



1 SUMMARY

Computes the optimal interpolation formula $\tilde{S}(x)$, of specified degree, which interpolates n prescribed function values. Specifically, given function values f_1, f_2, \dots, f_n at the n data points $x_1 < x_2 < \dots < x_n$ this subroutine computes the knots $\eta_1, \dots, \eta_{n-k}$ and the coefficients a_1, \dots, a_n of the spline function

$$\tilde{S}(x) = \sum_{i=1}^n a_i N_{k,i}(x)$$

of degree $k-1$, which satisfies the interpolation conditions

$$\sum_{i=1}^n a_i N_{k,i}(x_j) = f_j, \quad j=1, 2, \dots, n$$

and which, whenever $|f^{(k)}|$, $1 \leq k \leq n$, is bounded, and the value of the bound is unknown, provides the smallest possible value of $B(x)$ in the error bound

$$|f(x) - \tilde{S}(x)| \leq B(x) \max_{x_1 \leq x \leq x_n} |f^{(k)}(x)|.$$

N.B. The function $N_{k,i}(x)$ is a normalised B-spline of degree $k-1$.

As a by-product of the calculation the subroutine also computes the value of the integral

$$\int_{x_1}^{x_n} \tilde{S}(x) dx.$$

The method is described in the reports Gaffney, AERE CSS.52 (1977) and Gaffney, AERE R.8781 (1977).

ATTRIBUTES — **Version:** 1.0.0. **Types:** TB07A, TB07AD. **Calls:** TB06, TB08. **Original date:** June 1977. **Origin:** P.W.Gaffney*, Harwell.

2 HOW TO USE THE PACKAGE

2.1 The argument list and calling sequence

The single precision version:

```
CALL TB07A(N, X, F, K, NK, ETA, IL, AN, ISW, WK, A)
```

The double precision version:

```
CALL TB07AD(N, X, F, K, NK, ETA, IL, AN, ISW, WK, A)
```

- N is an INTEGER variable which is set by the user to the number n of data points x_i , $i=1, n$. This argument is not altered by the subroutine. **Restriction:** $n \geq 2$.
- X is a REAL (DOUBLE PRECISION in the D version) array of length at least n , which must be set by the user to the data points x_i , $i=1, n$. This argument is not altered by the subroutine. **Restriction:** These must be ordered so that $x_1 < x_2 < \dots < x_n$. This argument is not altered by the subroutine.
- F is a REAL (DOUBLE PRECISION in the D version) array of length at least n , which must be set by the user to the function values f_1, \dots, f_n . This argument is not altered by the subroutine.
- K is an INTEGER variable which must be set by the user to the number k , where the degree of $\tilde{S}(x)$ is $k-1$. This argument is not altered by the subroutine. **Restriction:** The value of k must be in the range $1 \leq k \leq n$.

- NK is an INTEGER variable which must be set by the user to the length of the array ETA. This argument is not altered by the subroutine.
- ETA is a REAL (DOUBLE PRECISION in the D version) array of length at least the maximum value of $n-k$ and 1. On exit from the subroutine $\text{ETA}(j)$ contains the value of η^*_k , when $n \neq k$. If $n=k$ the contents of ETA are ignored by the subroutine.
- IL is an INTEGER array of length at least n , which is used by the subroutine as workspace.
- AN is a two-dimensional REAL (DOUBLE PRECISION in the D version) array whose first dimension must be n and whose second dimension must be k . It is used to store the coefficient matrix $N_{k,i}(x_j)_{1 \leq i,j \leq n}$, in compact form. On exit from the subroutine AN is overwritten by its triangular decomposition.
- ISW is an INTEGER variable which the user must set to the length of the array WK. This argument is not altered by the subroutine.
- WK is a REAL (DOUBLE PRECISION in the D version) array of length at least $4n+3k+1$, which is used as workspace. On exit from the subroutine the value of the integral

$$\int_{x_1}^{x_n} \tilde{S}(x) dx$$

is stored in $\text{WK}(N+K+1)$.

- A is a REAL (DOUBLE PRECISION in the D version) array of length at least n which will be set by the subroutine to the values of the coefficients a_1, \dots, a_n .

2.2 The Common area and diagnostic messages

The subroutine uses a Common area which the user may also reference. To do this the calling program will require a Common statement of the form

Single precision version:

```
COMMON/TB07B/ IMAX,LP,IFAIL
```

Double precision version:

```
COMMON/TB07BD/ IMAX,LP,IFAIL
```

- IMAX is an INTEGER variable which is defaulted to the value 1,000. It is a limit imposed on the number of Newton iterations performed in TB08A/AD, see §4.
- LP is an INTEGER variable which specifies the Fortran stream number to be used for error messages. The default value is 6 (line printer). To suppress the printing of error messages set LP to zero.
- IFAIL is an INTEGER variable which is always set by the subroutine to indicate success or failure. On exit from the subroutine IFAIL will take one of the following values:

- 0 successful entry.
- 1 $n < 2$.
- 2 $k < 1$ or $k > n$.
- 3 $x_i \geq x_{i+1}$ for some i .
- 4 IMAX too small.
- 5 The continuation method used by the subroutine failed to start. This is usually because k is too large or the problem is ill-conditioned.

2.3 The contents of the workspace

On exit from the subroutine the workspace array `IL` and the first $n+k$ locations of `WK` contain information which may be useful to the user. This information is described below.

The contents of `IL` are the integers which identify the knot intervals where the data points lie. That is `IL(I)`, $I=2, N-1$ contain the unique integrals, r_i , say, such that

$$\eta^*_{r_i-k} \leq x_i < \eta^*_{r_i+1-k}, \quad i=1, n-1$$

where $\eta^*_0 = x_1$ and $\eta^*_{n-k+1} = x_n$, and `IL(1)` contains the value k and `IL(N)` the value n .

The first $n+k$ locations of `WK` contain the complete knot set which is required in order to write $\tilde{S}(x)$ as a linear combination of B-splines. They have the values

$$\begin{aligned} \text{WK}(1) &= \dots = \text{WK}(k) = x_1, \\ \text{WK}(k+i) &= \eta^*_i, \quad i=1, n-k \end{aligned}$$

and

$$\text{WK}(n+1) = \dots = \text{WK}(n+k) = x_n.$$

3 GENERAL INFORMATION

Use of Common: The subroutine uses a Common area `TB07B/BD`, see §2.2.

Workspace: The user provides the workspace through the arguments `WK` and `IL`.

Other subroutines: `TB06A/AD` is called to compute the coefficients a_1, \dots, a_n of $\tilde{S}(x)$, and `TG04A/AD` is used to evaluate B-splines. `TB08A/AD` is also called.

Input/Output: In the event of errors diagnostic messages are printed. The output stream for these may be changed or the messages suppressed by altering the Common variable `LP`, see §2.2.

Restrictions:

$$n \geq 2,$$

$$1 \leq k \leq n.$$

$$x_1 < x_2 < \dots < x_{n-1} < x_n.$$

4 METHOD

The subroutine first calls `TB08A/AD` to obtain the knots $\eta^*_1, \dots, \eta^*_{n-k}$ and then it calls `TB06A/AD` to compute the n linear parameters of \tilde{S} . Further details are given by Gaffney (1977a and 1977b).

References

Gaffney, P.W. (1977a) 'To compute the Optimal Interpolation Formula'. Harwell Report C.S.S. 52.

Gaffney, P.W. (1977b). 'Fortran Subroutines for computing the Optimal Interpolation Formula'. Harwell Report No. R.8781.