



1 SUMMARY

To **calculate automatically a smooth curve fit to given weighted data**. The output is in a form which allows easy evaluation of the fitted function at any point in the range of the data.

The user must provide only the M data points (x_i, y_i) $i = 1, 2, \dots, M$ and the corresponding weights w_i , $i = 1, 2, \dots, M$. The subroutine calculates a cubic spline fit $s(x)$ which attempts to follow trends in the data but ignores random errors. The function $s(x)$ is chosen automatically by the subroutine and is defined only in the range $x_i \leq x \leq x_M$. To extend the range of validity of $s(x)$ beyond either or both of these points extra data may be provided with zero weight w_k (since if $w_k = 0$ the data point is ignored by the fitting process).

The subroutine fits $s(x)$, in $[x_1, x_M]$, which makes the following expression small

$$\sum_{i=1}^M [w_i (y_i - s(x_i))]^2 + \sum_{j=2}^{N-1} [\theta_j d_j]^2$$

This expression consists of the usual least squares term (the first term) and a smoothing term which is determined automatically by VC03A using statistical tests on errors.

$s(x)$ is a cubic spline with knots $\xi_1, \xi_2, \xi_3, \dots, \xi_N$, and d_i represents the discontinuity in $s'''(x)$ at ξ_i i.e.

$$d_i = s'''(\xi_i + 0) - s'''(\xi_i - 0)$$

θ_i are weight factors used for smoothing $s(x)$. Output from the subroutine consists of N, the number of knots, the knot positions, the values of $s(\xi_i)$, $s'(\xi_i)$ $i = 1, 2, \dots, N$, the smoothing term parameters θ_i and the residuals, $y_i - s(x_i)$. Since VC03A is automatic in choosing $s(x)$, the storage space required for the defining parameters is not known, the user is asked to indicate how much space has been made available. If the routine needs more than has been indicated, an error return is made.

NOTE The algorithm assumes that the data represent measured values of a smooth function and makes statistical tests on this assumption, at best therefore $s(x)$ will be a good estimate of this underlying function and the user should be critical of the fit provided.

ATTRIBUTES — **Version:** 1.0.0. **Types:** VC03A, VC03AD **Calls:** VB06. **Original date:** October 1967. **Origin:** M.J.D. Powell.

2 HOW TO USE THE PACKAGE

2.1 The argument list and calling sequence

The single precision version

```
CALL VC03A(M,N,XD,YD,WD,RD,XN,GN,DN,THETA,IPRINT,W)
```

The double precision version

```
CALL VC03AD(M,N,XD,YD,WD,RD,XN,GN,DN,THETA,IPRINT,W)
```

All arguments except M, N, IPRINT are arrays, the calling program must supply the appropriate dimension statements.

The following arguments must be set by the program before VC03A is called.

M INTEGER variable set at the number of data points

XD REAL (DOUBLE PRECISION in the D version) array, of minimum length M, containing the data positions i.e.

$$XD(J) = x_j$$

YD REAL (DOUBLE PRECISION in the D version) array, of minimum length M, containing the data values i.e. $YD(J) = y_j$

WD REAL (DOUBLE PRECISION in the D version) array, of minimum length M, containing the weights i.e. $WD(J) = w_j$

IPRINT is an integer parameter specifying the printing required from the subroutine as follows:

IPRINT = 0 no printing

IPRINT > 0 the subroutine prints details of the final fit only

IPRINT < 0 details of the fit are printed at every iteration using new knots.

N this parameter must be set by the user to indicate the storage space available to the subroutine. N is determined as follows: the dimensions of the arrays XN, FN, GN, DN, THETA, W will depend on the number of knot positions in the final fit $s(x)$. Since this number is unknown at the time the user sets up the dimension information, an over-estimate of these array dimensions will generally be made. N should be set to an over-estimate of the number of knots in the final fit therefore (see §3 for estimating N). If the subroutine requires more than indicated a return to the calling program is made with N negative, all output arguments being set to give the current state of the fitting process.

On a normal return N will contain the number of knots used in the fitting function $s(x)$. In an error return N will contain the negative of the number of knots.

W is an array of length $7M + 9N + 6$ words used by the subroutine as working space. The following arguments are set by VC03A.

XN, FN, GN, DN, THETA are arrays of length at least N, RD is of length M.

XN the knot positions: $XN(J) = \xi_j \quad J=1,2,\dots,N$

FN the values of $s(x)$ at the knots: $FN(J) = s(\xi_j) \quad J=1,2,\dots,N$

GN the values of $s'(x)$ at the knots: $GN(J) = s'(\xi_j) \quad J=1,2,\dots,N$

DN the third derivative discontinuities: $DN(J) = s'''(\xi_j+0) - s'''(\xi_j-0) \quad J=2\dots N$

THETA the weight factors in the smoothing term: $THETA(J) = \theta_j \quad J=2,\dots,N-1$

RD is an array of length M which is set by VC03A to contain the residuals: $RD(J) = y_j - s(x_j) \quad J=1,2,\dots,M$

Of the arguments set by the calling program only N is changed.

3 ESTIMATING N: WORKING SPACE AND ARRAY DIMENSIONS

Since $s(x)$, the final fit is determined automatically, the number of knots, N, is initially unknown, however the user is responsible for dimensioning arrays depending on N. The following remarks are intended to help the user make an overestimate of the space required.

(1) If a large number of data points fairly uniformly distributed over that range $x_1 < x < x_M$, then $N = \frac{1}{2}M$ should be an over-estimate.

(2) Data concentrated in a small region of the range may require $N \approx M$.

(3) It is not impossible for N to be greater than M.

4 RESTRICTIONS

$$M > 3$$

$$x_1 < x_2 < \dots < x_M$$

5 OTHER SUBROUTINES

Calls VB06.

6 RECOMMENDATION

Although zero weights w_k , are permitted to cause the subroutine to ignore data points, non zero weights that are much smaller than average should be avoided. However it is in order to give a few data values larger weights to force $s(x)$ to pass near to these points, in such cases a factor of 10^4 greater than average is suggested.

7 METHOD

The method is described by M. J. D. Powell in 'Curve Fitting by Cubic Splines' Report T.P.307 (1967).

8 THE FITTED CURVE $s(x)$

The fit provided by VC03A is a cubic spline in the range $[x_1, x_M]$ i.e. is a function of the form

$$s(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + \frac{1}{6} \sum_{j=2}^{N-1} b_j (x - \xi_j)_+^3$$

where ξ_j are the knot positions, and

$$\begin{aligned} (x - \xi_j)_+ &= 0 & x < \xi_j \\ &= x - \xi_j & x > \xi_j \end{aligned}$$

This implies that in each interval $[\xi_j, \xi_{j+1}]$, $s(x)$ is a segment of a cubic curve, and these segments are smoothly jointed at the knots. 'Smoothly jointed' here means that $s(x)$, $s'(x)$, $s''(x)$ are all continuous functions. The value of $s(x)$ is easily calculated if the cubics can easily be found, and convenient data for specifying a cubic over an interval $[\xi_j, \xi_{j+1}]$ is to give the values $s(\xi_j)$, $s'(\xi_j)$, $s(\xi_{j+1})$, $s'(\xi_{j+1})$, hence the form of the output from VC03A.

To enable the values of $s(x)$ to be calculated for arbitrary x , the library subroutine TG01B is available.

The third derivative discontinuities and the weighting factors indicate the error behaviour of the fit, see M. J. D. Powell's report mentioned in §7 above.