Chapter C05

Roots of One or More Transcendental Equations

Contents

1 Scope of the Chapter

This chapter is concerned with the calculation of real zeros of continuous real functions of one or more variables. (Complex equations must be expressed in terms of the equivalent larger system of real equations.)

2 Background to the Problems

The chapter divides naturally into two parts.

2.1 A Single Equation

The first deals with the real zeros of a real function of a single variable $f(x)$.

There are three routines with simple calling sequences. The first assumes that the user can determine an initial interval $[a,b]$ within which the desired zero lies, that is $f(a) \times f(b) < 0$, and outside which all other zeros lie. The routine then systematically subdivides the interval to produce a final interval containing the zero. This final interval has a length bounded by the user's specified error requirements; the end of the interval where the function has smallest magnitude is returned as the zero. This routine is guaranteed to converge to a **simple** zero of the function. (Here we define a simple zero as a zero corresponding to a sign-change of the function; none of the available routines are capable of making any finer distinction.) However, as with the other routines described below a non-simple zero might be determined and it is left to the user to check for this. The algorithm used is due to Bus and Dekker.

The two other routines are both designed for the case where the user is unable to specify an interval containing the simple zero. The first routine starts from an initial point and performs a search for an interval containing a simple zero. If such an interval is computed then the method described above is used next to determine the zero accurately. The second method uses a 'continuation' method based on a secant iteration. A sequence of subproblems is solved, the first of these is trivial and the last is the actual problem of finding a zero of $f(x)$. The intermediate problems employ the solutions of earlier problems to provide initial guesses for the secant iterations used to calculate their solutions.

Three other routines are also supplied. They employ reverse communication and are called by the routines described above.

2.2 Systems of Equations

The routines in the second part of this chapter are designed to solve a set of nonlinear equations in n unknowns

$$f_i(x) = 0, \quad i = 1,2,\ldots,n, \quad x = (x_1, x_2, \ldots, x_n)^T, \tag{1}$$

where T stands for transpose.

It is assumed that the functions are continuous and differentiable so that the matrix of first partial derivatives of the functions, the **Jacobian** matrix $J_{ij}(x) = (\partial f_i / \partial x_j)$ evaluated at the point x, exists, though it may not be possible to calculate it directly.

The functions f_i must be independent, otherwise there will be an infinity of solutions and the methods will fail. However, even when the functions are independent the solutions may not be unique. Since the methods are iterative, an initial guess at the solution has to be supplied, and the solution located will usually be the one closest to this initial guess.

3 Recommendations on Choice and Use of Available Routines

Note. Refer to the Users' Note for your implementation to check that a routine is available.

3.1 Zeros of Functions of One Variable

The routines can be divided into two classes. There are three routines (C05AVF, C05AXF and C05AZF) all written in reverse communication form and three (C05ADF, C05AGF and C05AJF) written in direct communication form. The direct communication routines are designed for inexperienced users and, in particular, for solving problems where the function $f(x)$ whose zero is to be calculated, can be coded as a user-supplied routine. These routines find the zero by making calls to one or more of the reverse communication routines. Experienced users are recommended to use the reverse communication routines directly as they permit the user more control of the calculation. Indeed, if the zero-finding process is embedded in a much larger program then the reverse communication routines should always be used.

The recommendation as to which routine should be used depends mainly on whether the user can supply an interval $[a, b]$ containing the zero, that is $f(a) \times f(b) < 0$. If the interval can be supplied, then C05ADF (or, in reverse communication, C05AZF) should be used, in general. This recommendation should be qualified in the case when the only interval which can be supplied is very long relative to the user's error requirements **and** the user can also supply a good approximation to the zero. In this case C05AJF (or, in reverse communication, C05AXF) **may** prove more efficient (though these latter routines will not provide the error bound available from C05AZF).

If an interval containing the zero cannot be supplied then the user must choose between C05AGF (or, in reverse communication, C05AVF followed by C05AZF) and C05AJF (or, in reverse communication, C05AXF). C05AGF first determines an interval containing the zero, and then proceeds as in C05ADF; it is particularly recommended when the user does not have a good initial approximation to the zero. If a good initial approximation to the zero is available then C05AJF is to be preferred. Since neither of these latter routines has guaranteed convergence to the zero, the user is recommended to experiment with both in case of difficulty.

3.2 Solution of Sets of Nonlinear Equations

The solution of a set of nonlinear equations

$$f_i(x_1, x_2, \ldots, x_n) = 0, \quad i = 1, 2, \ldots, n \tag{2}$$

can be regarded as a special case of the problem of finding a minimum of a sum of squares

$$s(x) = \sum_{i=1}^{m} [f_i(x_1, x_2, \ldots, x_n)]^2, \quad (m \geq n). \tag{3}$$

So the routines in Chapter E04 are relevant as well as the special nonlinear equations routines.

