nag_ode_bvp_fd_lin_gen (d02gbc)

1. Purpose

nag_ode_bvp_fd_lin_gen (d02gbc) solves a general linear two-point boundary value problem for a system of ordinary differential equations using a deferred correction technique.

2. Specification

3. Description

This function solves the linear two-point boundary value problem for a system of **neq** ordinary differential equations in the interval [a, b]. The system is written in the form

$$y' = F(x)y + g(x) \tag{1}$$

and the boundary conditions are written in the form

$$Cy(a) + Dy(b) = \gamma \tag{2}$$

Here F(x), C and D are **neq** by **neq** matrices, and g(x) and γ are **neq** component vectors. The approximate solution to (1) and (2) is found using a finite-difference method with deferred correction. The algorithm is a specialisation of that used in the function nag_ode_bvp_fd_nonlin_gen (d02rac) which solves a nonlinear version of (1) and (2). The nonlinear version of the algorithm is described fully in Pereyra (1979).

The user supplies an absolute error tolerance and may also supply an initial mesh for the construction of the finite-difference equations (alternatively a default mesh is used). The algorithm constructs a solution on a mesh defined by adding points to the initial mesh. This solution is chosen so that the error is everywhere less than the user's tolerance and so that the error is approximately equidistributed on the final mesh. The solution is returned on this final mesh.

If the solution is required at a few specific points then these should be included in the initial mesh. If, on the other hand, the solution is required at several specific points, then the user should use the interpolation routines provided in Chapter e01 if these points do not themselves form a convenient mesh.

4. Parameters

neg

Input: the number of equations; that is **neq** is the order of system (1). Constraint: $\mathbf{neq} \geq 2$.

fcnf

The function **fcnf**, supplied by the user, must evaluate the matrix F(x) in (1) at a general point x.

The specification of **fcnf** is:

fcng

a

b

the vector γ in (2).

conditions are in the order:

```
void fcnf (Integer neq, double x, double f[], Nag_User *comm)
           neq
                 Input: the number of differential equations.
           X
                 Input: the value of the independent variable x.
           f[neq*neq]
                 Output: the (i, j)th element of the matrix F(x), for i, j = 1, 2, \dots, neq where F_{ij}
                 is set by \mathbf{f}[(i-1) * \mathbf{neq} + (j-1)]. (See Section 8 for an example.)
           comm
                 Input/Output: pointer to a structure of type Nag_User with the following
                 \mathbf{p} - Pointer
                       Input/Output: The pointer comm->p should be cast to the required type,
                       e.g. struct user *s = (struct user *)comm->p, to obtain the original
                       object's address with appropriate type. (See the argument comm below.)
     The function fcng, supplied by the user, must evaluate the vector q(x) in (1) at a general
     point x.
     The specification of fcng is:
      void fcng (Integer neq, double x, double g[], Nag_User *comm)
           neq
                 Input: the number of differential equations.
           \mathbf{x}
                 Input: the value of the independent variable x.
           g[neq]
                 Output: the ith element of the vector g(x), for i = 1, 2, \dots, neq. (See Section 8)
                 for an example.)
           comm
                 Input/Output: pointer to a structure of type Nag_User with the following
                 p - Pointer
                       Input/Output: The pointer comm->p should be cast to the required type,
                       e.g. struct user *s = (struct user *)comm->p, to obtain the original
                       object's address with appropriate type. (See the argument comm below.)
     If the user does not wish to supply fcng the actual argument fcng must be the NAG defined
     null funtion pointer NULLFN.
     Input: the left-hand boundary point, a.
     Input: the right-hand boundary point, b.
     Constraint: b > a.
c[neq][neq]
d[neq][neq]
gam[neq]
```

 $3.d02 \mathrm{gbc}.2$ [NP3275/5/pdf]

Input: the arrays \mathbf{c} and \mathbf{d} must be set to the matrices C and D in (2). gam must be set to

Output: the rows of \mathbf{c} and \mathbf{d} and the components of \mathbf{gam} are re-ordered so that the boundary

- (i) conditions on y(a) only;
- (ii) condition involving y(a) and y(b); and
- (iii) conditions on y(b) only.

The routine will be slightly more efficient if the arrays c, d and gam are ordered in this way before entry, and in this event they will be unchanged on exit.

