VC11

PACKAGE SPECIFICATION HSL ARCHIVE

1 SUMMARY

To find the **weighted least squares fit to** N **given data points** (x_i, y_i) by a polynomial of degree $M, M<N$. The polynomial, $P_M(x)$, is chosen so that

$$\sum_{i=1}^{N} w_i [y_i - P_M(x_i)]^2$$

is minimized, where w_i, $i=1,2,...,N$ are the weights.

The polynomial $P_M(x)$ is defined as a linear combination of orthogonal polynomials $Q_K(x)$, $K=0,1,..., M$,

$$P_M(x) = \sum_{K=0}^{M} C_K Q_K(x)$$

where the $Q_K(x)$ are defined by the recurrence relations

$$Q_K(x) = (x - a_K) Q_{K-1}(x) - b_K Q_{K-2}(x), \quad K=2,3,..., M,$$

$$Q_0(x) = 1,$$

$$Q_1(x) = x - a_1$$

and a_K, b_K, $K=1,2,..., M$ are determined by the subroutine from the orthogonality relations

$$\sum_{i=1}^{N} w_i Q_K(x_i) Q_J(x_i) = 0 \quad J \neq K$$

ATTRIBUTES — **Version:** 1.0.0. **Types:** `VC11A`; `VC11AD`. **Calls:** None. **Original date:** February 1993. **Origin:** E.J. York, Harwell, modified by M.J. Hopper, Rutherford Appleton Laboratory. **Remark:** This is a rewritten version of `VC01A`.

2 HOW TO USE THE PACKAGE

2.1 The argument list and calling sequence

The single precision version:

```
CALL VC11A(X,Y,W,Z,N,A,B,C,G,H,L,M,U,LP)
```

The double precision version:

```
CALL VC11AD(X,Y,W,Z,N,A,B,C,G,H,L,M,U,LP)
```

`X` is a `REAL` (`DOUBLE PRECISION` in the D version) array, minimum length N, containing the data positions x_i as in section 1, such that

$$X(J) = x_J, \quad J=1,2,...,N$$

`Y` is a `REAL` (`DOUBLE PRECISION` in the D version) array, minimum length N, containing the data values y_i as in section 1.

`W` is a `REAL` (`DOUBLE PRECISION` in the D version) array, minimum length N, containing the weights w_i as in section 1.

`Z` is a `REAL` (`DOUBLE PRECISION` in the D version) array of length N set to the values

$$\sum_{J=0}^{M} C_J Q_J(x_i).$$

N is an INTEGER, the number of data points.

A is a REAL (DOUBLE PRECISION in the D version) array of length M+1 containing the parameters a_K in the recurrence relations.

B is a REAL (DOUBLE PRECISION in the D version) array of length M+1 containing the parameters b_K in the recurrence relations.

C is a REAL (DOUBLE PRECISION in the D version) array of length M+1 containing the coefficients c_K, so that $C(K)=c_{K-1}$, K=1,2,..., M+1.

G is a REAL (DOUBLE PRECISION in the D version) array of length M+1 set so that G(I) is the variance of C(I).

H is a REAL (DOUBLE PRECISION in the D version) array of length M+1 set to the residual sum of squares, as follows

$$H(I)=\sum_{J=1}^{N} W(J)[Y(J)-\sum_{K=1}^{I} C(K)Q_{K-1}(X(J))]^2.$$

L is an INTEGER array of length M+1 such that L(I) contains the number of changes of sign in the residuals when the fitting function is

$$\sum_{K=1}^{I} C(K)Q_{K-1}(x).$$

M is an INTEGER, the degree of the polynomial to be fitted.

U is a REAL (DOUBLE PRECISION in the D version) array of length 2N and is used by VC11A/VC11AD as working space.

LP is an INTEGER variable which specifies the stream number on which results appear: to suppress these messages set LP negative or zero.

3 GENERAL INFORMATION

Use of common: Makes no use of common areas.

Workspace: Passed through the argument list (see definition of U above).

Other routines called directly: None.

Input/output: Results may be printed (see definition of LP above).

Restrictions: $m < N$, $m \leq 19$.

4 METHOD

See G.E. Forsythe, Generation and use of orthogonal polynomials for data fitting, *Journal of SIAM*, **5** , pp.74- 78 (1957).

Note that the library subroutines PE07A/AD can be used to compute values of $P_M(x)$ and the routines PE08A/AD can be used to obtain the coefficients d_K, K=0,1,..., M in the power series expansion

$$P_M(x)=\sum_{K=0}^{M} d_K x^K.$$