[1] = 39838;
  seed[2] = 881818;
  seed[3] = 45812;
  lstate = mstate;
  nag_rand_init_repeatable(Nag_WichmannHill_I, subid, seed, lseed, state,
                           &lstate, &fail);
  if (fail.code == NE_NOERROR)
    nag_rand_basic(*n, state, *x, &fail);
  if (fail.code == NE_NOERROR)
    nag_rand_basic(*n, state, *y, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error in obtaining repeatable data from\nnag_rand_init_repeatable "
           "(g05kfc) and nag_rand_basic (g05sac).\nError message is:\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }

  for (i = 0; i < *n; i++)
    (*f)[i] = 0.75*
              exp(-(pow((9.*(*x)[i]-2.), 2)+pow((9.*(*y)[i]-2.), 2))/4.) +
    0.75*exp(-pow((9.*(*x)[i]+1.), 2)/49.-(9.*(*y)[i]+1.)/10.) +
    0.5*exp(-(pow((9.*(*x)[i]-7.), 2)+pow((9.*(*y)[i]-3.), 2))/4.) -
    0.2*exp(-pow((9.*(*x)[i]-4.), 2)-pow((9.*(*y)[i]-7.), 2));

  /* Grid size for the approximation. */
  *nxcels = 6;
  *nycels = *nxcels;

  /* Identify the computation. */
  printf("\n"
         "Computing the coefficients of a C^1 spline approximation to "
         "Franke's function\n"
         "Using a %ld by %ld grid\n", *nxcels, *nycels);

  /* Local-approximation control parameters. */
  *lsminp = 3;
  *lsmaxp = 100;

  /* Set up the array to hold the computed spline coefficients. */
  *lcoefs = (((*nxcels+2)*(*nycels+2)+1)/2)*10 + 1;
  if (!(*coefs = NAG_ALLOC(*lcoefs, double)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }

 END:

  return exit_status;
}
static Integer handle_options(Integer iopts[], const Integer liopts,
                              double opts[], const Integer lopts)
{
  /* Auxiliary routine for initializing the options arrays and
   * for demonstrating how to set and get optional parameters using
   * nag_fit_opt_set (e02zkc) and nag_fit_opt_get (e02zlc) respectively.
   */

  /* Scalars */
  Integer          exit_status = 0;
  double           rvalue;
  Integer          ivalue, lcvalue;
  /* Arrays */
```

```
  char             cvalue[3+1], optstr[80+1];
  /* Nag Types */
  Nag_VariableType optype;
  NagError         fail;

  INIT_FAIL(fail);

  /* Set some non-default parameters for the local approximation method. */
  sprintf(optstr, "Minimum Singular Value LPA = %16.9e", 1./32.);

  nag_fit_opt_set("Initialize = e02jdc", iopts, liopts, opts, lopts, &fail);
  if (fail.code == NE_NOERROR)
    nag_fit_opt_set(optstr, iopts, liopts, opts, lopts, &fail);
  if (fail.code == NE_NOERROR)
    nag_fit_opt_set("Polynomial Starting Degree = 3", iopts, liopts, opts,
                    lopts,  &fail);

  /* Set some non-default parameters for the global approximation method. */
  if (fail.code == NE_NOERROR)
    nag_fit_opt_set("Averaged Spline = Yes", iopts, liopts, opts, lopts,
                    &fail);

  /* As an example of how to get the value of an optional parameter,
   * display whether averaging of local approximations is in operation.
   */
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_fit_opt_set (e02zkc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }
  lcvalue = 3 + 1;
  nag_fit_opt_get("Averaged Spline", &ivalue, &rvalue, cvalue, lcvalue,
                  &optype, iopts, opts, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_fit_opt_get (e02zlc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  if (!strcmp(cvalue, "YES"))
    printf("Using an averaged local approximation\n");

 END:
  return exit_status;
}

static Integer evaluate_at_vector(const double coefs[], const Integer iopts[],
                                  const double opts[], const double pmin[],
                                  const double pmax[])
{
  /* Evaluates the approximation at a vector of values using
   * nag_2d_spline_ts_eval (e02jec).
   */

  /* Scalars */
  Integer   exit_status = 0;
  Integer   i, nevalv;
  /* Arrays */
  double    *fevalv = 0, *xevalv = 0, *yevalv = 0;
  /* Nag Types */
  NagError  fail;

  INIT_FAIL(fail);
  scanf("%ld%*[^\n] ", &nevalv);

  if (!(xevalv = NAG_ALLOC(nevalv, double)) ||
      !(yevalv = NAG_ALLOC(nevalv, double)) ||
      !(fevalv = NAG_ALLOC(nevalv, double)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
```

```
      goto END;
    }
  for (i = 0; i < nevalv; i++) scanf("%lf%lf%*[^\n]", &xevalv[i], &yevalv[i]);

  /* Force the points to be within the bounding box of the spline. */
  for (i = 0; i < nevalv; i++)
    {
      xevalv[i] = MAX(xevalv[i], pmin[0]);
      xevalv[i] = MIN(xevalv[i], pmax[0]);
      yevalv[i] = MAX(yevalv[i], pmin[1]);
      yevalv[i] = MIN(yevalv[i], pmax[1]);
    }

