NAG Library Chapter Introduction

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 is one function with simple calling sequences. It 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 function 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 function 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 functions are capable of making any finer distinction.) However, 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).

Finally, a function is provided that uses the iterative method described in Barry *et al.* (1995) to return values from the real branches of Lambert's W function (sometimes known as the 'product log' or 'Omega' function), which is the inverse function of

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

that is, if Lambert's W function $W(x) = a$ for $x, a \in C$, then a is a zero of the function $F(w) = we^w - x$. In this chapter we restrict $x, a \in R$.

2.2 Systems of Equations

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

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

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

3.1 Zeros of Functions of One Variable

If you can supply an interval $[a, b]$ containing the zero; that is where $f(a) \times f(b) < 0$, then nag_zero_cont_func_bd_1 (c05sdc) can be used.

3.2 Solution of Sets of Nonlinear Equations

The solution of a set of nonlinear equations

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

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

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

So the functions in Chapter e04 are relevant as well as the special nonlinear equations functions.

nag_zero_nonlin_eqns_deriv_1 (c05ubc) requires you to provide the derivatives, whilst nag_zero_nonlin_eqns_1 (c05tbc) does not.

Firstly, the calculation of the functions and their derivatives should be ordered so that **cancellation errors** are avoided. This is particularly important in a function 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 function. 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.

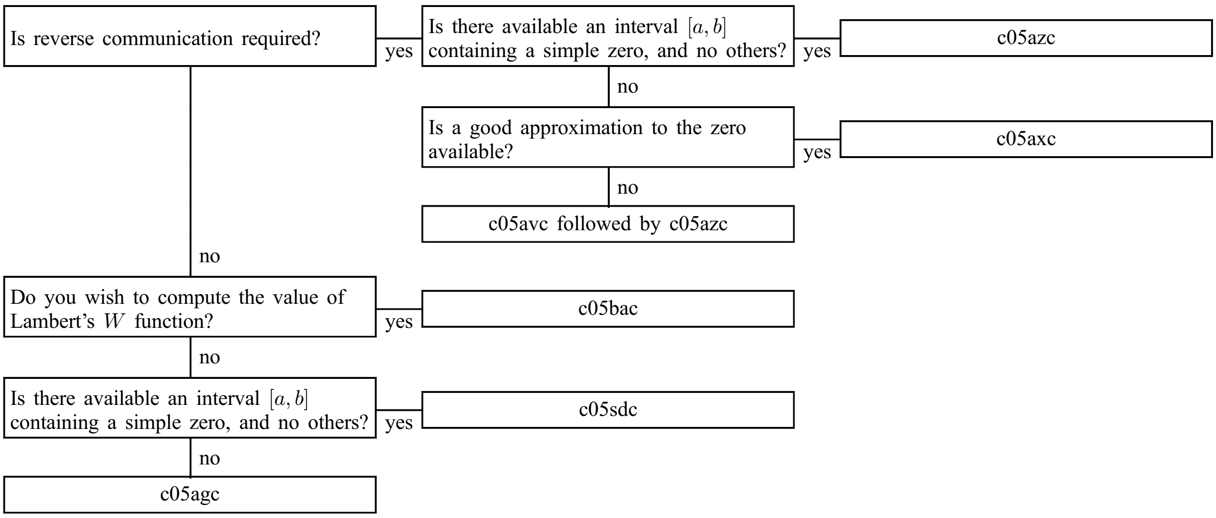
The accuracy is usually determined by the accuracy arguments of the functions, but the following points may be useful.

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

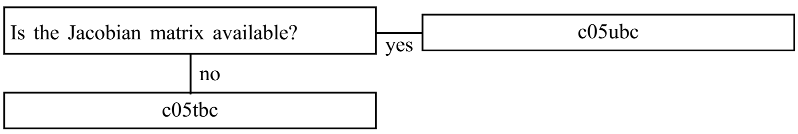
(ii) Some idea of the accuracies of the x_i may be obtained by monitoring the progress of the function to see how many figures remain unchanged during the last few iterations.

4 Decision Trees

Tree 1: Functions of One Variable



Tree 2: Functions of several variables



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6 Functions Withdrawn or Scheduled for Withdrawal

Withdrawn Function	**Mark of Withdrawal**	**Replacement Function(s)**
nag_zero_cont_func_bd (c05adc)	11	nag_zero_cont_func_bd_1 (c05sdc)
nag_zero_nonlin_eqns (c05nbc)	11	nag_zero_nonlin_eqns_1 (c05tbc)
nag_zero_nonlin_eqns_deriv (c05pbc)	11	nag_zero_nonlin_eqns_deriv_1 (c05ubc)
nag_check_deriv (c05zbc)	11	nag_check_deriv_1 (c05zcc)

7 References

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Brent R P (1973) *Algorithms for Minimization Without Derivatives* Prentice–Hall

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

Moré J J, Garbow B S and Hillstrom K E (1980) User guide for MINPACK-1 *Technical Report ANL-80-74* Argonne National Laboratory

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

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