A bracketing technique for computing a zero of a function

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An iterative technique for determining a real zero of a differentiable function is presented. At every stage the zero is bracketed, and as *either* bound approaches the zero, the method exhibits quadratic convergence. Numerical examples are given.

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1. Introduction

Many methods for determining a real zero of a function $f(x)$ first isolate a zero between lower and upper bounds, and then employ an iterative technique that brackets the zero at each stage. Examples of such iterative methods are the bisection method and the *regula falsi.* These methods employ function values only. We consider here the case where the derivative $f'(x)$ can also be employed in the determination of a zero of $f(x)$, assuming that the zero has first been isolated between bounds a and b. An iterative method for treating this case is presented. The method converges (as do those mentioned above) when there is an odd number of zeros between a and b; moreover it resembles Newton's rule when either bound approaches a zero, while possessing significant advantages in circumstances in which Newton's rule is unsatisfactory. Newton's rule, of course, demands rather restrictive conditions (Henrici, 1964) to guarantee convergence, although it is usually possible to incorporate safeguards to avoid possible divergence.

2. Choice of interpolating function

At the ith step of the iterative process, suppose we have bounds p and q on the required zero ξ, so that $p < \xi < q$ and $f(p)$, $f(q)$ have opposite signs. Initially $p = a$ and $q = b$.

We now consider the computation of an interpolating function with four parameters; these will be determined by equating $y(x)$ and $y'(x)$ with $f(x)$ and $f'(x)$, respectively, at both $x = p$ and $x = q$. We then solve $y(x) = 0$. The root so obtained then replaces p or q (depending on the sign of the corresponding $f(x)$) in the next cycle. Among the simplest forms for $y(x)$ are (a) a cubic polynomial in x, (b) a rational function with quadratic numerator and linear denominator, and (c) a rational function with linear numerator and quadratic denominator. We cannot expect any one of these to give a better interpolating function than the others in general, so we make our choice on the grounds of simplicity and convenience. The form (c) has the great virtue that unlike (a) and (b) it gives the zero of $y(x)$ directly, without the solution of a polynomial equation and selection of the appropriate root. This choice was also considered by Jarratt and Nudds (1965) and Jarratt (1966), but their techniques were not concerned with bracketing the zero.

3. The iterative formula

We therefore fit the interpolating function of the form

$$y(x) = (x - c)/(d_0 + d_1 x + d_2 x^2) \qquad (1)$$

to $f(x)$ so that function and derivative agree at $x = p$ and $x = q$. Solving the resulting four linear simultaneous equations yields

$$c = \frac{(p + q)f_p f_q(f_q - f_p) - (q - p)(pf_q^2 f'_p + qf_p^2 f'_q)}{2f_p f_q(f_q - f_p) - (q - p)(f_q^2 f'_p + f_p^2 f'_q)}, \qquad \ldots (2)$$

where $f_p = f(x_p)$, $f'_p = f'(x_p)$, etc.

This is the basic formula, which at each step gives the zero of $y(x)$, viz. $x = c$, as an estimate of ξ. We preserve accuracy as $p \to \xi$ by writing (2) in the form

$$c = p + \frac{(q - p)f_p f_q(f_q - f_p) - (q - p)^2 f_p^2 f'_q}{2f_p f_q(f_q - f_p) - (q - p)(f_q^2 f'_p + f_p^2 f'_q)}, \qquad (3)$$

or in the similar form with p and q interchanged as $q \to \xi$. If it transpires that c falls outside (p, q) then we discard this value and use instead the simple bisection given by

$$c = \tfrac{1}{2}(p + q). \qquad (4)$$

If $f(c)$ now has the same sign as $f(p)$, we proceed to the next cycle with c replacing the previous p; otherwise it replaces the previous q.

It is of interest to consider the conditions under which the value of c given by (2) lies outside (p, q), so that we turn to (4). Since $y(p)$ and $y(q)$ have opposite signs, this can happen only if $y(x)$ has exactly one pole in (p, q). We can rule out the possibility of such a single pole if $d_0 + d_1 x + d_2 x^2$ has neither, or both, of its zeros in (p, q); that is, if this quadratic has the same sign at p as it has at q. This yields

$$\{f_q(f_q - f_p) - hf_p f'_q\}\{f_p(f_q - f_p) - hf_q f'_p\} < 0, \qquad (5)$$

where $h = q - p$, as a necessary and sufficient condition for c to lie in (p, q).