Note that the boundary conditions must be of boundary value type, that is neither C nor D may be identically zero. Note also that the rank of the matrix [C, D] must be **neq** for the problem to be properly posed. Any violation of these conditions will lead to an error exit.

mnp

Input: the maximum permitted number of mesh points.

Constraint: mnp > 32.

np

Input: determines whether a default or user-supplied initial mesh is used. If $\mathbf{np} = 0$, then \mathbf{np} is set to a default value of 4 and a corresponding equispaced mesh $\mathbf{x}[0], \mathbf{x}[1], \dots, \mathbf{x}[\mathbf{np}-1]$ is used. If $\mathbf{np} \geq 4$, then the user must define an initial mesh using the array \mathbf{x} as described.

Constraint: $\mathbf{np} = 0$ or $4 \leq \mathbf{np} \leq \mathbf{mnp}$.

Output: the number of points in the final (returned) mesh.

x[mnp]

Input: if $\mathbf{np} \geq 4$ (see \mathbf{np} above), the first \mathbf{np} elements must define an initial mesh. Otherwise the elements of \mathbf{x} need not be set.

Constraint:
$$\mathbf{a} = \mathbf{x}[0] < \mathbf{x}[1] < \dots < \mathbf{x}[\mathbf{np}-1] = \mathbf{b}$$
, for $\mathbf{np} \ge 4$. (3)

Output: $\mathbf{x}[0], \mathbf{x}[1], \dots, \mathbf{x}[\mathbf{np}-1]$ define the final mesh (with the returned value of \mathbf{np}) satisfying the relation (3).

y[neq][mnp]

Output: the approximate solution $z_i(x_i)$ satisfying (4), on the final mesh, that is

$$\mathbf{y}[j-1][i-1] = z_j(x_i) \;,\; i=1,2,\ldots,\mathbf{np}; j=1,2,\ldots,\mathbf{neq},$$

where **np** is the number of points in the final mesh.

The remaining columns of \mathbf{y} are not used.

tol

Input: a positive absolute error tolerance. If

$$a = x_1 < x_2 < \ldots < x_{np} = b$$

is the final mesh, $z_j(x_i)$ is the jth component of the approximate solution at x_i , and $y_j(x_i)$ is the jth component of the true solution of equation (1) (see Section 3) and the boundary conditions, then, except in extreme cases, it is expected that

$$|z_j(x_i) - y_j(x_i)| \le \text{tol} , i = 1, 2, \dots, \text{np}; j = 1, 2, \dots, \text{neq}$$
 (4)

Constraint: tol > 0.0.

comm

Input/Output: pointer to a structure of type Nag_User with the following member:

p - Pointer

Input/Output: The pointer **p**, of type Pointer, allows the user to communicate information to and from the user-defined functions **fcnf()** and **fcng()**. An object of the required type should be declared by the user, e.g. a structure, and its address assigned to the pointer **p** by means of a cast to Pointer in the calling program, e.g. **comm.p** = (Pointer)&s. The type pointer will be void * with a C compiler that defines void * and **char** * otherwise.

fail

The NAG error parameter, see the Essential Introduction to the NAG C Library.

5. Error Indications and Warnings

NE_INT_ARG_LT

On entry, **neq** must not be less than 2: $\mathbf{neq} = \langle value \rangle$.

On entry, **mnp** must not be less than 32: $\mathbf{mnp} = \langle value \rangle$.

NE_REAL_ARG_LE

On entry, **tol** must not be less than or equal to 0.0: **tol** = $\langle value \rangle$.

NE_2_REAL_ARG_LE

On entry, $\mathbf{b} = \langle value \rangle$ while $\mathbf{a} = \langle value \rangle$. These parameters must satisfy $\mathbf{b} > \mathbf{a}$.

NE_INT_RANGE_CONS_2

On entry, $\mathbf{np} = \langle value \rangle$ and $\mathbf{mnp} = \langle value \rangle$. The parameter \mathbf{np} must satisfy either $4 \leq \mathbf{np} \leq \mathbf{mnp}$ or $\mathbf{np} = 0$.

NE_BOUND_COND_ROW

Row $\langle value \rangle$ of the array **c** and the corresponding row of array **d** are identically zero. i.e., the boundary conditions are rank deficient.

NE_BOUND_COND_COL

More than **neq** columns of the **neq** by $2 \times \text{neq}$ matrix [C, D] are identically zero. i.e., the boundary conditions are rank deficient. The number of non-identically zero columns is $\langle value \rangle$.

