NAG Fortran Library Routine Document

E04ZCF/E04ZCA

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of *bold italicised* terms and other implementation-dependent details.

1 Purpose

E04ZCF/E04ZCA checks that user-supplied routines for evaluating an objective function, constraint functions and their first derivatives, produce derivative values which are consistent with the function and constraint values calculated.

E04ZCA is a version of E04ZCF that has additional parameters in order to make it safe for use in multithreaded applications (see Section 5 below).

2 Specifications

2.1 Specification for E04ZCF

SUBROUTINE E04ZCF(N, NCNLN, NROWJ, CONFUN, OBJFUN, C, CJAC, OBJF,1OBJGRD, X, WORK, LWORK, IFAIL)INTEGERN, NCNLN, NROWJ, LWORK, IFAILrealC(NCNLN), CJAC(NROWJ,N), OBJF, OBJGRD(N), X(N),1WORK(LWORK)EXTERNALCONFUN, OBJFUN

2.2 Specification for E04ZCA

SUBROUTINE	E04ZCA(N, NCNLN, NROWJ, CONFUN, OBJFUN, C, CJAC, OBJF,
1	OBJGRD, X, WORK, LWORK, IUSER, RUSER, IFAIL)
INTEGER <i>real</i> 1	N, NCNLN, NROWJ, LWORK, IUSER(*), IFAIL C(NCNLN), CJAC(NROWJ,N), OBJF, OBJGRD(N), X(N), WORK(LWORK), RUSER(*)
EXTERNAL	CONFUN, OBJFUN

3 Description

Routines for minimizing a function of several variables subject to general equality and/or inequality constraints may require the user to provide subroutines to evaluate the objective function $F(x_1, x_2, \ldots, x_n)$, constraint functions $c_i(x_1, x_2, \ldots, x_n)$, for $i = 1, 2, \ldots, m$, and their first derivatives. E04ZCF/E04ZCA is designed to check the derivatives calculated by such user-supplied routines. As well as the routines to be checked (CONFUN and OBJFUN), you must supply a point $x = (x_1, x_2, \ldots, x_n)^T$ at which the checks will be made.

To check the first derivatives of F, the routine first calls OBJFUN to evaluate F and its first derivatives $g_j = \frac{\partial F}{\partial x_j}$, for j = 1, 2, ..., n at x. The components of the user-supplied derivatives 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, the error indicator IFAIL (see Section 6) is set to 2.

When n = 1 only p_1 and v_1 are generated.

Input

Input

Input

External Procedure

Similar checks are made of whether components of the first derivatives

$$\frac{\partial c_i}{\partial x_j}, \quad i = 1, 2, \dots, m; \ j = 1, 2, \dots, n$$

(as calculated by CONFUN at x) are consistent with difference approximations to the same quantities.

4 References

Gill P E, Murray W and Wright M H (1981) Practical Optimization Academic Press

5 Parameters

1: N - INTEGER

On entry: the number n of independent variables in the objective and constraint functions. Constraint: N > 1.

2: NCNLN – INTEGER

On entry: the number m of constraint functions.

Constraint: NCNLN ≥ 0 .

3: NROWJ – INTEGER

On entry: the first dimension of the array CJAC as declared in the (sub)program from which E04ZCF/E04ZCA is called.

Constraint: NROWJ $\geq \max(1, \text{NCNLN})$.

4: CONFUN – SUBROUTINE, supplied by the user.

CONFUN must calculate the vector c(x) of nonlinear constraint functions and its Jacobian for a specified *n*-vector *x*. If there are no nonlinear constraints (NCNLN = 0), CONFUN will not be called by E04ZCF/E04ZCA and CONFUN may be the dummy routine E04VDM/E54VDM. (E04VDM/E54VDM is included in the NAG Fortran Library and so need not be supplied by the user. Its name may be implementation-dependent: see the Users' Note for your implementation for details.) If there are nonlinear constraints, E04ZCF/E04ZCA always calls CONFUN and OBJFUN together, in that order.

