THEOREM 1 Theorem on Bisection Method

If $[a_0, b_0], [a_1, b_1], \ldots, [a_n, b_n], \ldots$ *denote the intervals in the bisection method, then the limits* $\lim_{n\to\infty} a_n$ *and* $\lim_{n\to\infty} b_n$ *exist, are equal, and represent a zero of* f. *If* $r = \lim_{n\to\infty} c_n$ *and* $c_n = \frac{1}{2}(a_n + b_n)$, *then*

$$|r - c_n| \le 2^{-(n+1)}(b_0 - a_0) \tag{2}$$

EXAMPLE 2 Suppose that the bisection method is started with the interval $[50, 63]$. How many steps should be taken to compute a root with relative accuracy of one part in 10^{-12}?

Solution The stated requirement on relative accuracy means that

$$|r - c_n|/|r| \le 10^{-12}$$

We know that $r \ge 50$, and thus it suffices to secure the inequality

$$|r - c_n|/50 \le 10^{-12}$$

By means of Theorem 1, we infer that the following condition is sufficient:

$$2^{-(n+1)} \times (13/50) \le 10^{-12}$$

Solving this for n, we conclude that $n \ge 37$. ∎

PROBLEMS 3.1

1. Find a positive root of
$$x^2 - 4x \sin x + (2 \sin x)^2 = 0$$
accurate to two significant figures. Use a hand calculator.

2. Consider the bisection method starting with the interval $[1.5, 3.5]$.
   a. What is the width of the interval at the nth step of this method?
   b. What is the maximum distance possible between the root r and the midpoint of this interval?

3. If the bisection method is used (in single precision) on the `Marc-32` starting with the interval $[128, 129]$, can we compute the root with absolute accuracy $< 10^{-6}$?

4. Determine the formula
$$n \ge \frac{\log(b_0 - a_0) - \log \varepsilon}{\log 2} - 1$$
involving $b_0 - a_0$ and ε for the number of steps that must be taken in the bisection method to guarantee that $|r - c_n| \le \varepsilon$.

5. Determine the formula
$$n \ge \frac{\log(b_0 - a_0) - \log \varepsilon - \log a_0}{\log 2} - 1$$
involving a_0, b_0, and ε for the number of steps that should be taken in the bisection algorithm to ensure that the root is determined with *relative* accuracy $\le \varepsilon$. Assume $a_0 > 0$.

6. (Continuation) What happens in the preceding problem if $a_0 < 0 < b_0$?

7. If the bisection method is used starting with the interval [2, 3], how many steps must be taken to compute a root with absolute accuracy $< 10^{-6}$? Answer the same question for the *relative* accuracy. What about to full single precision on the `Marc-32` in each case?

8. Let $c_n = \frac{1}{2}(a_n + b_n)$, $r = \lim_{n\to\infty} c_n$, and $e_n = r - c_n$. Here $[a_n, b_n]$, with $n \geq 0$, denotes the successive intervals that arise in the bisection method when it is applied to a continuous function f.

   a. Show that $|e_n| \leq 2^{-n}(b_1 - a_1)$.

   b. Show that $e_n = \mathcal{O}(2^{-n})$ as $n \to \infty$.

   c. Is it true that $|e_0| \geq |e_1| \geq \cdots$? Explain.

   d. Show that $|c_n - c_{n+1}| = 2^{-n-2}(b_0 - a_0)$.

   e. Show that for all n and m, $a_m \leq b_n$.

   f. Show that r is the unique element in $\bigcap_{n=0}^{\infty}[a_n, b_n]$.

   g. Show that for all n, $[a_n, b_n] \supset [a_{n+1}, b_{n+1}]$.

9. In the bisection method, an interval $[a_{n-1}, b_{n-1}]$ is divided in half, and one of these halves is chosen for the next interval. Define $d_n = 0$ if $[a_n, b_n]$ is the left half of the interval $[a_{n-1}, b_{n-1}]$, and let $d_n = 1$ otherwise. Express the root determined by the algorithm in terms of the sequence $d_1, d_2, \ldots$. *Hint:* Consider the case $[a_0, b_0] = [0, 1]$ first, and think about the binary representation of the root.