  /* Evaluate using nag_2d_spline_ts_eval (e02jec). */
  nag_2d_spline_ts_eval(nevalv, xevalv, yevalv, coefs, fevalv, iopts, opts,
                        &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_2d_spline_ts_eval (e02jec).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
  }

  printf("\nValues of computed spline at (x_i,y_i):\n"
         "\n%12s%12s%12s\n", "x_i", "y_i", "f(x_i,y_i)");

  for (i = 0; i < nevalv; i++)
    printf("%12.2f%12.2f%12.2f\n", xevalv[i], yevalv[i], fevalv[i]);

 END:

  NAG_FREE(xevalv);
  NAG_FREE(yevalv);
  NAG_FREE(fevalv);

  return exit_status;
}

static Integer evaluate_on_mesh(const double coefs[], const Integer iopts[],
                                const double opts[], const double pmin[],
                                const double pmax[])
{
  /* Evaluates the approximation on a mesh of n_x * n_y values. */

  /* Scalars */
  Integer     exit_status = 0;
  Integer     i, j, nxeval, nyeval;
  /* Arrays */
  char        print_mesh[9+1];
  double      *fevalm = 0, *xevalm = 0, *yevalm = 0;
  double      h[2], ll_corner[2], ur_corner[2];
  /* Nag Types */
  Nag_Boolean print_mesh_enum;
  NagError    fail;

  INIT_FAIL(fail);
  scanf("%ld%ld%*[^\n] ", &nxeval, &nyeval);

  if (!(xevalm = NAG_ALLOC(nxeval, double)) ||
      !(yevalm = NAG_ALLOC(nyeval, double)) ||
      !(fevalm = NAG_ALLOC(nxeval*nyeval, double)))
    {
      printf("Allocation failure\n");
      exit_status = -1;
      goto END;
    }

  /* Define the mesh by its lower-left and upper-right corners, which must
   * lie within the bounding box of the spline.
   */
  scanf("%lf%lf%*[^\n] ", &ll_corner[0], &ll_corner[1]);
  scanf("%lf%lf%*[^\n] ", &ur_corner[0], &ur_corner[1]);
```

```
  for (i = 0; i < 2; i++) {
    ll_corner[i] = MAX(ll_corner[i], pmin[i]);
    ur_corner[i] = MIN(ur_corner[i], pmax[i]);
  }

  /* Set the mesh spacing and the evaluation points. */
  h[0] = (ur_corner[0]-ll_corner[0])/(double) (nxeval-1);
  h[1] = (ur_corner[1]-ll_corner[1])/(double) (nyeval-1);

  for (i = 0; i < nxeval; i++) xevalm[i] = ll_corner[0] + (double) i*h[0];
  for (j = 0; j < nyeval; j++) yevalm[j] = ll_corner[1] + (double) j*h[1];

  /* Evaluate using nag_2d_spline_ts_eval_rect (e02jfc). */
  nag_2d_spline_ts_eval_rect(nxeval, nyeval, xevalm, yevalm, coefs, fevalm,
                             iopts, opts, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_2d_spline_ts_eval_rect (e02jfc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }

  /* Output the computed function values? */
  scanf("%9s%*[^\n] ", print_mesh);
  print_mesh_enum = (Nag_Boolean) nag_enum_name_to_value(print_mesh);

  printf("\n");
  if (!print_mesh_enum) {
    printf("Outputting of the function values on the mesh is disabled\n");
  } else {
    printf("Values of computed spline at (x_i,y_j):\n"
           "\n%12s%12s%12s\n", "x_i", "y_j",  "f(x_i,y_j)");
    for (j = 0; j < nyeval; j++)
      for (i = 0; i < nxeval; i++)
        printf("%12.2f%12.2f%12.2f\n", xevalm[i], yevalm[j],
               fevalm[j*nxeval+i]);
  }

 END:

  NAG_FREE(xevalm);
  NAG_FREE(yevalm);
  NAG_FREE(fevalm);