The specification of CONFUN for E04ZCF is: SUBROUTINE CONFUN(MODE, NCNLN, N, NROWJ, X, C, CJAC, NSTATE) INTEGER MODE, NCNLN, N, NROWJ, NSTATE real X(N), C(NROWJ), CJAC(NROWJ,N) The specification of CONFUN for E04ZCA is: SUBROUTINE CONFUN(MODE, NCNLN, N, NROWJ, X, C, CJAC, NSTATE, IUSER, 1 RUSER) MODE, NCNLN, N, NROWJ, NSTATE, IUSER(*) INTEGER real X(N), C(NROWJ), CJAC(NROWJ,N), RUSER(*) MODE – INTEGER 1: Input/Output MODE is a flag that you may set within CONFUN to indicate a failure in the evaluation of the nonlinear constraints.

On entry: MODE is always non-negative.

On exit: if MODE is negative on exit from CONFUN, then execution of E04ZCF/E04ZCA will be terminated with IFAIL containing the negative value of MODE.

2:	NCNLN – INTEGER Input
	On entry: the number m of nonlinear constraints, as input to E04ZCF/E04ZCA.
3:	N – INTEGER Input
	On entry: the number n of variables, as input to E04ZCF/E04ZCA.
4:	NROWJ – INTEGER Input
	<i>On entry</i> : the first dimension of the array CJAC and the length of the array C, as input to E04ZCF/E04ZCA.
5:	X(N) – <i>real</i> array Input
	On entry: the vector x of variables at which the constraint functions are to be evaluated
6:	C(NROWJ) – <i>real</i> array Output
	On exit: C must contain the NCNLN nonlinear constraint values, with the value of the <i>j</i> th nonlinear constraint in $C(j)$.
7:	CJAC(NROWJ,N) – <i>real</i> array Output
	On exit: CJAC must contain the Jacobian of the nonlinear constraint functions with the <i>i</i> th row of CJAC containing the gradient of the <i>i</i> th nonlinear constraint, i.e., $CJAC(i, j)$ must contain the partial derivative of c_i with respect to x_j . If CJAC contains any constant elements, a saving in computation can be made by setting them once only, when NSTATE = 1 (see below).
8:	NSTATE – INTEGER Input
	On entry: NSTATE will be 1 on the first call to CONFUN by E04ZCF/E04ZCA, and is 0 for the two subsequent calls. Thus, if the user wishes, NSTATE may be tested within CONFUN in order to perform certain calculations once only. For example, you may read data or initialise COMMON blocks when NSTATE = 1. In addition, the constant elements of CJAC can be set in CONFUN when NSTATE = 1, and need not be defined on subsequent calls.
Note: the following are additional parameters for specific use of CONFUN with E04ZCA. Users of E04ZCF therefore need not read the remainder of this description.	
9: 10:	IUSER(*) - INTEGER arrayUser WorkspaceRUSER(*) - real arrayUser WorkspaceUser Workspace
	CONFUN is called from E04ZCA with the parameters IUSER and RUSER as supplied to E04ZCA. You are free to use the arrays IUSER and RUSER to supply information to

CONFUN must be declared as EXTERNAL in the (sub)program from which E04ZCF/E04ZCA is called. Parameters denoted as Input must not be changed by this procedure.

OBJFUN - SUBROUTINE, supplied by the user. 5:

CONFUN.

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OBJFUN must calculate the objective function F(x) and its gradient for a specified *n*-element vector x.

