1 SUMMARY

To **find a minimum of a function,** $f(x)$**, of the single variable** x**.** The method is iterative and a starting approximation to the required value of x must be provided. When values of $f(x)$ are required by the subroutine, a return to the calling program is made (see section 2 below).

ATTRIBUTES — Version: 1.0.0. **Types:** VD01A, VD01AD **Original date:** May 1964. **Origin:** M.J.D. Powell.

2 HOW TO USE THE PACKAGE

2.1 The argument list and calling sequence

The single precision version

```
CALL VD01A(K,X,F,MAXF,ABSACC,RELACC,XSTEP)
```

The double precision version

```
CALL VD01AD(K,X,F,MAXF,ABSACC,RELACC,XSTEP)
```

The calling sequence for this routine would normally be of the form

```
     K=2 (or 3)
5    CALL VD01A(K,X,F,MAXF,ABSACC,RELACC,XSTEP)
     GO TO (1,2,3,4),K
1    [Instructions to set F=f(X)]
     GO TO 5
2    [Minimum value found to required accuracy]
3    [Error return.  Rounding errors have made it
      impossible to achieve the required accuracy]
4    [Error return.  MAXF evaluations of f(x) have been
      made and the required minimum not yet found].
```

The calling program must set the following arguments before VD01A is first called.

X is a REAL (DOUBLE PRECISION in the D version) variable giving a starting approximation to the minimum position. On return from the subroutine X will be set to a value for which $f(x)$ must be calculated (K=1) or the subroutine's latest estimate of the minimum position (K=2,3,4).

MAXF is an INTEGER set by the calling program as an upper limit on the number of evaluations of $f(x)$ that are allowed. An error return is made if the required accuracy is not achieved within MAXF evaluations (K=4).

ABSACC, RELACC are REAL (DOUBLE PRECISION in the D version) parameters specifying the accuracy to which the required minimum x is to be found. The subroutine executes a normal return (K=2) when, if X, x are two consecutive estimates

$$|X-x| \le \text{ABSACC} \text{ or } |X-x| \le |x| \cdot \text{RELACC},$$

XSTEP is a REAL (DOUBLE PRECISION in the D version) variable set to indicate a reasonable change to be made in the variable x in beginning the search for a minimum. A bad estimate will cause more function values to be requested than necessary, but should not affect the final convergence.

K is an INTEGER control variable. At the first call of VD01A this integer parameter is set to 2 or 3. If the value of $f(x)$ at the starting approximation is available then set K=3. On return K will be set to one of the values 1,2,3,4

as shown in the calling sequence above.

F is a REAL (DOUBLE PRECISION in the D version) variable which may be set by the calling program before VD01A is called (K=3 on entry). On a final (or error) return K=2,3,4, F will be set to the value of $f(x)$ at the latest estimate of the minimum. When K=1 the calling program must set F=$f(x)$ and return to the subroutine as shown in the calling sequence.

3 METHOD

The minimum position is predicted by constructing a quadratic function defined by 3 consecutive estimates. Precautions are taken to prevent convergence to a maximum and to present an excessive step being taken. Obvious bounds on the minimum position are noted and used. If unreasonable high accuracy is requested many function evaluations will be required.