10. Using the notation of the previous two problems, find the formulas that relate a_n, b_n, and c_n to d_n.

11. Give an example (or prove that none exists) in which $a_0 < a_1 < a_2 < \cdots$.

12. Give an example in which $a_0 = a_1 < a_2 = a_3 < a_4 = a_5 < a_6 = \cdots$.

13. In the bisection method, does $\lim_{n\to\infty} |r - c_{n+1}|/|r - c_n|$ exist? Explain.

14. Let the bisection method be applied to a continuous function, resulting in intervals $[a_0, b_0]$, $[a_1, b_1]$, and so on. Let $r = \lim_{n\to\infty} a_n$. Which of these statements can be false?

   a. $a_0 \leq a_1 \leq a_2 \leq \cdots$

   b. $|r - 2^{-1}(a_n + b_n)| \leq 2^{-n}(b_0 - a_0) \qquad (n \geq 0)$

   c. $|r - 2^{-1}(a_{n+1} + b_{n+1})| \leq |r - 2^{-1}(a_n + b_n)| \qquad (n \geq 0)$

   d. $[a_{n+1}, b_{n+1}] \subseteqq [a_n, b_n] \qquad (n \geq 0)$

   e. $|r - a_n| = \mathcal{O}(2^{-n})$ as $n \to \infty$

   f. $|r - c_n| < |r - c_{n-1}| \qquad (n \geq 1)$

15. Prove that the point c computed in the bisection method is the point where the line through $(a, \text{sign}(f(a)))$ and $(b, \text{sign}(f(b)))$ intersects the x-axis.

16. Suppose that $|a_n - b_n| \leq \lambda_n |a_{n-1} - b_{n-1}|$ for all n with $\lambda_n < 1$. Find an upper bound on $|a_n - b_n|$ in terms of $|a_0 - b_0|$ and $\lambda = \max_{1\leq i\leq n}\{\lambda_i\}$.

COMPUTER PROBLEMS 3.1

1. Write and test a subprogram or procedure to implement the bisection algorithm. Test the program on these functions and intervals:

   a. $x^{-1} - \tan x$ on $[0, \pi/2]$

   b. $x^{-1} - 2^x$ on $[0, 1]$

Taking partial derivatives, we get the Jacobian matrix

$$F'(X) = \begin{bmatrix} x_2 & x_1 & -2x_3 \\ x_2x_3 - 2x_1 & x_1x_3 + 2x_2 & x_1x_2 \\ e^{x_1} & -e^{x_2} & 1 \end{bmatrix}$$

Using the starting value $X^{(0)} = (1, 1, 1)^T$, we carry out the nonlinear Newton's method given in Equations (11) and (12) and obtain the following:

n	x_1	x_2	x_3
0	1.00000 00	1.00000 00	1.00000 00
1	2.18932 60	1.59847 51	1.39390 06
2	1.85058 96	1.44425 14	1.27822 40
3	1.78016 11	1.42443 59	1.23929 24
4	1.77767 47	1.42396 09	1.23747 38
5	1.77767 19	1.42396 05	1.23747 11
6	1.77767 19	1.42396 05	1.23747 11

■

The solution of systems such as (8) is often challenging. The standard reference on the subject is Ortega and Rheinboldt [1970]. See also Rheinboldt [1974], Ostrowski [1966], Byrne and Hall [1973], Schnabel and Frank [1984], Eaves, Gould, Peitgen, and Todd [1983], and Allgower, Glasshoff, and Peitgen [1981]. For a discussion of the convergence of Newton's method in higher dimensions, refer to Goldstein [1966] or Ortega and Rheinboldt [1970].

