VB01

PACKAGE SPECIFICATION HSL ARCHIVE

1 SUMMARY

If $y_1, y_2, ..., y_n$ are a set of observations of a function $f(x, v_1, v_2, ..., v_m)$ at discrete values $x_1, x_2, ..., x_n$, then VB01A finds the value of **v** which minimizes

$$S = \sum_{i=1}^{n} w_i (y_i - f(x_i, \mathbf{v}))^2$$

where $w_1, w_2, ..., w_n$ are weights provided by the user. The method used is a modified Marquardt routine (see R. Fletcher, 'A modified Marquardt subroutine for nonlinear least squares', AERE-R 6799, 1971).

The user must provide initial estimates of the parameters v_j $j=1,2,...,m$ and a subroutine to calculate values of the functions $f(x,\mathbf{v})$ and its derivatives with respect to the parameters $\partial f/\partial v_j$, $j=1,2,...,m$.

The routine returns to the calling program

(1) The final values of the v_i.

(2) The standard deviations of the v_i.

(3) The variance covariance matrix.

(4) The fitted values $f(x_i,\mathbf{v})$.

It also prints out a history of the iterative process and full details of the solution and its statistical properties, including standard deviations and a chi-squared test on the variance ratio.

ATTRIBUTES — Version: 1.0.0. **Types:** VB01A, VB01AD. **Calls:** MA10, _DOT, OA01, SA01 and DERIV (a user subroutine). **Original date:** June 1972. **Origin:** R. Fletcher, Harwell.

2 HOW TO USE THE PACKAGE

2.1 The argument list and calling sequence

The single precision version

```
CALL VB01A(X,Y,W,Z,N,V,E,M,A,IA,MAXFN)
```

The double precision version

```
CALL VB01AD(X,Y,W,Z,N,V,E,M,A,IA,MAXFN)
```

X is a REAL (DOUBLE PRECISION in the D version) array of n elements to be set by the user to the data points $x_1, x_2, ..., x_n$.

Y is a REAL (DOUBLE PRECISION in the D version) array of n elements to be set by the user to the observations $y_1, y_2, ..., y_n$.

W is a REAL (DOUBLE PRECISION in the D version) array of n elements to be set by the user to the weights $w_1, w_2, ..., w_n$.

Z is a REAL (DOUBLE PRECISION in the D version) array of n elements in which the fitted estimates $f(x_i,\mathbf{v})$ $i=1,2,...,n$ are returned.

N is an INTEGER to be set to n the number of observations.

V is a REAL (DOUBLE PRECISION in the D version) array of m elements or more in which an initial estimate of $v_1, v_2, ..., v_m$ must be set. The optimum value of **v** is returned on exit. In addition, V(M+1), V(M+2),... may be used to communicate constants between the calling routine and the user subroutine DERIV.

E is a REAL (DOUBLE PRECISION in the D version) array of m elements in which the standard deviations of the v_i are returned on exit.

M is an INTEGER to be set to m the number of variables; $2 \le m \le 25$.

A is a REAL (DOUBLE PRECISION in the D version) array of two dimensions, at least m^2, in which the variance-covariance matrix is returned on exit.

IA is an INTEGER set to the first dimension of A, i.e. the dimension statement in the calling program will have the form A(IA,).

MAXFN is an INTEGER set to the maximum number of times which the sum of squares can be evaluated.

3 THE USER SUBROUTINE

The user must provide a subroutine headed

```
SUBROUTINE DERIV(X,V,F,FUNC,IFL)
REAL F(*),V(*)
```

which is passed a value x in X (one of the x_i) and a vector **v** in V. The subroutine should calculate the value of $f(x, v_1, v_2,..., v_m)$ and return it in FUNC and calculate the values $\partial f/\partial v_i$ i=1,2,...,m and return them in F(I) = I=1,M. If the vector **v** is unsatisfactory in any way (for instance V(I) may be negative when it is known to be positive from physical considerations) then IFL should be set equal to 1 and a RETURN made without setting FUNC or F. Finally constants may be communicated to DERIV from the calling routine by using V(M+1), V(M+2),....

4 PRINTING

Printing occurs on stream 6 (line printer) although this can be changed (to stream 8 say) by including the statements

```
COMMON/VB01B/IP
IP=8
```

in the calling program. The print out commences with a history of each iteration of the iterative process given in the form

iteration number	*number of evaluations of S*
S	
V(1),V(2),...,V(M)	(8 to a line)
G(1),G(2),...,G(M)	(8 to a line)

where 2*G(I) is the derivative ∂S/∂V(I). The fact that G(I) → 0 for all I is an indication that the iteration has converged. Once the iteration has converged (the criterion being that the change in each V(I) is less than one tenth of its standard deviation) then the following information is printed out: the optimum V(I) and their standard deviations, the variance covariance matrix, the values x_i, y_i and $f(x_i,\mathbf{v})$ for each i, and finally the weighted sum of squares S, the number of degrees of freedom N-M, the variance ratio, and the probability of chance occurrence of a variance ratio as least as large as that obtained.

5. GENERAL

Use of common: A COMMON area named VB01B/BD is used. This need only be referenced if the user requires the output from VB01A/AD to be written on an output stream other than stream 6, see section 4.

Workspace: 800 words local to VB01A/AD.

Input/output: no input, for output see section 4.

Restrictions: $2 \le m \le 25$.