

NAG Library Chapter Introduction**C05 – Roots of One or More Transcendental Equations****Contents**

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1 Scope of the Chapter

This chapter is concerned with the calculation of zeros of continuous functions of one or more variables. The majority of problems considered are for real-valued functions of real variables, in which case 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 you can determine an initial interval $[a, b]$ within which the desired zero lies, (that is, where $f(a) \times f(b) < 0$), 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 your 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 you to check for this. The algorithm used is due to Brent (1973).

The two other routines are both designed for the case where you are unable to specify an interval containing the simple zero. One 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 other 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 use the same core algorithms as the routines described above.

Finally, two routines are provided to return values of Lambert’s W function (sometimes known as the ‘product log’ or ‘Omega’ function), which is the inverse function of

$$f(w) = we^w \quad \text{for} \quad w \in C;$$

that is, if Lambert’s W function $W(x) = a$ for $x, a \in C$, then a is a zero of the function $F(w) = we^w - x$. One routine uses the iterative method described in Barry *et al.* (1995) to return values from the real branches of W (restricting $x, a \in R$). The second routine enforces no such restriction, and uses the approach described in Corless *et al.* (1996).

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

$$f_i(x) = 0, \quad i = 1, 2, \dots, n, \quad x = (x_1, x_2, \dots, x_n)^T, \quad (1)$$

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 $J_{ij}(x) = \left(\frac{\partial f_i}{\partial x_j} \right)$ 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

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 (C05AUF, C05AWF and C05AYF) 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 (sub)program. These routines find the zero by using the same core algorithms as the reverse communication routines. Experienced users are recommended to use the reverse communication routines directly as they permit you 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 you can supply an interval $[a, b]$ containing the zero; that is, where $f(a) \times f(b) < 0$. If the interval can be supplied, then C05AYF (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 your error requirements **and** you can also supply a good approximation to the zero. In this case C05AWF (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 you must choose between C05AUF (or, in reverse communication, C05AVF followed by C05AZF) and C05AWF (or, in reverse communication, C05AXF). C05AUF first determines an interval containing the zero, and then proceeds as in C05AYF; it is particularly recommended when you do not have a good initial approximation to the zero. If a good initial approximation to the zero is available then C05AWF is to be preferred. Since neither of these latter routines has guaranteed convergence to the zero, you are 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

$$f_i(x_1, x_2, \dots, x_n) = 0, \quad i = 1, 2, \dots, n \quad (2)$$

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

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

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 five routines (C05QBF, C05QCF, C05QSF, C05RBF and C05RCF) all written in direct communication form and two (C05QDF and C05RDF) 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 subroutines. 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 you 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 you have to make 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.

C05RBF, C05RCF and C05RDF require you to provide the derivatives, whilst C05QBF, C05QCF, C05QDF and C05QSF do not. C05QBF, C05QSF and C05RBF are easy-to-use routines; greater flexibility may be obtained using C05QCF and C05RCF (or, in reverse communication, C05QDF and C05RDF), but these have longer parameter lists.

C05QSF is an easy-to-use routine specially adapted for sparse problems, that is, problems where each function depends on a small subset of the n variables so that the Jacobian matrix has many zeros. It

employs sparse linear algebra methods and consequently is expected to take significantly less time to complete than the other routines, especially if n is large.

C05ZDF is provided for use in conjunction with C05RBF, C05RCF and C05RDF to check the user-supplied derivatives for consistency with the functions themselves. You are strongly advised to make use of this routine whenever C05RBF, C05RCF or C05RDF 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 is given by e where e is the solution to the set of linear equations

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

where $f(x) = (f_1(x), f_2(x), \dots, f_n(x))^T$.

Note that the QR decomposition of J is available from C05QCF and C05RCF (or, in reverse communication, C05QDF and C05RDF) so that

$$Re = -Q^T f$$

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 $i = 1, 2, \dots, n$, then the corresponding change in the solution x is given approximately by σ , where σ is the solution of the set of linear equations