PROBLEMS 3.2

1. Find the smallest positive starting point for which Newton's method diverges when it is applied to $f(x) = \tan^{-1} x$.
2. Let Newton's method be used on $f(x) = x^2 - q$ (where $q > 0$). Show that if x_n has k correct digits after the decimal point, then x_{n+1} will have at least $2k - 1$ correct digits after the decimal point, provided that $q > 0.006$ and $k \geq 1$.
3. Prove that if Newton's method is used on a function f for which f'' is continuous and $f(r) = 0 \neq f'(r)$, then $\lim_{n\to\infty} e_{n+1}e_n^{-2}$ exists and equals $f''(r)/[2f'(r)]$. How can this fact be used in a program to test whether convergence is quadratic?
4. **(Steffensen's method)** Consider the iteration formula

$$x_{n+1} = x_n - f(x_n)/g(x_n)$$

where

$$g(x) = [f(x + f(x)) - f(x)]/f(x)$$

Show that this is quadratically convergent, under suitable hypotheses.

5. What is the purpose of the following iteration formula?

$$x_{n+1} = 2x_n - x_n^2 y$$

Identify it as the Newton iteration for a certain function.

6. To compute reciprocals without division, we can solve $x = 1/R$ by finding a zero of the function $f(x) = x^{-1} - R$. Write a short algorithm to find $1/R$ by Newton's method applied to f. Do not use division or exponentiation in your algorithm. For positive R, what starting points are suitable?

7. Define $x_0 = 0$ and $x_{n+1} = x_n - [(\tan x_n - 1)/\sec^2 x_n]$. What is $\lim_{n\to\infty} x_n$ in this example? Relate this to Newton's method.

8. Perform four iterations of Newton's method for the polynomial

$$p(x) = 4x^3 - 2x^2 + 3$$

starting with $x_0 = -1$. Use a hand calculator.

9. If Newton's method is used on $f(x) = x^3 - 2$ starting with $x_0 = 1$, what is x_2?

10. Devise a Newton iteration formula for computing $\sqrt[3]{R}$ where $R > 0$. Perform a graphical analysis of your function $f(x)$ to determine the starting values for which the iteration will converge.

11. Devise a Newton algorithm for computing the fifth root of any positive real number.

12. The function $f(x) = x^2 + 1$ has zeros in the complex plane at $x = \pm i$. Is there a *real* starting point for complex Newton's method such that the iterates converge to either of these zeros? What complex starting points will work?

13. If Newton's method is used with $f(x) = x^2 - 1$ and $x_0 = 10^{10}$, how many steps are required to obtain the root with accuracy 10^{-8}? (Solve analytically, not experimentally.)

14. Suppose that r is a double zero of the function f. Thus, $f(r) = f'(r) = 0 \neq f''(r)$. Show that if f'' is continuous, then in Newton's method we shall have $e_{n+1} \approx \frac{1}{2} e_n$ (linear convergence).

15. Consider a variation of Newton's method in which only one derivative is needed; that is,

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_0)}$$

Find C and s such that

$$e_{n+1} = C e_n^s$$

16. Prove that Newton's iteration will diverge for these functions, no matter what (real) starting point is selected.

   a. $f(x) = x^2 + 1$

   b. $f(x) = 7x^4 + 3x^2 + \pi$

17. Which of these sequences converges quadratically?

   a. $1/n^2$

   b. $1/2^{2^n}$

   c. $1/\sqrt{n}$

   d. $1/e^n$

   e. $1/n^n$

18. Find the conditions on α to ensure that the iteration

$$x_{n+1} = x_n - \alpha f(x_n)$$

will converge linearly to a zero of f if started near the zero.

19. Prove that if r is a zero of multiplicity k of the function f, then quadratic convergence in Newton's iteration will be restored by making this modification:

$$x_{n+1} = x_n - kf(x_n)/f'(x_n)$$

20. (Continuation) In the course of using Newton's method, how can a multiple zero be detected by examining the behavior of the points $(x_n, f(x_n))$?