The routines for solving a set of nonlinear equations can also be divided into classes. There are four routines (C05NBF, C05NCF, C05PBF and C05PCF) all written in direct communication form and two (C05NDF and C05PDF) written in reverse communication form. The direct communication routines are designed for inexperienced users and, in particular, these routines require the f_i (and possibly their derivatives) to be calculated in user-supplied routines. These should be set up carefully so the Library routines can work as efficiently as possible. Experienced users are recommended to use the reverse communication routines as they permit the user more control of the calculation. Indeed, if the zero-finding process is embedded in a much larger program then the reverse communication routines should always be used.

The main decision which has to be made by the user is whether to supply the derivatives $\frac{\partial f_i}{\partial x_j}$. It is advisable to do so if possible, since the results obtained by algorithms which use derivatives are generally more reliable than those obtained by algorithms which do not use derivatives.

C05PBF and C05PCF (or, in reverse communication, C05PDF) require the user to provide the derivatives, whilst C05NBF and C05NCF (or, in reverse communication, C05NDF) do not. C05NBF and C05PBF are easy-to-use routines; greater flexibility may be obtained using C05NCF and C05PCF, (or, in reverse communication, C05NDF and C05PDF), but these have longer parameter lists. C05ZAF is provided for use in conjunction with C05PBF and C05PCF to check the user-provided derivatives for consistency with the functions themselves. The user is strongly advised to make use of this routine whenever C05PBF or C05PCF is used.

Firstly, the calculation of the functions and their derivatives should be ordered so that **cancellation errors** are avoided. This is particularly important in a routine that uses these quantities to build up estimates of higher derivatives.

Secondly, **scaling** of the variables has a considerable effect on the efficiency of a routine. The problem should be designed so that the elements of x are of similar magnitude. The same comment applies to the functions, i.e., all the f_i should be of comparable size.

The accuracy is usually determined by the accuracy parameters of the routines, but the following points may be useful:

(i) Greater accuracy in the solution may be requested by choosing smaller input values for the accuracy parameters. However, if unreasonable accuracy is demanded, rounding errors may become important and cause a failure.

(ii) Some idea of the accuracies of the x_i may be obtained by monitoring the progress of the routine to see how many figures remain unchanged during the last few iterations.

(iii) An approximation to the error in the solution x, given by e where e is the solution to the set of linear equations

$$J(x)e = -f(x)$$

where $f(x) = (f_1(x), f_2(x), \ldots, f_n(x))^T$ (see Chapter F04).

Note that the QR decomposition of J is available from C05NCF and C05PCF (or, in reverse communication, C05NDF and C05PDF) so that

$$R\,e = -Q^T f$$

and $Q^T f$ is also provided by these routines.

(iv) If the functions $f_i(x)$ are changed by small amounts ϵ_i, for $i = 1, 2, \ldots, n$, then the corresponding change in the solution x is given approximately by σ, where σ is the solution of the set of linear equations

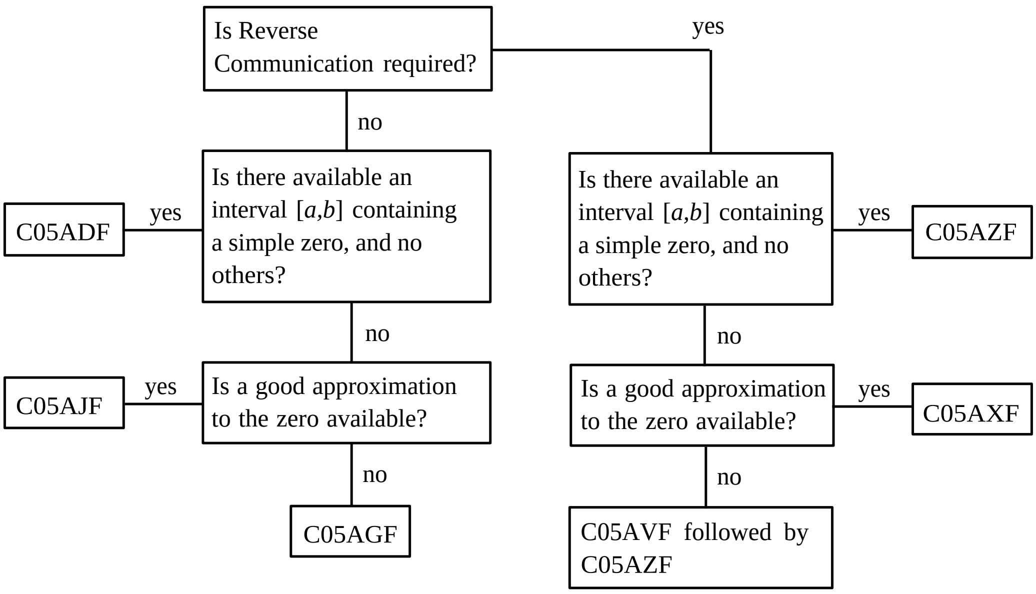
$$J(x)\sigma = -\epsilon,$$

(see Chapter F04).