External Procedure

E04ZCF/E04ZCA.3

The specification of OBJFUN for E04ZCF is: SUBROUTINE OBJFUN(MODE, N, X, OBJF, OBJGRD, NSTATE) INTEGER MODE, N, NSTATE real X(N), OBJF, OBJGRD(N) The specification of OBJFUN for E04ZCA is: SUBROUTINE OBJFUN(MODE, N, X, OBJF, OBJGRD, NSTATE, IUSER, RUSER) MODE, N, NSTATE, IUSER(*) INTEGER real X(N), OBJF, OBJGRD(N), RUSER(*) 1: MODE – INTEGER Input/Output MODE is a flag that you may set within OBJFUN to indicate a failure in the evaluation of the objective function. On entry: MODE is always non-negative. On exit: if MODE is negative on exit from OBJFUN, then execution of E04ZCF/E04ZCA will be terminated with IFAIL set to MODE. N - INTEGER 2: Input On entry: the number n of variables as input to E04ZCF/E04ZCA. 3: X(N) - real array Input On entry: the vector x of variables at which the objective function is to be evaluated. OBJF - real 4: Output On exit: OBJF must be set to the value of the objective function. 5: OBJGRD(N) - real array Output On exit: OBJGRD must contain the gradient vector of the objective function, with OBJGRD(j) containing the partial derivative of F with respect to x_i . NSTATE - INTEGER 6: Input On entry: NSTATE will be 1 on the first call to OBJFUN by E04ZCF/E04ZCA, and is 0 on the two subsequent calls. Thus, if the user wishes, NSTATE may be tested in order to perform certain calculations only on the first call of OBJFUN, e.g., read data or initialise COMMON blocks. Note that if there are any nonlinear constraints, CONFUN and OBJFUN are called together, in that order. Note: the following are additional parameters for specific use of OBJFUN with E04ZCA. Users of E04ZCF therefore need not read the remainder of this description. IUSER(*) - INTEGER array User Workspace 7: 8: RUSER(*) - real array User Workspace OBJFUN is called from E04ZCA with the parameters IUSER and RUSER as supplied to E04ZCA. You are free to use the arrays IUSER and RUSER to supply information to **OBJFUN**.

OBJFUN must be declared as EXTERNAL in the (sub)program from which E04ZCF/E04ZCA is called. Parameters denoted as *Input* must **not** be changed by this procedure.

C(NCNLN) - real array 6:

On exit: unless you set MODE < 0 in the first call of CONFUN, C(i) contains the value of $c_i(x)$ at the point given in X, for $i = 1, 2, \ldots, m$.

If NCNLN = 0, C is not referenced.

7: CJAC(NROWJ,N) - *real* array

> On exit: unless you set MODE < 0 in the first call of CONFUN, CJAC(i, j) contains the value of the derivative $\frac{\partial c_i}{\partial x_j}$ at the point given in X, as calculated by CONFUN, for j = 1, 2, ..., n; $i = 1, 2, \ldots, m.$

If NCNLN = 0, CJAC is not referenced.

8: OBJF - real

On exit: unless you set MODE < 0 in the first call of OBJFUN, OBJF contains the value of the objective function F(x) at the point given in X.

9: OBJGRD(N) - real array

> On exit: unless you set MODE < 0 in the first call of OBJFUN, OBJGRD(j) contains the value of the derivative $\frac{\partial F}{\partial x_i}$ at the point given in X, as calculated by OBJFUN, for j = 1, 2, ..., n.

10: X(N) - real array

> On entry: X(j), for j = 1, 2, ..., n must be set to the co-ordinates of a suitable point x at which to check the derivatives calculated by CONFUN and OBJFUN. 'Obvious' settings such as 0 or 1, should not be used since, at such points, incorrect terms may take correct values (particularly zero), so that errors could go undetected. Similarly, it is preferable that no two elements of x should be equal.

- WORK(LWORK) real array 11:
- 12: LWORK – INTEGER

On entry: the dimension of the array WORK as declared in the (sub)program from which E04ZCF/E04ZCA is called.

Constraint: LWORK $\geq 4 \times N + NCNLN + N \times NROWJ$.

13: IFAIL - INTEGER

Note: for E04ZCA, IFAIL does not occur in this position in the parameter list. See the additional parameters described below.

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, because for this routine the values of the output parameters may be useful even if IFAIL $\neq 0$ on exit, the recommended value is -1. When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.

Output

Output

Input

Output

Output

Workspace

Input

Input/Output

Note: the following are additional parameters for specific use with E04ZCA. Users of E04ZCF therefore need not read the remainder of this section.