NE_BOUND_COND_LC

At least one row of the **neq** by $2 \times \mathbf{neq}$ matrix [C, D] is a linear combination of the other rows, i.e., the boundary conditions are rank deficient. The index of the first such row is $\langle value \rangle$.

NE_BOUND_COND_NLC

At least one row of the **neq** by $2 \times$ **neq** matrix [C, D] is a linear combination of the other rows determined up to a numerical tolerance, i.e., the boundary conditions are rank deficient. The index of first such row is $\langle value \rangle$.

There is some doubt as to the rank deficiency of the boundary conditions. However even if the boundary conditions are not rank deficient they are not posed in a suitable form for use with this routine.

For example, if

$$C = \begin{pmatrix} 1 & 0 \\ 1 & \varepsilon \end{pmatrix}, \qquad D = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \qquad \gamma = \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix}$$

and ε is small enough, this error exit is likely to be taken. A better form for the boundary conditions in this case would be

$$C = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad D = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad \gamma = \begin{pmatrix} \gamma_1 \\ \varepsilon^{-1}(\gamma_2 - \gamma_1) \end{pmatrix}$$

NE_LF_B_MESH

On entry, the left boundary value **a**, has not been set to $\mathbf{x}[0]$: $\mathbf{a} = \langle value \rangle$, $\mathbf{x}[0] = \langle value \rangle$.

NE_RT_B_MESH

On entry, the right boundary value **b**, has not been set to $\mathbf{x}[\mathbf{np}-1]$: $\mathbf{b} = \langle value \rangle$, $\mathbf{x}[\mathbf{np}-1] = \langle value \rangle$.

NE_NOT_STRICTLY_INCREASING

The sequence \mathbf{x} is not strictly increasing: $\mathbf{x}[\langle value \rangle] = \langle value \rangle$, $\mathbf{x}[\langle value \rangle] = \langle value \rangle$.

NE_BOUND_COND_MAT

One of the matrices C or D is identically zero, i.e., the problem is of initial value and not of the boundary type.

NE_ALLOC_FAIL

Memory allocation failed.

NE_CONV_MESH

A finer mesh is required for the accuracy requested; that is mnp is not large enough.

3.d02gbc.4 [NP3275/5/pdf]

NE_CONV_MESH_INIT

The Newton iteration failed to converge on the initial mesh. This may be due to the initial mesh having too few points or the initial approximate solution being too inaccurate. Try using nag_ode_bvp_fd_nonlin_gen (d02rac).

NE_CONV_ROUNDOFF

Solution cannot be improved due to roundoff error. Too much accuracy might have been requested.

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 consult NAG for assistance.

6. Further Comments

The time taken by the function depends on the difficulty of the problem, the number of mesh points (and meshes) used and the number of deferred corrections.

In the case where the user wishes to solve a sequence of similar problems, the use of the final mesh from one case is strongly recommended as the initial mesh for the next.

6.1. Accuracy

The solution returned by the function will be accurate to the user's tolerance as defined by the relation (4) except in extreme circumstances. If too many points are specified in the initial mesh, the solution may be more accurate than requested and the error may not be approximately equidistributed.

6.2. References

Pereyra V (1979) PASVA3: An Adaptive Finite-Difference Fortran Program for First Order Nonlinear, Ordinary Boundary Problems. In: 'Codes for Boundary Value Problems in Ordinary Differential Equations'. Lecture Notes in Computer Science. (ed B Childs, M Scott JW Daniel, E Denman and P Nelson) 76 Springer-Verlag.

7. See Also

nag_ode_bvp_fd_nonlin_fixedbc (d02gac) nag_ode_bvp_fd_nonlin_gen (d02rac)

8. Example

We solve the problem (written as a first order system)

$$\varepsilon y'' + y' = 0$$

with boundary conditions

$$y(0) = 0, \ y(1) = 1$$

for the cases $\varepsilon = 10^{-1}$ and $\varepsilon = 10^{-2}$ using the default initial mesh in the first case, and the final mesh of the first case as initial mesh for the second (more difficult) case. We give the solution and the error at each mesh point to illustrate the accuracy of the method given the accuracy request tol = 1.0e-3.

