

## 1 SUMMARY

To calculate the **minimum of a general function** of several variables when values of the **derivatives** with respect to the variables can be provided, that is, find  $\mathbf{x} = x_1, x_2, \dots, x_n$  to minimize a function  $F(\mathbf{x})$  given  $\partial F / \partial x_j, j=1, 2, \dots, n$ .

The subroutine uses the BFGS variable metric method without exact line searches of the type analysed by Powell, AERE Report CSS.15, (1975).

**ATTRIBUTES** — **Version:** 1.0.0. **Types:** VA13A, VA13AD. **Calls:** MC11. **Original date:** May 1975. **Origin:** M.J.D.Powell, Harwell.

## 2 HOW TO USE THE PACKAGE

### 2.1 Argument List

*The single precision version*

```
CALL VA13(FUNC,N,X,F,G,SCALE,ACC,W)
```

*The double precision version*

```
CALL VA13D(FUNC,N,X,F,G,SCALE,ACC,W)
```

**FUNC** The name of the subroutine provided by the user which is considered in Section 2.2. It must be declared in an **EXTERNAL** statement.

**N** is an **INTEGER** variable whose value must be set by the user to  $n$  the number of variables.

**X** is a **REAL** (**DOUBLE PRECISION** in the D version) array of at least  $n$  elements, set by the user to initial values of the variables  $(x_1, x_2, \dots, x_n)$ . Usually computing time is saved if these estimates are close to the final solution. They are changed automatically to the values that give the least calculated value of the objective function.

**F** is a **REAL** (**DOUBLE PRECISION** in the D version) variable that is set by the subroutine to the least calculated value of the objective function.

**G** is a **REAL** (**DOUBLE PRECISION** in the D version) array of at least  $n$  elements that are set automatically to the components of the first derivative vector of **F** for the final values of the variables. Small values indicate a successful calculation.

**SCALE** is a **REAL** (**DOUBLE PRECISION** in the D version) array of at least  $n$  elements, whose  $i$ -th component ( $1 < i < n$ ) must be set to a *positive* value that is a suitable change to make to  $x_i$  initially in the minimization calculation. About 10% of the total expected change in  $x_i$  is often a good value. This array is called **SCALE** because its elements should reflect the relative sizes of  $(x_1, x_2, \dots, x_n)$ .

**ACC** is a **REAL** (**DOUBLE PRECISION** in the D version) variable which must be set by the user to the required accuracy. The calculation finishes when, for  $i=1, 2, \dots, n$ , changes in  $x_i$  of size  $ACC * SCALE(i)$  do not reduce the objective function. When in doubt about the value of **ACC** it is usually best to choose a small value.

**W** is a **REAL** (**DOUBLE PRECISION** in the D version) array of at least  $\frac{1}{2}n(n+13)$  elements that is used as working space. On exit from the subroutine the first  $\frac{1}{2}n(n+1)$  locations of **W** give the final approximation of the second derivative matrix, stored in the factored form used by subroutine MC11A.

## 2.2 User subroutine

The user must provide a subroutine to calculate the finished values and first derivative values.

```
SUBROUTINE XXX(N,X,F,G)
  DIMENSION X(N),G(N)
```

The arguments  $N$ ,  $X$ ,  $F$  and  $G$  correspond to the arguments with these same names described in Section 2.1.  $N$  and the elements of  $X$  are given to the user subroutine by VA13A/AD. The user subroutine must set  $F$  and  $G(I)$ ,  $I=1,N$ , to the value of the objective function and the components of its first derivative for the given vector of variables in  $X$ . The user should check the accuracy of these derivatives independently, because if they are wrong the convergence of VA13A becomes much slower than necessary, or VA13A/AD may fail to converge to a minimum of the objective function.

## 2.3 BLOCK COMMON

VA13A contains a common block VA13B (VA13BD in the double precision version).

*The single precision version*

```
COMMON/VA13B/ IPRINT,LP,MAXFUN,MODE,NFUN
```

*The double precision version*

```
COMMON/VA13BD/ IPRINT,LP,MAXFUN,MODE,NFUN
```

The five integers called  $IPRINT$ ,  $LP$ ,  $MAXFUN$ ,  $MODE$  and  $NFUN$  are present in a common block in order that they can be reached by the user. In most calculations they can be ignored, but sometimes they are useful, their purpose being as follows.

$IPRINT$  is an INTEGER variable used to control printing, it has a default value of zero, and is unchanged by VA13A/AD. If  $IPRINT=0$ , then no printing occurs except perhaps the diagnostic message mentioned below. Otherwise the value of the objective function is printed every  $|IPRINT|$  iterations. If  $IPRINT > 0$  the values in  $X$  and  $G$  are printed also. If  $IPRINT \neq 0$  the final values of  $F$ ,  $X$  and  $G$  are always printed.

$LP$  is an INTEGER variable with a default value of 6, and is the stream number for any output from VA13A/AD.

$MAXFUN$  is an INTEGER variable with a default value of zero, in which case it does not influence the calculation. However, if it is positive, then VA13A/AD finishes automatically when the user subroutine (see Section 2.2) is called  $MAXFUN$  times. Normal convergence can occur earlier.

$MODE$  is an INTEGER variable with a default value of one, in which case the initial approximation to the second derivative matrix is set automatically to a positive diagonal matrix. However, if a suitable positive definite approximation is known, then it may be passed to VA13A/AD in the first  $\frac{1}{2}n(n+1)$  locations of  $W$  by setting  $MODE=2$  or  $MODE=3$ . When  $MODE=2$  these elements of  $W$  must contain the lower triangle of the Hessian approximation,  $\mathbf{B} = \{b_{ij}\}_{n \times n}$  say, in the order  $b_{1,1}, b_{2,1}, b_{3,1}, \dots, b_{n,1}, b_{2,2}, b_{3,2}, \dots, b_{n-1,n-1}, b_{n,n-1}, b_{n,n}$ . When  $MODE=3$  the Hessian approximation must be given in the factored form used by subroutine MC11A/AD, which is also the form used to provide the Hessian approximation in  $W$  at the return from VA13A/AD. A check for positive definiteness is made automatically by VA13A/AD, and if it fails a diagnostic message is printed. In this case the calculation proceeds as though  $MODE=1$ , but the actual value of  $MODE$  is not changed.

$NFUN$  is an INTEGER variable which is set by the subroutine to the number of times the user subroutine of Section 2.2 is called.

### 3 GENERAL INFORMATION

**Use of common:** See Section 2.3.

**Workspace:** None.

**Other routines called directly:** MC11.

**Input/output:** Occurs on stream LP. See the purpose of IPRINT and LP in Section 2.3.

**Restrictions:** The elements of SCALE must be positive.

### 4 METHOD

The subroutine uses the BFGS variable metric method without exact line searches of the type analysed by Powell (Report CSS 15, AERE Harwell, 1975). The line search combines safeguards based on brackets with cubic polynomial interpolation and quadratic spline extrapolation. It maintains positive definiteness of the second derivative matrix by calling subroutine MC11A, which employs and revises an **LDL**<sup>T</sup> factorization.