nag_check_deriv (c05zbc)

1. Purpose

nag_check_deriv (c05zbc) checks that a user-supplied C function for evaluating a vector of functions and the matrix of their first derivatives produces derivative values which are consistent with the function values calculated.

2. Specification

```
#include <nag.h>
#include <nagc05.h>

void nag_check_deriv(Integer n, double x[], double fvec[], double fjac[],
            Integer tdfjac,
            void (*f)(Integer n, double x[],double fvec[],
                      double fjac[], Integer tdfjac, Integer *userflag),
            NagError *fail)
```

3. Description

nag_check_deriv checks the derivatives calculated by user-supplied C functions, e.g. functions of the form required for nag_zero_nonlin_eqns_deriv (c05pbc). As well as the C function to be checked **f**, the user must supply a point $x = (x_1, x_2, \ldots, x_n)^T$ at which the check will be made.

nag_check_deriv first calls **f** to evaluate both the $f_i(x)$ and their first derivatives, and uses these to calculate the sum of squares

$$F(x) = \sum_{i=1}^{n} [f_i(x)]^2,$$

and its first derivatives

$$g_j = \left.\frac{\partial F}{\partial x_j}\right|_x, \quad \text{for } j = 1, 2, \ldots, n.$$

The components of g along two orthogonal directions (defined by unit vectors p_1 and p_2, say) are then calculated; these will be $g^T p_1$ and $g^T p_2$ respectively. The same components are also estimated by finite differences, giving quantities

$$v_k = \frac{F(x + hp_k) - F(x)}{h}, \quad k = 1, 2$$

where h is a small positive scalar. If the relative difference between v_1 and $g^T p_1$ or between v_2 and $g^T p_2$ is judged too large, an error indicator is set.

4. Parameters

n

Input: the number n of variables, x_j, for use with nag_zero_nonlin_eqns_deriv (c05pbc).
Constraint: $\mathbf{n} > 0$.

x[n]

Input: $\mathbf{x}[j-1]$, for $j = 1, 2, \ldots, n$ must be set to the co-ordinates of a suitable point at which to check the derivatives calculated by **f**. 'Obvious' settings, such as 0 or 1, should not be used since, at such particular points, incorrect terms may take correct values (particularly zero), so that errors can go undetected. For a similar reason, it is preferable that no two elements of **x** should have the same value.

fvec[n]

Output: unless **userflag** is set negative when evaluating f_i at the point given in **x**, $\mathbf{fvec}[i-1]$ contains the value of f_i at the point given by the user in **x**, for $i = 1, 2, \ldots, n$.

fjac[n][tdfjac]

Output: unless **userflag** is set negative when evaluating the Jacobian at the point given in **x**, **fjac**$[i-1][j-1]$ contains the value of the first derivative $\partial f_i/\partial x_j$ at the point given in **x**, as calculated by **f**, for $i = 1, 2, \ldots, n$; $j = 1, 2, \ldots, n$.

tdfjac

Input: the last dimension of array **fjac** as declared in the function from which nag_check_deriv is called.
Constraint: **tdfjac** $\geq$ **n**.

f

f must calculate the values of the functions at a point **x** or return the Jacobian at **x**. nag_zero_nonlin_eqns_deriv (c05pbc) gives the user the option of resetting a parameter to terminate immediately. nag_check_deriv (c05zbc) will also terminate immediately, without finishing the checking process, if the parameter in question is reset.)
The specification of **f** is:

```
void f(Integer n, double x[], double fvec[], double fjac[],
       Integer tdfjac, Integer *userflag)
```

n

Input: the number of equations, n

x[n]

Input: the components of the point x at which the functions or the Jacobian must be evaluated.

fvec[n]

Output: if **userflag** $= 1$ on entry, **fvec** must contain the function values $f_i(x)$ (unless **userflag** is set to a negative value by **f**).
If **userflag** $= 2$ on entry, **fvec** must not be changed.

fjac[n∗tdfjac]

Output: if **userflag** $= 2$ on entry, **fjac**$[(i-1)*$**tdfjac**$+j-1]$ must contain the value of $\partial f_i/\partial x_j$ at the point x, for $i = 1, 2, \ldots, n$; $j = 1, 2, \ldots, n$ (unless **userflag** is set to a negative value by **f**).
If **userflag** $= 1$ on entry, **fjac** must not be changed.

tdfjac

Input: the last dimension of array **fjac** as declared in the function from which nag_check_deriv is called.

userflag

Input: **userflag** $= 1$ or 2.
If **userflag** $= 1$, **fvec** is to be updated.
If **userflag** $= 2$, **fjac** is to be updated.

Output: in general, **userflag** should not be reset by **f**. If, however, the user wishes to terminate execution (perhaps because some illegal point **x** has been reached), then **userflag** should be set to a negative integer. This value will be returned through **fail.errnum**.

fail

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

5. Error Indications and Warnings

NE_INT_ARG_LE

On entry, **n** must not be less or equal to 0: **n** $= \langle$*value*$\rangle$.