21. **Halley's method** for solving the equation $f(x) = 0$ uses the iteration formula

$$x_{n+1} = x_n - \frac{f_n f_n'}{(f_n')^2 - (f_n f_n'')/2}$$

where $f_n = f(x_n)$, and so on. Show that this formula results when Newton's iteration is applied to the function $f/\sqrt{f'}$.

22. Starting with (0, 0, 1), carry out an iteration of Newton's method for nonlinear systems on

$$\begin{cases} xy - z^2 = 1 \\ xyz - x^2 + y^2 = 2 \\ e^x - e^y + z = 3 \end{cases}$$

Explain the results.

23. Perform two iterations of Newton's method on these systems.

a. Starting with (0, 1)

$$\begin{cases} 4x_1^2 - x_2^2 = 0 \\ 4x_1x_2^2 - x_1 = 1 \end{cases}$$

b. Starting with (1, 1)

$$\begin{cases} xy^2 + x^2y + x^4 = 3 \\ x^3y^5 - 2x^5y - x^2 = -2 \end{cases}$$

COMPUTER PROBLEMS 3.2

1. Write a computer program to solve the equation $x = \tan x$ by means of Newton's method. Find the roots nearest 4.5 and 7.7.

2. (Continuation) Write and test a program to compute the first ten roots of the equation $\tan x = x$. (This is much more difficult than the preceding computer problem.) *Cultural note:* If $\lambda_1, \lambda_2, \ldots$ are *all* the positive roots of this equation, then $\sum_{i=1}^{\infty} \lambda_i^{-2} = 1/10$. (*Amer. Math. Monthly*, Oct. 1986, p. 660.)

3. Find the positive minimum point of the function $f(x) = x^{-2} \tan x$ by computing the zeros of f' using Newton's method.

4. Write a brief computer program to solve the equation $x^3 + 3x = 5x^2 + 7$ by Newton's method. Take ten steps starting at $x_0 = 5$.

5. The equation $2x^4 + 24x^3 + 61x^2 - 16x + 1 = 0$ has two roots near 0.1. Determine them by means of Newton's method.

6. In the first example of this section, investigate the sensitivity of the root to perturbations in the constant term.

7. For the function $f(z) = z^4 - 1$, carry out the complex Newton's method using as starting values all grid points on the mesh with uniform spacing 0.1 in the circle $|z| < 2$ in the complex plane. Assign the same color to all grid points that engender sequences

convergent to the same zero. Display the resulting four-color mesh on a color graphics computer terminal or on a color plotter.

8. Program the Newton algorithm in complex arithmetic, and test it on these functions with the given starting points.

   a. $f(z) = z^2 + 1, \quad z = 3 + i$

   b. $f(z) = z + \sin z - 3, \quad z = 2 - i$

   c. $f(z) = z^4 + z^2 + 2 + 3i, \quad z = 1$

9. Program and test Steffensen's method (Problem **3.2.4**, p. 90) using the test functions in Computer Problems **3.2.1–2** (p. 92).

10. The polynomial $p(x) = x^3 + 94x^2 - 389x + 294$ has zeros 1, 3, and -98. The point $x_0 = 2$ should therefore be a good starting point for computing either of the small zeros by the Newton iteration. Carry out the calculation and explain what happens.

11. Carry out five iterations of the complex Newton's method applied to the complex-valued function $f(z) = 1 + z^2 + e^z$, using the starting value $z_0 = -1 + 4i$.

12. Find the first four zeros of the function $f(z) = 1 + z^2 + e^z$ ordered according to increasing complex absolute values. How do you know these are the *first* four zeros and that you have not missed some?

13. Carry out five iterations of Newton's method (for two nonlinear functions in two variables) on the following system:

$$\begin{cases} f_1(x, y) = 1 + x^2 - y^2 + e^x \cos y \\ f_2(x, y) = 2xy + e^x \sin y \end{cases}$$

Use starting values $x_0 = -1$ and $y_0 = 4$. Is this problem related to Computer Problem **11** above, and do they have similar numerical behavior? Explain.