8.1. Program Text

```
/* nag_ode_bvp_fd_lin_gen(d02gbc) Example Program
 * Copyright 1994 Numerical Algorithms Group.
 * Mark 3, 1994.
 */
#include <nag.h>
#include <math.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nagd02.h>
#ifdef NAG_PROTO
static void fcnf(Integer neq, double x, double f[], Nag_User *comm);
static void fcnf();
#endif
#define NEQ 2
#define MNP 70
main()
{
  double a, b, c[NEQ][NEQ], d[NEQ][NEQ];
  Integer i, j;
  double eps;
  double x[MNP], y[NEQ][MNP];
  Integer neq, mnp, np;
  double gam[NEQ], tol;
  Nag_User comm;
  Vprintf("d02gbc Example Program Results\n");
  /* For communication with function fcnf()
   * assign address of eps to comm.p.
  comm.p = (Pointer)&eps;
  neq = NEQ;
  mn\bar{p} = MNP;
  tol = 1.0e-3;
  np = 0;
  a = 0.0;
  b = 1.0;
  for (i=0; i<neq; ++i)
      gam[i] = 0.0;
      for (j=0; j<neq; ++j)
          c[i][j] = 0.0;
          d[i][j] = 0.0;
  c[0][0] = 1.0;
  d[1][0] = 1.0;
  gam[1] = 1.0;
  for (i=1; i<=2; ++i)
      eps = pow (10.0, (double) -i);
      Vprintf ("\nProblem with epsilon = %7.4f\n", eps);
d02gbc(neq, fcnf, NULLFN, a, b, (double *)c, (double *)d, gam,
              mnp, &np, x, (double *)y, tol, &comm, NAGERR_DEFAULT);
      Vprintf ("\nApproximate solution on final mesh of %ld points\n", np);
```

3.d02gbc.6 [NP3275/5/pdf]

```
Vprintf ("
                                     Y(1,I)\n");
                        X(I)
           for (j=0; j<np; ++j)
Vprintf ("%9.4f %9.4f\n", x[j], y[0][j]);
      exit(EXIT_SUCCESS);
    #ifdef NAG_PROTO
     static void fcnf(Integer neq, double x, double f[], Nag_User *comm)
     #else
          static void fcnf(neq, x, f, comm)
          Integer neq;
          double x;
          double f[];
          Nag_User *comm;
     #endif
     #define F(I, J) f[(I)*neq+J]
       double *eps = (double *)comm->p;
      F(0,0) = 0.0;
      F(0,1) = 1.0;
      F(1,0) = 0.0;
       F(1,1) = -1.0/ *eps;
8.2. Program Data
     None.
8.3. Program Results
     d02gbc Example Program Results
     Problem with epsilon = 0.1000
     Approximate solution on final mesh of 15 points
                    Y(1,I)
        X(I)
        0.0000
                    0.0000
        0.0278
                    0.2425
        0.0556
                    0.4263
        0.1111
                    0.6708
       0.1667
                    0.8112
        0.2222
                    0.8917
        0.2778
                    0.9379
        0.3333
                    0.9644
       0.4444
                    0.9883
       0.5556
                    0.9962
        0.6667
                    0.9988
        0.7500
                    0.9995
        0.8333
                    0.9998
                    0.9999
        0.9167
        1.0000
                    1.0000
    Problem with epsilon = 0.0100
     Approximate solution on final mesh of 49 points
         X(I)
                     Y(1,I)
        0.0000
                    0.0000
        0.0009
                    0.0884
       0.0019
                    0.1690
        0.0028
                    0.2425
        0.0037
                    0.3095
        0.0046
                    0.3706
       0.0056
                    0.4262
        0.0065
                    0.4770
        0.0074
                    0.5232
        0.0083
                    0.5654
```

0.0093 0.0111 0.0130 0.0148 0.0167 0.0185 0.0204 0.0222 0.0241 0.0259 0.0278 0.0306 0.0333 0.0361 0.0389 0.0417 0.0444 0.0472 0.0500 0.0528 0.0556 0.0648 0.0741 0.0833 0.0926 0.1019 0.1111 0.1389 0.1667 0.2222 0.2778 0.3333 0.4444 0.5556 0.6667 0.7500	0.6038 0.6708 0.7265 0.7727 0.8111 0.8431 0.8696 0.8916 0.9100 0.9252 0.9378 0.9529 0.9643 0.9730 0.9795 0.9845 0.9883 0.9911 0.9933 0.9949 0.9961 0.9985 0.9994 0.9999 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000 1.0000
0.5556	1.0000
1.0000	1.0000

 $3. d02 gbc. 8 \\ [NP3275/5/pdf]$