13: IUSER(*) – INTEGER array

Note: the dimension of the array IUSER must be at least 1.

IUSER is not used by E04ZCA, but is passed directly to the external procedure QPHX and may be used to pass information to that routine.

14: RUSER(*) – *real* array

Note: the dimension of the array RUSER must be at least 1.

RUSER is not used by E04ZCA, but is passed directly to the external procedure QPHX and may be used to pass information to that routine.

15: IFAIL – INTEGER

Note: see the parameter description for IFAIL above.

6 Error Indicators and Warnings

If on entry IFAIL = 0 or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL < 0

A negative value of IFAIL indicates an exit from E04ZCF/E04ZCA because the user has set MODE negative in OBJFUN or CONFUN. The value of IFAIL will be the same as the user's setting of MODE. The checks on OBJFUN and CONFUN will not have been completed.

IFAIL = 1

IFAIL = 2

You should check carefully the derivation and programming of expressions for the derivatives of F(x), because it is very unlikely that OBJFUN is calculating them correctly.

IFAIL = 2 + i, for $i = 1, 2, \dots$, NCNLN

You should check carefully the derivation and programming of expressions for the derivatives of $c_i(x)$, because it is very unlikely that CONFUN is calculating them correctly. See also Section 7.

7 Accuracy

IFAIL is set to 2 if

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

for k = 1 or 2. (See Section 3 for definitions of the quantities involved.) The scalar h is set equal to $\sqrt{\epsilon}$, where ϵ is the *machine precision* (see X02AJF).

IFAIL is set to 2 + i if a relation analogous to that given above holds for c_i and its calculated derivatives.

User Workspace

User Workspace

Input/Output

8 Further Comments

The user-supplied routines CONFUN and OBJFUN are both called three times unless NCNLN = 0, in which case CONFUN is not called.

Before using E04ZCF/E04ZCA to check the calculation of first derivatives, you should be confident that CONFUN and OBJFUN are calculating F and the c_i correctly. The usual way of checking the calculation of these function values is to compare values of F(x) and the $c_i(x)$ calculated by OBJFUN and CONFUN at non-trivial points x with values calculated independently. ('Non-trivial' means that, as when setting x before calling E04ZCF/E04ZCA, co-ordinates such as 0 or 1 should be avoided.)

9 Example

The example problem has nine variables, finite bounds on six of the variables, four general linear constraints, and fifteen nonlinear constraints.

The objective function is

$$F(x) = -x_2x_6 + x_1x_7 - x_3x_7 - x_5x_8 + x_4x_9 + x_3x_8$$

and the fifteen nonlinear constraint functions are

The example checks the gradients at two separate points.

9.1 Program Text

Note: the listing of the example program presented below uses *bold italicised* terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*
      E04ZCF Example Program Text
      Mark 14 Revised. NAG Copyright 1989.
*
      .. Parameters ..
*
                       NIN, NOUT
      INTEGER
      PARAMETER
                        (NIN=5,NOUT=6)
      .. Local Scalars ..
     real
                       OBJF
      INTEGER
                       I, IFAIL, J, K, LWORK, N, NCNLN, NROWJ
      .. Local Arrays ..
*
                       C(20), CJAC(20,9), OBJGRD(9), WORK(351), X(9)
      real
      .. External Subroutines ...
*
     EXTERNAL
                       CONFUN, E04ZCF, OBJFUN
      .. Data statements ..
*
                       NROWJ/20/, LWORK/351/
      DATA
      .. Executable Statements ..
      WRITE (NOUT, *) 'E04ZCF Example Program Results'
      Skip heading in data file
+
      READ (NIN, *)
     N = 9
```

