8.1 Find a Zero of a Univariate Function

A. Purpose
Find a zero of a univariate function, \( f(x) \).

B. Usage
This subroutine uses reverse communication, i.e., it returns to the calling program each time it needs to have \( f() \) evaluated at a new value of \( x \).

B.1 Program Prototype, Single Precision

```plaintext
REAL X1, F1, X2, F2, TOL
INTEGER MODE

Assign values to X1, X2, and TOL.

MODE = 0
F2 = The value of \( f() \) evaluated at X2.
10 F1 = The value of \( f() \) evaluated at X1.

CALL SZERO(X1, F1, X2, F2, MODE, TOL)

IF ( MODE .EQ. 1) go to 10

Computed quantities are returned in MODE, X1, F1, X2, and F2.

B.2 Argument Definitions

X1, F1, X2, F2 [inout] On the initial entry, F1 = \( f(X1) \) and F2 = \( f(X2) \). If F1 and F2 are of opposite sign, the zero will be found in the interval spanned by X1 and X2. If \( F1 \times F2 > 0 \), and \( X2 \neq X1 \) then \( |X2 - X1| \) will be used in setting the step size for the initial search. If \( X2 = X1 \) on entry, then one must also have F2 = F1, and the search is started as described in Section D.

On returns with MODE = 1, X1 is a new trial abscissa. The calling program must set F1 = \( f(X1) \) and call SZERO again.

On return with MODE = 2 or 3, X1 is the abscissa at which \( |f()| \) had the smallest value, and F1 = \( f(X1) \). If F1 \neq 0, X2 is the nearest abscissa to X1 at which \( f() \) was evaluated and found to have the opposite sign from F1, and F2 = \( f(X2) \).

MODE [inout] Current state of computation. The user must initially set MODE = 0, and after that should not change its value, except to control detailed printing as explained in Section D. On each return, MODE will have one of the following values:

= 1 The calling program is to compute F1 = \( f(X1) \) and call SZERO again.
= 2 Normal termination. Error tolerance criterion is satisfied.
= 3 Normal termination. Error tolerance criterion is not satisfied.
= 4 Apparently \( f \) has a discontinuity between X1 and X2. No zero has been identified.
= 5 Set when \( F1 \times F2 > 0 \), and SZERO was unable to find function values with different signs.
= 6 SZERO was called with MODE > 1, or called initially with MODE > 0. This causes execution to stop.

TOL [in] Error tolerance.

> 0 the zero is to be isolated to an interval of length less than TOL.
< 0 an \( x \) is desired for which \( |f(x)| \leq |TOL| \).
= 0 the iteration continues until the zero of \( f() \) is isolated as accurately as possible. In this case SZERO will never set MODE = 3.

B.3 Modifications for Double Precision
For double-precision usage change the name SZERO to DZERO, and change the REAL declaration to DOUBLE PRECISION.

C. Examples and Remarks
The program DRSZERO illustrates the use of SZERO to compute the root of the function, \( f(x) = 2^x - 8 \), for which the exact answer is \( x = 3 \). Output is shown in ODSZERO.

D. Functional Description
When \( F1 \times F2 > 0 \) at the initial point, iterates are generated according to the formula \( x = x_{\text{min}} + (x_{\text{min}} - x_{\text{max}}) \times \rho \), where the subscript “min” is associated with the \((x, f)\) pair that has the smallest value for \( |f| \), and \( \rho \) is 8 if \( r = f_{\text{min}} / (f_{\text{max}} - f_{\text{min}}) \geq 8 \), else \( \rho = \max(\kappa/4, r) \), where \( \kappa \) is a count of the number of iterations that have been taken without finding \( f \)'s with opposite signs. If \( X1 \) and \( X2 \) have the same value initially (and \( F1 \) and \( F2 \) equal \( F(X1) \)), then the next \( x \) is a distance 0.008 ± \( |x_{\text{min}}|/4 \) from \( x_{\text{min}} \) taken toward 0. (If \( X1 = X2 = 0 \), the next \( x \) is \( -0.008 \).

Let \( x_1 \) and \( x_2 \) denote the first two \( x \) values that give \( f \) values with different signs. Let \( A < B \) be

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the two values of $x$ that bracket the zero as tightly as is known. Thus $A = x_1$ or $A = x_2$ and $B$ is the other when computing $x_3$. The next point $x_3$ is generated treating $x$ as the linear function $q(f)$ that interpolates the points $(f(x_1), x_1)$ and $(f(x_2), x_2)$, and computing $x_3 = q(0)$, subject to the condition that $A + \varepsilon \leq x_3 \leq B - \varepsilon$, where $\varepsilon = 0.875$ times the accuracy to which the root has been requested. (This condition on $x_3$ with updated values for $A$ and $B$ is also applied to future iterates.)

Let $x_4, x_5, \ldots, x_m$ denote the abscissae on the following iterations. Let $a = x_m, b = x_{m-1}$, and $c = x_{m-2}$. Either $A$ or $B$ (defined as above) will coincide with $a$, and $B$ will frequently coincide with either $b$ or $c$. Let $p(x)$ be the quadratic polynomial in $x$ that passes through the values of $f$ evaluated at $a$, $b$, and $c$. Let $q(f)$ be the quadratic polynomial in $f$ that passes through the points $(f(a), a)$, $(f(b), b)$, and $(f(c), c)$.

Let $C = A$ or $B$, selected so that $C \neq a$. If the sign of $f$ has changed in the last 4 iterations and $p'(a) \times q'(f(a))$ and $p'(C) \times q'(f(C))$ are both in the interval $[1/4, 4]$, then $x$ is set to $q(0)$. (Note that if $p$ is replaced by $f$ and $q$ is replaced by $x$, then both products have the value 1.) Otherwise $x$ is set to $a - (a - C)(\varphi/(1 + \varphi))$, where $\varphi$ is selected based on past behavior and on the ratio of $f(a)$ with values of $f()$ having the same sign as $f(a)$, and different sign from $f(a)$, evaluated at nearby values of $x$. The method of selecting $\varphi$ is sufficiently complicated that we simply refer interested readers to the code. The algorithm is such that $0 < \varphi$, and if the sign of $f()$ does not change for an extended period, $\varphi$ gets large.

Reference [1] compares a number of algorithms for finding a zero of a continuous function. Dr. Shi has kindly used the same test program, ENCL0FX, on DZERO. With Dr. Shi’s permission, results from Table II of that paper are given on the next page with an additional column added for the results he obtained with DZERO. With the exception of DE and M, all codes solved all of the problems. See [1] for more details.

Detailed printing

Before the initial call with MODE = 0, or at any time during the iterative process, the user may set a counter for detailed output by calling SZERO with a negative value of MODE. There is no problem-solving action on such a call. A saved counter is set so detailed output will be written using the message processor described in Chapter 19.3 on the next |MODE|−1 normal calls. To resume normal computation with the detailed print on, the calling program must set MODE = 0 if a new problem sequence is being started or MODE = 1 if an iterative sequence is being continued. (Detailed print can be turned off by setting MODE = −1 as is implied by the above.)

The detailed output consists of X1, F1, KTYP, DIV, and KS. KTYP is 0 if $\varphi$ above was used on the previous iteration, and KTYP is 1 if $x$ was set to $q(0)$. DIV is the name of the program variable corresponding to $\varphi$, and KS is the number of iterations since there has been a change in the sign of $f()$.

References


E. Error Procedures and Restrictions

The user must initially set MODE = 0 and must not alter MODE after that while iterating on the same problem (except as described in Section D for detailed output.) Entering SZERO with MODE > 0 when SZERO has not set MODE to 1 results in an error condition and an error message will be issued using the system error handler SMESS (or DMESS). In such a case, if MODE ≠ 6, SZERO will set MODE = 6 and return, whereas if MODE = 6, SZERO will STOP.

SZERO uses the Fortran 77 SAVE statement to save values of internal variables between the successive calls needed to solve a problem. Thus SZERO cannot be used to work on more than one problem at a time. In particular, calling SZERO with MODE = 0 will always initialize it for a new problem and no data will be retained from a previous problem (except for the internal detailed print counter described in Section D.)

F. Supporting Information

The source language is ANSI Fortran 77.

Entry Required Files
SZERO AMACH, DMESS, DZERO, MESS

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Revised to allow $F1 \times F2 > 0$ on initial entry, and to change error handling, November 1991.
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DRSZERO