14. Using Newton's method, find the roots of the nonlinear systems.

   a. $\begin{cases} 4y^2 + 4y + 52x = 19 \\ 169x^2 + 3y^2 + 111x - 10y = 10 \end{cases}$

   b. $\begin{cases} x + e^{-1x} + y^3 = 0 \\ x^2 + 2xy - y^2 + \tan(x) = 0 \end{cases}$

3.3 Secant Method

Recall that the Newton iteration is defined by the equation

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{1}$$

One of the drawbacks of Newton's method is that it involves the derivative of the function whose zero is sought. To overcome this disadvantage, a number of methods have been proposed. For example, Steffensen's iteration (Problem **3.2.4**, p. 90).

$$x_{n+1} = x_n - \frac{[f(x_n)]^2}{f(x_n + f(x_n)) - f(x_n)}$$

In all scientific computing tasks, established software packages are recommended over programs written by oneself, except for special applications. For the root-finding problem, the best software is rather complicated because it must incorporate several procedures to secure both global convergence and locally rapid convergence. These goals conflict somewhat with each other, as mentioned previously.

Unfortunately, there are too many methods, and variations of them, to include them all in this book. Examples of algorithms of interest that we do not discuss are ones developed by Brent [1973], Dekker [1969], and Le [1985]. They combine the good features of the bisection and secant methods and assume nothing about the function whose root is sought, other than $f(a)f(b) \leq 0$. The idea behind Brent's method is to combine the bisection method with the secant method and include an inverse quadratic interpolation to get a more robust procedure. Le's algorithm combines the bisection method with second- and third-order methods that use derivative estimates from the objective function values. The interested reader is encouraged to refer to the papers cited above for a complete description of these algorithms. Since the resulting codes are rather long and complicated, we recommend obtaining the software for them via the Internet. Our general advice, to use established and proven software whenever possible, holds true here. Usually such software is freely available and has been carefully written and tested. For example, using a browser to the World Wide Web, we can connect to the address `http://gams.nist.gov`, which is a "Guide to Available Mathematical Software." A problem decision tree is found there, and we go down it from *F. Solution of Nonlinear Equations* to *F1. Single Equation* to *F1b. Nonpolynomial*. There we find that on `Netlib` a version of Brent's algorithm in the C-language (for finding a minimum or a zero of a univariate function within a given range) is available. (See also Appendix A, "An Overview of Mathematical Software.")

PROBLEMS 3.3

1. Establish Equation (4).
2. In the secant method, prove that if $x_n \to q$ as $n \to \infty$, and if $f'(q) \neq 0$, then q is a zero of f.
3. Using Taylor expansions for $f(x+h)$ and $f(x+k)$, derive the following approximation to $f'(x)$:
$$f'(x) \approx \frac{k^2 f(x+h) - h^2 f(x+k) + (h^2 - k^2) f(x)}{(k-h)kh}$$
4. If the secant method is applied to the function $f(x) = x^2 - 2$, with $x_0 = 0$ and $x_1 = 1$, what is x_2?
5. What is x_2 if $x_0 = 1$, $x_1 = 2$, $f(x_0) = 2$, and $f(x_1) = 1.5$ in an application of the secant method?
6. The relation of asymptotic equality between two sequences is written $x_n \sim y_n$ and signifies that $\lim_{n\to\infty}(x_n/y_n) = 1$. Prove that if $x_n \sim y_n$, $u_n \sim v_n$, and $c \neq 0$, then
   a. $cx_n \sim cy_n$
   b. $x_n^r \sim y_n^r$
   c. $x_n u_n \sim y_n v_n$

d. if $y_n \sim u_n$, then $x_n \sim v_n$

e. $y_n \sim x_n$

7. Prove that the formula for the secant method can be written in the form

$$x_{n+1} = \frac{f(x_n)x_{n-1} - x_n f(x_{n-1})}{f(x_n) - f(x_{n-1})}$$

Explain why this formula is inferior to Equation (3) in practice.