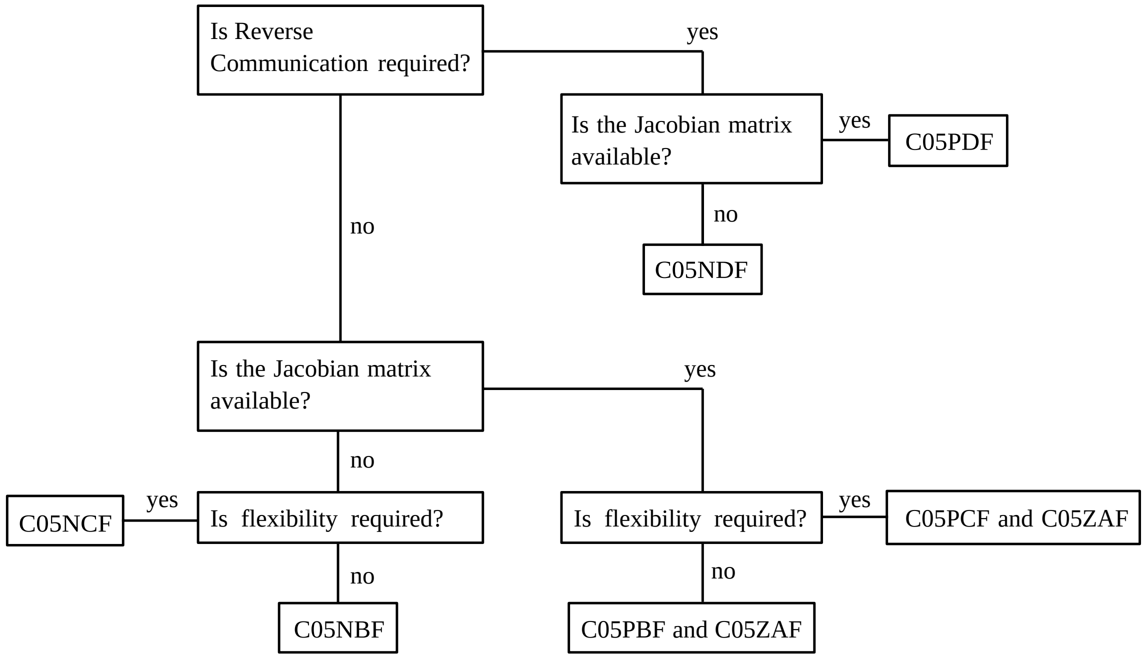
Thus one can estimate the sensitivity of x to any uncertainties in the specification of $f_i(x)$, for $i = 1, 2, \ldots, n$. As noted above, the sophisticated routines C05NCF and C05PCF (or, in reverse communication, C05NDF and C05PDF) provide the QR decomposition of J.

4 Decision Trees

(i) Functions of One Variable



(ii) Functions of Several Variables



5 Index

Zeros of functions of one variable:
Direct communication:

binary search followed by Bus and Dekker algorithm	C05AGF
Bus and Dekker algorithm	C05ADF
continuation method	C05AJF

Reverse communication:

binary search	C05AVF
Bus and Dekker algorithm	C05AZF
continuation method	C05AXF

Zeros of functions of several variables:
Direct communication:

easy-to-use	C05NBF
easy-to-use, derivatives required	C05PBF
sophisticated	C05NCF
sophisticated, derivatives required	C05PCF

Reverse Communication:

sophisticated	C05NDF
sophisticated, derivatives required	C05PDF

Checking Routine:

Checks user-supplied Jacobian	C05ZAF

6 Routines Withdrawn or Scheduled for Withdrawal

None since Mark 13.

7 References

[1] Gill P E and Murray W (1976) Algorithms for the solution of the nonlinear least-squares problem *Report NAC 71* National Physical Laboratory

[2] Moré J J, Garbow B S, and Hillstrom K E (1974) User guide for MINPACK–1 *Technical Report ANL–80–74* Argonne National Laboratory

[3] Ortega J M and Rheinboldt W C (1970) *Iterative Solution of Nonlinear Equations in Several Variables* Academic Press

[4] Rabinowitz P (1970) *Numerical Methods for Nonlinear Algebraic Equations* Gordon and Breach

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