NAG Toolbox for MATLAB

e04ab

1 Purpose

e04ab searches for a minimum, in a given finite interval, of a continuous function of a single variable, using function values only. The method (based on quadratic interpolation) is intended for functions which have a continuous first derivative (although it will usually work if the derivative has occasional discontinuities).

2 Syntax

```
[e1, e2, a, b, maxcal, x, f, user, ifail] = e04ab(funct, e1, e2, a, b, maxcal, 'user', user)
```

3 Description

e04ab is applicable to problems of the form:

Minimize
$$F(x)$$
 subject to $a \le x \le b$.

It normally computes a sequence of x values which tend in the limit to a minimum of F(x) subject to the given bounds. It also progressively reduces the interval [a,b] in which the minimum is known to lie. It uses the safeguarded quadratic-interpolation method described in Gill and Murray 1973.

You must supply a user-supplied (sub)program funct to evaluate F(x). The parameters **e1** and **e2** together specify the accuracy

$$Tol(x) = \mathbf{e1} \times |x| + \mathbf{e2}$$

to which the position of the minimum is required. Note that **funct** is never called at any point which is closer than Tol(x) to a previous point.

If the original interval [a, b] contains more than one minimum, e04ab will normally find one of the minima.

4 References

Gill P E and Murray W 1973 Safeguarded steplength algorithms for optimization using descent methods NPL Report NAC 37 National Physical Laboratory

5 Parameters

5.1 Compulsory Input Parameters

1: funct – string containing name of m-file

You must supply this function to calculate the value of the function F(x) at any point x in [a, b]. It should be tested separately before being used in conjunction with e04ab.

[fc, user] = funct(xc, user)

Input Parameters

1: xc – double scalar

The point x at which the value of F is required.

2: user – Any MATLAB object

funct is called from e04ab with user as supplied to e04ab

[NP3663/21] e04ab.1

e04ab NAG Toolbox Manual

Output Parameters

1: fc – double scalar

Must be set to the value of the function F at the current point x.

2: user - Any MATLAB object

funct is called from e04ab with user as supplied to e04ab

2: e1 – double scalar

The relative accuracy to which the position of a minimum is required. (Note that, since e1 is a relative tolerance, the scaling of x is automatically taken into account.)

e1 should be no smaller than 2ϵ , and preferably not much less than $\sqrt{\epsilon}$, where ϵ is the *machine* precision.

3: **e2 – double scalar**

The absolute accuracy to which the position of a minimum is required. **e2** should be no smaller than 2ϵ .

4: a - double scalar

The lower bound a of the interval containing a minimum.

5: **b – double scalar**

The upper bound b of the interval containing a minimum.

6: maxcal – int32 scalar

The maximum number of calls of F(x) to be allowed.

Constraint: $maxcal \ge 3$. (Few problems will require more than 30.)

There will be an error exit (see Section 6) after maxcal calls of user-supplied (sub)program funct

5.2 Optional Input Parameters

1: user - Any MATLAB object

user is not used by e04ab, but is passed to **funct**. Note that for large objects it may be more efficient to use a global variable which is accessible from the m-files than to use **user**.

5.3 Input Parameters Omitted from the MATLAB Interface

None.

5.4 Output Parameters

1: e1 – double scalar

If you set **e1** to 0.0 (or to any value less than ϵ), **e1**will be reset to the default value $\sqrt{\epsilon}$ before starting the minimization process.

2: **e2 – double scalar**

If you set e2 to 0.0 (or to any value less than ϵ), e2 will be reset to the default value $\sqrt{\epsilon}$.

3: **a – double scalar**

An improved lower bound on the position of the minimum.

e04ab.2 [NP3663/21]

4: **b** – **double scalar**

An improved upper bound on the position of the minimum.

5: maxcal – int32 scalar

The total number of times that user-supplied (sub)program funct was actually called.

6: x - double scalar

The estimated position of the minimum.

7: f - double scalar

The function value at the final point given in \mathbf{x} .

8: user – Any MATLAB object

user is not used by e04ab, but is passed to **funct**. Note that for large objects it may be more efficient to use a global variable which is accessible from the m-files than to use **user**.

9: ifail – int32 scalar

0 unless the function detects an error (see Section 6).

6 Error Indicators and Warnings

Note: e04ab may return useful information for one or more of the following detected errors or warnings.

ifail = 1

```
On entry, (\mathbf{a} + \mathbf{e2}) \ge \mathbf{b}, or \mathbf{maxcal} < 3.
```

ifail = 2

The number of calls of user-supplied (sub)program **funct** has exceeded **maxcal**. This may have happened simply because **maxcal** was set too small for a particular problem, or may be due to a mistake in **funct**. If no mistake can be found in **funct**, restart e04ab (preferably with values of **a** and **b** given on exit from the previous call of e04ab).

7 Accuracy

If F(x) is δ -unimodal for some $\delta < Tol(x)$, where $Tol(x) = \mathbf{e1} \times |x| + \mathbf{e2}$, then, on exit, x approximates the minimum of F(x) in the original interval [a,b] with an error less than $3 \times Tol(x)$.

8 Further Comments

Timing depends on the behaviour of F(x), the accuracy demanded and the length of the interval [a,b]. Unless F(x) can be evaluated very quickly, the run time will usually be dominated by the time spent in user-supplied (sub)program **funct**.

If F(x) has more than one minimum in the original interval [a, b], e04ab will determine an approximation x (and improved bounds a and b) for one of the minima.

If e04ab finds an x such that $F(x - \delta_1) > F(x) < F(x + \delta_2)$ for some $\delta_1, \delta_2 \ge Tol(x)$, the interval $[x - \delta_1, x + \delta_2]$ will be regarded as containing a minimum, even if F(x) is less than $F(x - \delta_1)$ and $F(x + \delta_2)$ only due to rounding errors in the (sub)program. Therefore user-supplied (sub)program **funct** should be programmed to calculate F(x) as accurately as possible, so that e04ab will not be liable to find a spurious minimum.

[NP3663/21] e04ab.3

e04ab NAG Toolbox Manual

9 Example

```
e04ab\_funct.m
 function [fc, user] = e04abf_funct(xc, user)
  fc = \sin(xc)/xc;
e1 = 0;
e2 = 0;
a = 3.5;
b = 5;
maxcal = int32(30);
[e1Out, e2Out, aOut, bOut, maxcalOut, x, f, user, ifail] = ...
    e04ab('e04ab_funct', e1, e2, a, b, maxcal)
e10ut =
   1.0542e-08
e2Out =
   1.0542e-08
aOut =
   4.4934
bOut =
   4.4934
maxcalOut =
   4.4934
f =
  -0.2172
user =
ifail =
           0
```

e04ab.4 (last) [NP3663/21]