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

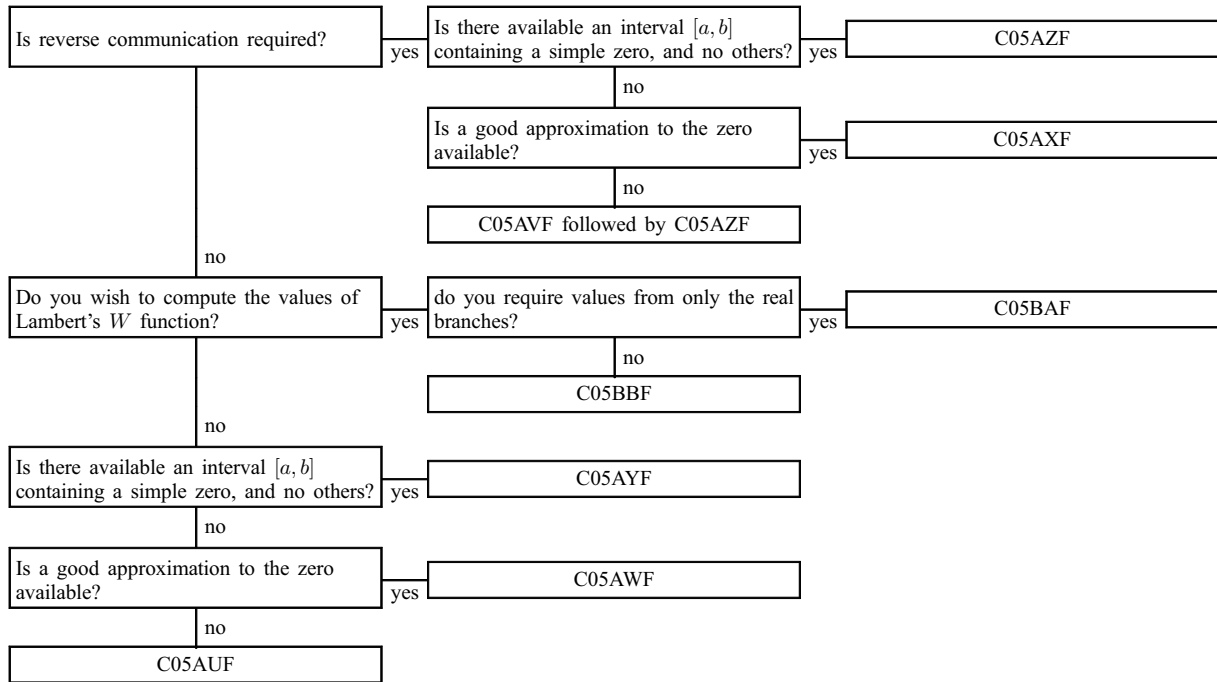
Thus one can estimate the sensitivity of x to any uncertainties in the specification of $f_i(x)$, for $i = 1, 2, \dots, n$. As noted above, the sophisticated routines C05QCF and C05RCF (or, in reverse communication, C05QDF and C05RDF) provide the QR decomposition of J .

3.3 Values of Lambert's W function

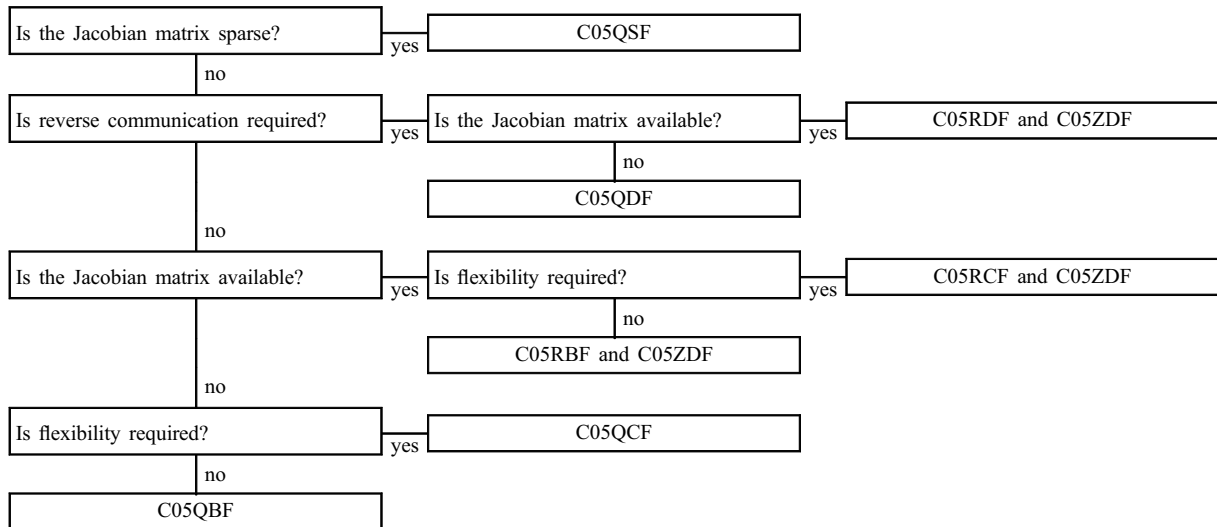
If you require purely-real values of W , these will be evaluated marginally more efficiently by C05BAF than C05BBF owing to the differing iterative procedures used by each routine.

4 Decision Trees

Tree 1: Functions of One Variable



Tree 2: Functions of several variables



5 Functionality Index

Lambert's W function,	
complex values	C05BBF
real values	C05BAF
Zeros of functions of one variable,	
direct communication,	
binary search followed by Brent algorithm	C05AUF
Brent algorithm	C05AYF
continuation method	C05AWF

reverse communication,	
binary search.....	C05AVF
Brent algorithm.....	C05AZF
continuation method	C05AXF
Zeros of functions of several variables,	
checking routine,	
checks user-supplied Jacobian	C05ZDF
direct communication,	
easy-to-use,	
derivatives required	C05RBF
no derivatives required.....	C05QBF
no derivatives required, sparse	C05QSF
sophisticated,	
derivatives required	C05RCF
no derivatives required.....	C05QCF
reverse communication,	
sophisticated,	
derivatives required	C05RDF
no derivatives required.....	C05QDF

6 Auxiliary Routines Associated with Library Routine Parameters

None.

7 Routines Withdrawn or Scheduled for Withdrawal

The following lists all those routines that have been withdrawn since Mark 17 of the Library or are scheduled for withdrawal at one of the next two marks.

Withdrawn Routine	Mark of Withdrawal	Replacement Routine(s)
C05ADF	25	C05AYF
C05AGF	25	C05AUF
C05AJF	25	C05AWF
C05NBF	25	C05QBF
C05NCF	25	C05QCF
C05NDF	25	C05QDF
C05PBF/C05PBA	25	C05RBF
C05PCF/C05PCA	25	C05RCF
C05PDF/C05PDA	25	C05RDF
C05ZAF	25	C05ZDF

8 References

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