  return exit_status;
}
```

10.2 Program Data

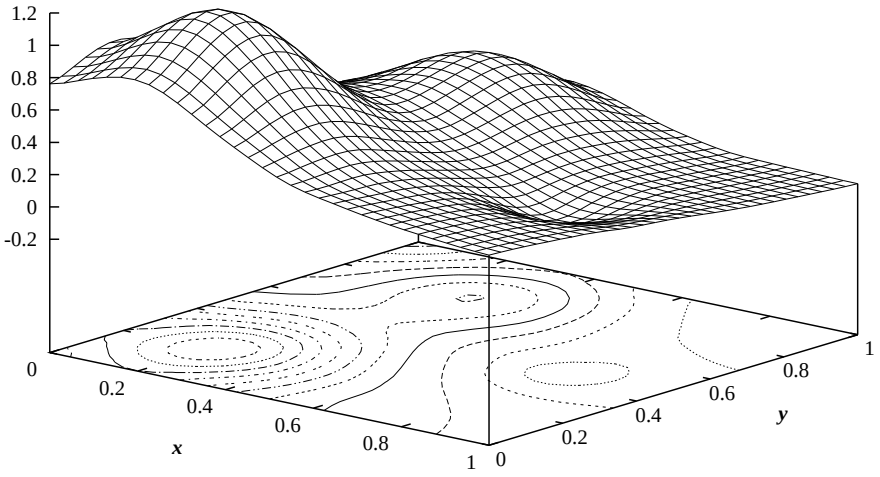
```
nag_2d_spline_fit_ts_scat (e02jdc) Example Program Data
 100                                          : number of data points to fit
  1                                           : no. points for vector evaluation
  0  0                                        : (x_i,y_i) vector to eval.
  101  101                                    : (n_x,n_y) size for mesh eval.
  0  0                                        : mesh lower-left corner
  1  1                                        : mesh upper-right corner
  Nag_FALSE                                   : display the computed mesh vals?
```

10.3 Program Results

```
nag_2d_spline_fit_ts_scat (e02jdc) Example Program Results

Computing the coefficients of a C^1 spline approximation to Franke's function
Using a 6 by 6 grid
Using an averaged local approximation

Values of computed spline at (x_i,y_i):

         x_i         y_i  f(x_i,y_i)
```

```
        0.01        0.01        0.73

Outputting of the function values on the mesh is disabled
```

Example Program
Calculation and Evaluation of Bivariate Spline Fit
from Scattered Data using Two-Stage Approximation



11 Optional Arguments

Several optional arguments in nag_2d_spline_fit_ts_scat (e02jdc) control aspects of the algorithm, methodology used, logic or output. Their values are contained in the arrays **iopts** and **opts**; these must be initialized before calling nag_2d_spline_fit_ts_scat (e02jdc) by first calling nag_fit_opt_set (e02zkc) with **optstr** set to `"Initialize = e02jdc"`.

Each optional argument has an associated default value; to set any of them to a non-default value, or to reset any of them to the default value, use nag_fit_opt_set (e02zkc). The current value of an optional argument can be queried using nag_fit_opt_get (e02zlc).

The remainder of this section can be skipped if you wish to use the default values for all optional arguments.

The following is a list of the optional arguments available. A full description of each optional argument is provided in Section 11.1.

Averaged Spline

Minimum Singular Value LPA

Polynomial Starting Degree

11.1 Description of the Optional Arguments

For each option, we give a summary line, a description of the optional argument and details of constraints.

The summary line contains:

the keywords;

a parameter value, where the letters a, i and r denote options that take character, integer and real values respectively;

the default value.

Keywords and character values are case insensitive.

For nag_2d_spline_fit_ts_scat (e02jdc) the maximum length of the parameter **cvalue** used by nag_fit_opt_get (e02zlc) is 6.

Averaged Spline a Default $=$ 'NO'

When the bounding box is triangulated there are 8 equivalent configurations of the mesh. Setting **Averaged Spline** $=$ 'YES' will use the averaged value of the 8 possible local polynomial approximations over each triangle in the mesh. This usually gives better results but at (about 8 times) higher computational cost.

Constraint: **Averaged Spline** $=$ 'YES' or 'NO'.

Minimum Singular Value LPA r Default $= 1.0$

A tolerance measure for accepting or rejecting a local polynomial approximation (LPA) as reliable.

The solution of a local least squares problem solved on each triangle subdomain is accepted as reliable if the minimum singular value σ of the matrix (of Bernstein polynomial values) associated with the least squares problem satisfies **Minimum Singular Value LPA** $\leq \sigma$.

In general the approximation power will be reduced as **Minimum Singular Value LPA** is reduced. (A small σ indicates that the local data has hidden redundancies which prevent it from carrying enough information for a good approximation to be made.) Setting **Minimum Singular Value LPA** very large may have the detrimental effect that only approximations of low degree are deemed reliable.

Minimum Singular Value LPA will have no effect if **Polynomial Starting Degree** $= 0$, and it will have little effect if the input data is 'smooth' (e.g., from a known function).

A calibration procedure (experimenting with a small subset of the data to be fitted and validating the results) may be needed to choose the most appropriate value for this parameter.

Constraint: **Minimum Singular Value LPA** ≥ 0.0.

Polynomial Starting Degree i Default $= 1$

The degree to be used in the initial step of each local polynomial approximation.

At the initial step the method will attempt to fit with local polynomials of degree **Polynomial Starting Degree**. If the approximation is deemed unreliable (according to **Minimum Singular Value LPA**), the degree will be decremented by one and a new local approximation computed, ending with a constant approximation if no other is reliable.

Polynomial Starting Degree is bounded from above by the maximum possible spline degree, 3.

The default value gives a good compromise between efficiency and accuracy. In general the best approximation can be obtained by setting **Polynomial Starting Degree** $= 3$.

Constraint: $0 \leq$ **Polynomial Starting Degree** ≤ 3.