```
NCNLN = 15
      Read in two points and check the derivatives at each point.
      DO 20 K = 1, 2
         READ (NIN,99999) (X(J),J=1,N)
         IFAIL = 1
*
         CALL E04ZCF(N,NCNLN,NROWJ,CONFUN,OBJFUN,C,CJAC,OBJF,OBJGRD,X,
     +
                      WORK, LWORK, IFAIL)
4
         WRITE (NOUT, *)
         IF (IFAIL.EQ.0) THEN
            WRITE (NOUT, *) 'Derivatives probably correct at the point'
            WRITE (NOUT, 99998) (X(J), J=1, N)
         ELSE IF (IFAIL.EQ.1) THEN
            WRITE (NOUT, *) 'Incorrect parameter supplied to E04ZCF'
            STOP
         ELSE IF (IFAIL.EQ.2) THEN
            WRITE (NOUT, *)
     +
              'Probable error in derivative of objective function'
            WRITE (NOUT, 99998) (X(J), J=1, N)
            WRITE (NOUT,*) 'The computed gradients are'
            WRITE (NOUT, 99998) (OBJGRD(J), J=1, N)
         ELSE
            I = IFAIL - 2
            WRITE (NOUT, 99997)
     +
               'Probable error in derivative of constraint', I,
              ' at the point'
     +
            WRITE (NOUT, 99998) (X(J), J=1, N)
            WRITE (NOUT, *)
              'The computed gradients of this constraint are'
     +
            WRITE (NOUT, 99998) (CJAC(I,J), J=1,N)
         END IF
   20 CONTINUE
      STOP
99999 FORMAT (1X,9F6.2)
99998 FORMAT (1X, 1P, 5e12.4)
99997 FORMAT (1X,A,I4,A)
      END
*
      SUBROUTINE OBJFUN (MODE, N, X, OBJF, OBJGRD, NSTATE)
      .. Scalar Arguments ..
*
      real
                         OBJF
      INTEGER
                         MODE, N, NSTATE
      .. Array Arguments ..
      real
                         OBJGRD(N), X(N)
      .. Executable Statements .
*
      OBJF = X(2) * X(6) - X(1) * X(7) + X(3) * X(7) + X(5) * X(8) - X(4) * X(9) -
     +
             X(3)*X(8)
      OBJF = -OBJF
      OBJGRD(1) = X(7)
      OBJGRD(2) = -X(6)
      OBJGRD(3) = -X(7) + X(8)
      OBJGRD(4) = X(9)
      OBJGRD(5) = -X(8)
      OBJGRD(6) = -X(2)
      OBJGRD(7) = -X(3) + X(1)
      OBJGRD(8) = -X(5) + X(3)
      OBJGRD(9) = X(4)
      RETURN
      END
      SUBROUTINE CONFUN(MODE, NCNLN, N, NROWJ, X, C, CJAC, NSTATE)
      .. Parameters ..
                         ZERO, TWO
      real
                         (ZERO=0.0e0,TWO=2.0e0)
      PARAMETER
      .. Scalar Arguments ..
*
                        MODE, N, NCNLN, NROWJ, NSTATE
      INTEGER
*
      .. Array Arguments ..
      real
                         C(NROWJ), CJAC(NROWJ,N), X(N)
      .. Local Scalars ..
```