4. Convergence

It is clear from (3) that

$$c \to p - f_p/f'_p \text{ as } p \to \xi. \qquad (6)$$

A similar result holds, of course, if q replaces p everywhere in (6). Thus as either bound approaches the required zero, the method essentially becomes Newton's rule, and therefore exhibits quadratic convergence. On the other hand, when the bounds are far from the zero, the methods have very different behaviour. In particular, Newton's rule fails when $f'_p = 0$, whereas our method is valid even when $f'_p = f'_q = 0$; in which case we find $c = \frac{1}{2}(p + q)$.

5. Practical tests

A class of test functions was devised for the method. A polynomial $p_n(x)$ of degree n was defined by taking a set of $n + 1$ pseudorandom numbers, rectangularly distributed in the range $(-1, 1)$, as its coefficients. If the values of the polynomial at $x = a$ and $x = b$ were of opposite sign the polynomial was used to test the method in finding a zero in (a, b); otherwise the polynomial was rejected and a new set of coefficients generated. The method was terminated when two successive estimates of the zero differed by ϵ or less, for a given value of ϵ, or when the function value became zero. This test was carried out 100 times for both $n = 10$ and $n = 30$. In each case the values $a = 0$, $b = 1$ and $\epsilon = \frac{1}{2} \times 10^{-8}$ were used. The average number of evaluations of both $p_n(x)$ and its derivative to determine a zero of $p_n(x)$ was 6·81 for the case $n = 10$ and 7·16 for $n = 30$. These figures include the evaluations of $p_n(x)$ and $p'_n(x)$ at $x = a$ and $x = b$. If a search procedure had previously been used to isolate the zeros, $p_n(a)$ and $p_n(b)$ would already have been determined. All 100 10th degree polynomials and 96 of the 30th degree polynomials were solved for a zero in 10 or less evaluations. The most common number of evaluations was 7 (with 6 coming a close second) in both cases. The frequency of usage of (2) relative to that of (4) was approximately 15 : 1 in both cases.

The method has also been tested on a number of nonpolynomial functions, and results similar to these detailed above obtained. An ALGOL procedure for the method is given in the appendix.

6. Conclusions

An iterative method employing derivatives that brackets the zero at each stage has been developed for determining a real zero of a function. Its ultimate convergence is quadratic, and judging by tests carried out on the method, the initial progress is generally good too. Only occasionally does the method predict a value outside the range, and in this case a simple bisection of the interval is made instead. The conditions for such an occurrence have been analysed.

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Appendix

Algol procedure

```
procedure zero of function (a, b, eps, evaluate, x, imax,
    fail);
value a, b, eps, imax; label fail;
real a, b, eps, x; integer imax; procedure evaluate;
comment zero of function determines a zero of the differ-
    entiable function f(x) lying in the range (a, b) by an
    iterative method that brackets the zero at each stage.
    The range (a, b) must be such that f(a) and f(b) are of
    opposite sign. The process terminates when two suc-
    cessive estimates of the zero differ by an amount less
    than or equal to eps, or when the function value becomes
    zero. If convergence is not achieved within imax
    (function + derivative) evaluations, or if f(a) and f(b)
    are of like sign, the procedure exits to label fail. f(x)
    and its derivative must be specified by procedure
    evaluate (fx, dfdx, x);
  begin
  real p, q, fp, fq, fx, dp, dq, dx, h, d, x old;
  integer i, s;
  x old := p := a; q := b;
  evaluate (fp, dp, p); evaluate (fq, dq, q);
  s := sign (fp); if sign (fq) = s then goto fail;
  for i := 3 step 1 until imax do
    begin
    h := q − p;
    d := 2×fp×fq×(fq − fp) −
          h×(dp×fq×fq + dq×fp×fp);
    x := if d = 0 then (p+q)/2·0 else
          if x old = p
          then p + h×fp×(fq×(fq − fp) −
            h×fp×dq)/d
          else q − h×fq×(fp×(fq − fp) −
            h×fq×dp)/d;
    if x < p ∨ x > q then x := (p+q)/2·0;
    if abs (x − x old) ⩽ eps then goto out;
    evaluate (fx, dx, x); if fx = 0 then goto out;
    if sign (fx) = s then
    begin x old := p := x; fp := fx; dp := dx
    end
    else
    begin x old := q := x; fq := fx; dq := dx
    end
  end i;
  goto fail;
out:
end zero of function
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