1 SUMMARY

Finds a **cubic spline approximation to a given smooth function** $f(x)$ within a prescribed accuracy ε, i.e. finds a cubic spline $S(x)$ with knots ξ_i $i=1,2,...,n$ such that

$$|S(x) - f(x)| \leq \varepsilon \quad a \leq x \leq b$$

The method is given in M.J.D. Powell, AERE R.7308.

The user must provide a subroutine to evaluate $f(x)$ in the range $a \leq x \leq b$. The spline, which is returned in terms of the knots, the function values and first derivative values at the knots, interpolates $f(x)$ at the knots. The accuracy bound ε may optionally be applied to relative accuracy.

ATTRIBUTES — **Version:** 1.0.0. **Remark:** `TG01` may be used to obtain values of the spline. **Types:** `TS01A`; `TS01AD`. **Original date:** December 1972. **Origin:** M.J.D.Powell, Harwell.

2 HOW TO USE THE PACKAGE

2.1 Argument List (absolute accuracy)

The single precision version

```
CALL TS01A(A,B,ACC,MAXFUN,N,XN,FN,GN,IPRINT,W,CALCFX)
```

The double precision version

```
CALL TS01AD(A,B,ACC,MAXFUN,N,XN,FN,GN,IPRINT,W,CALCFX)
```

A   is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to the lower limit a of the range of x of the required approximation of $f(x)$. The argument is not changed by the subroutine.

B   is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to the upper limit b of the range of x of the required approximation of $f(x)$. The argument is not changed by the subroutine.

ACC is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to the bound ε on the required absolute accuracy of the computed approximation. The subroutine changes the value of `ACC` to be the predicted accuracy in the approximation.

MAXFUN is an `INTEGER` variable which must be set by the user to an upper limit on the number of times `TS01` may call for values of $f(x)$. However, in order to provide an approximation, at least 13 values of $f(x)$ are always used. If the final spline is not sufficiently accurate due to the value of `MAXFUN`, a diagnostic message is printed. This case can be recognised automatically because the final value of `ACC` will be greater than the original ε. The argument `MAXFUN` is not altered by the subroutine.

N   is an `INTEGER` variable which must be set by the user. It serves two purposes. First it regulates the number of knots of the first trial spline approximation. Specifically, for the first iteration of the algorithm a trial spline is used that has max(9,N) equally spaced knots, unless this number is constrained by `MAXFUN`. Because it is usually adequate to begin by dividing the range [a,b] into eight segments, we recommend that the user sets N=0. The second purpose of N is that when the subroutine finishes, the value of N will be changed to the number of knots of the final spline approximation.

XN   is a `REAL` (`DOUBLE PRECISION` in the D version) array of length at least `MAXFUN` which is set by the subroutine to the final knot values ξ_i, $i=1,2,...,n$. Note that $\xi_1 = a$ and $\xi_n = b$.

FN   is a `REAL` (`DOUBLE PRECISION` in the D version) array of length at least `MAXFUN` which is set by the subroutine to the final values of the spline approximation $S(\xi_i)$ at the knots ξ_i, $i=1,2,...,n$.

GN   is a REAL (DOUBLE PRECISION in the D version) array of length at least MAXFUN which is set by the subroutine to the final values of the spline derivative $S'(\xi_i)$ at the knots ξ_i, i=1,2,...,n.

IPRINT is an INTEGER variable which must be set by the user to control the printing from TS01A/AD. If IPRINT≤0 then no spline approximations will be printed, if IPRINT≥2 then only the final spline approximation will be printed, but if IPRINT=1 then the spline approximation at every iteration of the algorithm will be printed, The printing will include estimates of the error $f(x)-S(x)$, which are particularly useful if there is any difficulty in achieving the required accuracy. If the printed error estimates seem to be irregular then the inexperienced user should seek expert advice. This argument is not altered by the subroutine.

W   is a REAL (DOUBLE PRECISION in the D version) array of length at least 1.25*MAXFUN which is used by the subroutine as workspace.

CALCFX is the name of a subroutine which the user must provide to calculate values of the function $f(x)$ in the range $a \le x \le b$. The name should be declared EXTERNAL in the calling program and the subroutine should take the form

The single precision version

```
       SUBROUTINE CALCFX(X,F)
```

The single precision version

```
       SUBROUTINE CALCFX(X,F)
       DOUBLE PRECISION X,F
```

The subroutine must set F to the value of $f(x)$ evaluated at the point x provided in X. The subroutine must not change X.

2.2 Use of common and printing

Any printed output from TS01A/AD is written to unit number LP, where the common variable LP is set to 6 automatically by a BLOCK DATA subprogram. This method is used in order that the destination of the output can be changed by the calling program by reference to the common block

The single precision version

```
       COMMON/TS01B/ LP
```

The double precision version

```
       COMMON/TS01BD/ LP
```

2.3 Requesting relative accuracy

To obtain an approximation based on relative accuracy rather than absolute accuracy a different entry to TS01 must be called.

The single precision version

```
       CALL TS01C(A,B,ACC,RELACC,MAXFUN,N,XN,FN,GN,IPRINT,W,CALCFX)
```

The double precision version

```
       CALL TS01CD(A,B,ACC,RELACC,MAXFUN,N,XN,FN,GN,IPRINT,W,CALCFX)
```

All the arguments except ACC and RELACC are as described for TS01A/AD.

The approximation $S(x)$ is calculated to satisfy the inequality

$$|f(x) - S(x)| \le \max\{\texttt{ACC},\texttt{RELACC}*|f(x)|\}, \qquad a \le x \le b,$$

The arguments ACC and RELACC defined in this expression must both be set to positive values by the user of the subroutine. In this case the value of ACC is changed to the predicted value of the quantity

$$\max_{a \le x \le b} \left\{ \min\left[|f(x) - S(x)|, \left| \frac{f(x) - S(x)}{f(x)} \right| \times \frac{\texttt{ACC}}{\texttt{RELACC}} \right] \right\}.$$

so again `ACC` is increased if and only if the requested accuracy is not satisfied according to the tests of the subroutine. The value of `RELACC` is not altered.

3 GENERAL INFORMATION

Workspace: see argument `W`.

Use of common: a common block `TS01B/BD` is used, see §2.2.

Other routines called directly: a user supplied subroutine is called to evaluate $f(x)$, see argument `CALCFX`.

Input/output: see argument `IPRINT` and §2.2.

4 METHOD

The method is described in detail in Harwell report R-7308 by M.J.D. Powell. Because tridiagonal matrices occur in the calculation of $S(x)$, the subroutine operations of `TS01` are so fast that usually the time spent in `TS01` is insignificant compared with the time spent in the subroutine `CALCFX` that calculates $f(x)$. Most applications require fewer than 100 evaluations of $f(x)$.