NE_2_INT_ARG_LT

On entry **tdfjac** $= \langle$*value*$\rangle$ while **n** $= \langle$*value*$\rangle$. These parameters must satisfy **tdfjac** $\geq$ **n**.

NE_ALLOC_FAIL

Memory allocation failed.

NE_DERIV_ERRORS

Large errors were found in the derivatives of the objective function.

The user should check carefully the derivation and programming of expressions for the $\partial f_i/\partial x_j$, because it is very unlikely that **f** is calculating them correctly.

NE_USER_STOP

User requested termination, user flag value = $\langle$*value*$\rangle$.

6. Further Comments

Before using nag_check_deriv (c05zbc) to check the calculation of the first derivatives, the user should be confident that **f** is evaluating the functions correctly.

6.1. Accuracy

fail.code is set to **NE_DERIV_ERRORS** if

$$(v_k - g^T p_k)^2 \geq h \times ((g^T p_k)^2 + 1)$$

for $k = 1$ or 2. (See Section 3 for definitions of the quantities involved.) The scalar h is set equal to $\sqrt{\varepsilon}$, where ε is the ***machine precision***.

7. See Also

nag_zero_nonlin_eqns_deriv (c05pbc)

8. Example

This example checks the Jacobian matrix for the problem solved in the example program for nag_zero_nonlin_eqns_deriv (c05pbc).

8.1. Program Text

```
/* nag_check_deriv(c05zbc) Example Program
 *
 * Copyright 1991 Numerical Algorithms Group.
 *
 * Mark 2, 1991.
 */

#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nagc05.h>

#ifdef NAG_PROTO
static void f(Integer n, double xc[], double fvecc[],
              double fjacc[], Integer tdj, Integer *userflag);
#else
static void f();
#endif

main()
{
#define NMAX 5

  double fjac[NMAX][NMAX], fvec[NMAX], x[NMAX];
  Integer i, j, n, tdfjac;
  static NagError fail;

  fail.print = TRUE;
  Vprintf("c05zbc Example Program Results\n");
  n = 3;
  tdfjac = NMAX;
```

```
    /* Set up an arbitrary point at which to check the 1st derivatives */
    x[0] = 9.2e-01;
    x[1] = 1.3e-01;
    x[2] = 5.4e-01;
    Vprintf("The test point is ");
    for (j=0; j<n; ++j)
      Vprintf("%13.3e", x[j]);
    Vprintf("\n\n");
    c05zbc(n, x, fvec, (double *)fjac, tdfjac, f, &fail);
    if (fail.code != NE_NOERROR) exit(EXIT_FAILURE);
    Vprintf("1st derivatives are consistent with residual values.\n\n");
    Vprintf("At the test point, f() gives\n\n");
    Vprintf("    Residuals            1st derivatives\n\n");
    for (i=0; i<n; ++i)
      {
        Vprintf("%13.3e", fvec[i]);
        for (j=0; j<n; ++j)
          Vprintf("%13.3e", fjac[i][j]);
        Vprintf("\n");
      }
    exit(EXIT_SUCCESS);
  }

  #ifdef NAG_PROTO
  static void f(Integer n, double x[], double fvec[], double fjac[],
                Integer tdfjac, Integer *userflag)
  #else
       static void f(n, x, fvec, fjac, tdfjac, userflag)
       Integer n;
       double x[], fvec[], fjac[];
       Integer tdfjac;
       Integer *userflag;
  #endif
  {
  #define FJAC(I,J) fjac[((I))*tdfjac+(J)]
    Integer j, k;

    if (*userflag != 2)
      {
        /* Calculate the function values */
        for (k=0; k<n; k++)
          {
            fvec[k] = (3.0-x[k]*2.0) * x[k] + 1.0;
            if (k>0)  fvec[k] -= x[k-1];
            if (k<n-1) fvec[k] -= x[k+1] * 2.0;
          }
      }
    else
      {
        /* Calculate the corresponding first derivatives */
        for (k=0; k<n; k++)
          {
            for (j=0; j<n; j++)
              FJAC(k,j)=0.0;
            FJAC(k,k) = 3.0 - x[k] * 4.0;
            if (k>0)
              FJAC(k,k-1) = -1.0;
            if (k<n-1)
              FJAC(k,k+1)= -2.0;
          }
      }
  }
```

8.2. Program Data

None.

8.3. Program Results

```
c05zbc Example Program Results
The test point is     9.200e-01    1.300e-01    5.400e-01

1st derivatives are consistent with residual values.

At the test point, f() gives

    Residuals            1st derivatives

    1.807e+00   -6.800e-01   -2.000e+00    0.000e+00
   -6.438e-01   -1.000e+00    2.480e+00   -2.000e+00
    1.907e+00    0.000e+00   -1.000e+00    8.400e-01
```