```
INTEGER
                           I, J
      .. Executable Statements ..
      The zero elements of Jacobian matrix are set only once. This
*
      occurs during the first call to CONFUN (NSTATE = 1).
      IF (NSTATE.EQ.1) THEN
         DO 40 J = 1, N
             DO 20 I = 1, NCNLN
                 CJAC(I,J) = ZERO
   20
             CONTINUE
   40
         CONTINUE
      END IF
      C(1) = X(1) * * 2 + X(6) * * 2
      CJAC(1,1) = TWO * X(1)
      CJAC(1,6) = TWO * X(6)
      C(2) = (X(2)-X(1)) * 2 + (X(7)-X(6)) * 2
      CJAC(2,1) = -TWO * (X(2) - X(1))
      CJAC(2,2) = TWO * (X(2) - X(1))
      CJAC(2, 6) = -TWO * (X(7) - X(6))
      CJAC(2,7) = TWO * (X(7) - X(6))
      C(3) = (X(3)-X(1)) * * 2 + X(6) * * 2
      CJAC(3, 1) = -TWO * (X(3) - X(1))
      CJAC(3,3) = TWO * (X(3) - X(1))
      CJAC(3,6) = TWO \star X(6)
      C(4) = (X(1)-X(4)) * 2 + (X(6)-X(8)) * 2
      CJAC(4,1) = TWO * (X(1) - X(4))
      CJAC(4, 4) = -TWO * (X(1) - X(4))
      CJAC(4, 6) = TWO * (X(6) - X(8))
      CJAC(4,8) = -TWO * (X(6) - X(8))
      C(5) = (X(1)-X(5)) * 2 + (X(6)-X(9)) * 2
      CJAC(5,1) = TWO * (X(1) - X(5))
      CJAC(5,5) = -TWO * (X(1) - X(5))
      CJAC(5,6) = TWO * (X(6) - X(9))
      CJAC(5,9) = -TWO * (X(6) - X(9))
      C(6) = X(2) * * 2 + X(7) * * 2
      CJAC(6,2) = TWO * X(2)
      CJAC(6,7) = TWO * X(7)
      C(7) = (X(3) - X(2)) * * 2 + X(7) * * 2
      CJAC(7,2) = -TWO*(X(3)-X(2))
      CJAC(7,3) = TWO * (X(3) - X(2))
      CJAC(7,7) = TWO * X(7)
      C(8) = (X(4)-X(2)) * 2 + (X(8)-X(7)) * 2
      CJAC(8,2) = -TWO * (X(4) - X(2))
      CJAC(8, 4) = TWO * (X(4) - X(2))
      CJAC(8,7) = -TWO * (X(8) - X(7))
      CJAC(8,8) = TWO * (X(8) - X(7))
      C(9) = (X(2)-X(5)) * 2 + (X(7)-X(9)) * 2
      CJAC(9,2) = TWO * (X(2) - X(5))
      CJAC(9,5) = -TWO*(X(2)-X(5))
      CJAC(9,7) = TWO * (X(7) - X(9))
      CJAC(9,9) = -TWO * (X(7) - X(9))
      C(10) = X(3) * * 2
      CJAC(10,3) = TWO * X(3)
      C(11) = (X(4) - X(3)) * 2 + X(8) * 2
      CJAC(11,3) = -TWO * (X(4) - X(3))
      CJAC(11, 4) = TWO * (X(4) - X(3))
      CJAC(11,8) = TWO * X(8)
      C(12) = (X(5)-X(3)) * * 2 + X(9) * * 2
      CJAC(12,3) = -TWO * (X(5) - X(3))
      CJAC(12,5) = TWO * (X(5) - X(3))
      CJAC(12,9) = TWO * X(9)
      C(13) = X(4) * * 2 + X(8) * * 2
      CJAC(13, 4) = TWO * X(4)
      CJAC(13,8) = TWO \times X(8)
      C(14) = (X(4)-X(5)) * 2 + (X(9)-X(8)) * 2
      CJAC(14, 4) = TWO * (X(4) - X(5))
      CJAC(14,5) = -TWO * (X(4) - X(5))
      CJAC(14,8) = -TWO * (X(9) - X(8))
      CJAC(14,9) = TWO * (X(9) - X(8))
      C(15) = X(5) * * 2 + X(9) * * 2
      CJAC(15,5) = TWO * X(5)
      CJAC(15,9) = TWO * X(9)
```

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RETURN END

9.2 Program Data

E04ZCF Example Program Data 1.10 1.20 1.30 1.40 1.50 1.60 1.70 1.80 1.90 1.10 2.20 3.30 4.40 5.50 6.60 7.70 8.80 9.90

9.3 **Program Results**

E04ZCF Example Program Results

Derivatives probably correct at the point 1.1000E+00 1.2000E+00 1.3000E+00 1.4000E+00 1.5000E+00 1.6000E+00 1.7000E+00 1.8000E+00 1.9000E+00 Derivatives probably correct at the point 1.1000E+00 2.2000E+00 3.3000E+00 4.4000E+00 5.5000E+00 6.6000E+00 7.7000E+00 8.8000E+00 9.9000E+00