1 SUMMARY

To **minimise the sum of squares of** m **given functions** each of n variables, i.e. to find $(x_1, x_2, ..., x_n)$ to minimise

$$S(x_1, x_2, ..., x_n) = \sum_{j=1}^{m} f_j(x_1, x_2, ..., x_n)^2 \qquad m \geq n$$

The user must supply a subroutine CALCFG (see section 3) to calculate the values of f_i, and the partial derivatives $\partial f_i / \partial x_j$ for any given values of the independent variables $(x_1, x_2, ..., x_n)$. The method is an iterative descent method with quadratic convergence and the user must supply an initial approximation to the required x_i.

ATTRIBUTES — **Version:** 1.0.0. **Types:** VB13A, VB13AD. **Calls:** MB01, VD02, and CALCFG (a user subroutine). **Original date:** May 1963. **Origin:** M.J.D. Powell. **Remark:** A version of VB03 with a modified argument list.

2 HOW TO USE THE PACKAGE

2.1 The argument list and calling sequence

The single precision version

        CALL VB13A(M,N,X,E,F,G,ESCALE,IPRINT,MAXIT,IG,W)

The double precision version

        CALL VB13AD(M,N,X,E,F,G,ESCALE,IPRINT,MAXIT,IG,W)

M   is an INTEGER variable specifying m the number of functions f_i in the sum of squares.

N   is an INTEGER variable specifying n the number of independent variables $(x_1, x_2, ..., x_n)$. Note that N may be changed by VB13A, in fact it will be set to 0 in the event of an error return (see section 5).

X   is a REAL (DOUBLE PRECISION in the D version) array, minimum length n, initially containing an approximation to the required minimum position, i.e. the user's guess of x_i must be stored in X(I) on entry to VB13A/AD. On exit, X will contain the final minimum position.

E   is a REAL (DOUBLE PRECISION in the D version) array of length n specifying the accuracy to which the minimum position is to be found. E(I) specifies the absolute accuracy to which X(I) is required.

F   is a REAL (DOUBLE PRECISION in the D version) array of length m, which on return from VB13A/AD will contain the values of f_i at the minimum position.

G   is a REAL (DOUBLE PRECISION in the D version) two-dimensional array (first dimension IG) which will be set by VB13A/AD to the partial derivatives at the minimum, i.e. G(i,j) = $\partial f_i / \partial x_j$.

ESCALE is a REAL (DOUBLE PRECISION in the D version) is a safety parameter used to control the size of step taken in each iteration. Its main function is to ensure that the minimum position nearest to the initial approximation is found and large steps away from this position are not taken. The change in X(I) at each iteration will not be more than ESCALE*E(I). Too small a value of ESCALE will cause slow convergence to the minimum.

IPRINT is an INTEGER variable controlling the printing from VB13A/AD. IPRINT=0 gives no printing, otherwise the value of S and of the variables X(I) will be printed at every IPRINT iterations.

MAXIT   is an integer parameter specifying the maximum number of iterations allowed. The subroutine will be left automatically after MAXIT iterations have been made.

IG   is the first dimension of the array G, i.e. the users DIMENSION statement will contain an entry G(IG,).

W   is a REAL (DOUBLE PRECISION in the D version) array of length at least $n(n+4)$ used by the routine as workspace.

3 SUBROUTINE CALCFG

A subroutine of the form

```
SUBROUTINE CALCFG(M,N,F,G,IG)
```

must be provided by the user. The arguments have the same meanings as the corresponding arguments of VB13A. For given values of the variables X(I), CALCFG must evaluate and set F(i), and G(i,j) to the values of $f_i(x_1, x_2, ..., x_n)$ and $\partial f_i/\partial x_j$, $i=1,2,...,m$, $j=1,2,...,n$. The values of X(I) will be set by VB13A to $x_1, x_2, ..., x_n$.

4 METHOD

See Fletcher and Powell, *Computer Journal,* July 1963.

5 OUTPUT AND DIAGNOSTICS

Apart from the printing controlled by IPRINT, output may arise in two other ways:

(i) when MAXIT iterations have been completed

(ii) when rounding errors have proved troublesome. The output is appropriate to each situation, but note that if either occurs then N is set to zero before return.

6 OTHER SUBROUTINES

This subroutine requires the use of Harwell Library routines MB01A and VD02A, in addition to the user supplied routine CALCFG.

7 GENERAL COMMENT

On average CALCFG will be called twice per iteration.