```c
program DRSZERO

>>> 1995–05–28 DRSZERO Krogh Changes to use M77CON
>>> 1993–05–05 DRSZERO Krogh Adjusted to simplify conversion to C.
>>> 1992–03–24 DRSZERO Krogh Added ",," to format statement.
<---S replaces ",": DRSZERO, ?ZERO

Demo driver for SZERO. Univariate zero finder.
```

```c
real X1, X2, F1, F2, A, B, TOL, TWO, EIGHT
parameter(A = 0.0E0, B = 4.0E0, TOL = 0.0E0)
parameter(TWO = 2.0E0, EIGHT = 8.0E0)
integer MODE

10 format(' Results from subroutine SZERO: '/' MODE = ', 13/
        ' Solution: X1 = ',F11.8/
        ' f(X1) = ',1P,G11.3/
        ' Accuracy: X1 - X2 = ',G11.3/
        ' f(X2) = ',G11.3)
```

```c
write(*,'(1x,a)')
* 'DRSZERO.. Demo driver for SZERO, univariate zero finder.,'
* 'Problem: Find zero of 2**X – 8. Exact result: X = 3.'
X2 = B
F2 = TWO**X2  - EIGHT
MODE = 0
X1 = A
20 F1 = TWO**X1  - EIGHT
    call SZERO(X1, F1, X2, F2, MODE, TOL)
    if ( MODE .eq. 1) go to 20
    write(*,10) MODE, X1, F1, X1–X2, F2
stop
end
```

ODSZERO

DRSZERO.. Demo driver for SZERO, univariate zero finder.
Results from subroutine SZERO:

```
MODE = 2
Solution: X1 = 3.00000024
    f(X1) = 9.537E-07
Accuracy: X1 – X2 = 4.768E-07
    f(X2) = -1.431E-06
```