8. (A polynomial of very high degree) An **annuity** is a fund of money to which payments (not necessarily equal in value) are made at regular intervals of time. In one form of annuity, the fund is invested at a constant rate of interest, r, per interval. The interest is compounded at the end of each interval. Let the payments be in amounts $a_1, a_2, \ldots$. Let V_i denote the accumulated value of the annuity, computed just after payment a_i has been made. Then $V_1 = a_1$ and

$$V_i = V_{i-1}(1 + r) + a_i \qquad (i = 2, 3, \ldots)$$

The factor $(1 + r)$ accounts for the interest rV_{i-1} earned on V_{i-1} during one time interval. Prove that $V_n = \sum_{i=1}^{n} a_i x^{n-i}$, where $x = 1 + r$. (Computer Problem 3.3.6, p. 100, is related.)

9. Two men follow two different savings strategies over a period of 44 years. The first saves \$1000 per year for six years and leaves the account to earn interest for the remaining 38 years. The second invests nothing in the first six years, but thereafter saves \$1000 per year. At the end of 44 years, the values of the two accounts are the same. Assume the earnings in both accounts are compounded annually at the same rate of interest. What is the rate and what is the value of each account?

10. How does the interchange in the secant method pseudocode affect the error analysis? Write out the details for a modified error analysis.

COMPUTER PROBLEMS 3.3

1. Write a subprogram to carry out the secant method on a function f, assuming that two starting points are given. Test the routine on these functions.

   a. $\sin(x/2) - 1$

   b. $e^x - \tan x$

   c. $x^3 - 12x^2 + 3x + 1$

2. Program and test a refinement of the secant method that uses the approximate value of $f'(x)$ given in Problem 3.3.3 (p. 98). That is, use this approximation for $f'(x)$ in the formula for the Newton method. Three starting points are now needed. The first two can be arbitrary, and the third can be obtained by the secant method.

3. Write subprograms for carrying out the bisection method, Newton's method, and the secant method. They should apply to an arbitrary function F. In each case, the calling sequence should include a parameter M for the maximum number of steps the user will allow. The user should be able to specify also the accuracy desired (ε and δ, as in the pseudocode in this section). These codes should be in single precision.

a. Test your subprograms on the function

$$f(x) = \tan^{-1} x - \frac{2x}{1+x^2}$$

Try to obtain the positive zero with full machine precision.

b. Use the zero found in part a as the starting point for Newton's method on the function

$$g(x) = \tan^{-1} x$$

c. Combine two of the programs that you have written to create a hybrid method that has good global and local characteristics.

4. Select a routine from the program library available on your computer for solving an equation $f(x) = 0$, without using derivatives. Test the code on these functions on the intervals given.

a. $x^{20} - 1$ on $[0, 10]$

b. $\tan x - 30x$ on $[1, 1.57]$

c. $x^2 - (1 - x)^{10}$ on $[0, 1]$

d. $x^3 + 10^{-4}$ on $[-0.75, 0.5]$

e. $x^{19} + 10^{-4}$ on $[-0.75, 0.5]$

f. x^5 on $[-1, 10]$

g. x^9 on $[-1, 10]$

h. xe^{-x^2} on $[-1, 4]$

(See Nerinckx and Haegemans [1976].)

5. Program and test the secant algorithm using the same example as in the text. Then repeat the computation using 3 and 10 as the initial points. Explain what happened.

6. (Refer to Problem **3.3.8**, p. 99.) A succession of 60 monthly payments is made into an annuity. In the first to fifth years, the payments are, respectively, \$200, \$275, \$312, \$380, and \$400. Just after the last payment has been made, the accumulated value of the annuity is \$24,738. What was the monthly rate of interest? Use the secant method to find the zero of the polynomial that arises.

3.4 Fixed Points and Functional Iteration

Newton's method and Steffensen's method are examples of procedures whereby a sequence of points is computed by a formula of the form

$$x_{n+1} = F(x_n) \qquad (n \geq 0) \tag{1}$$

The algorithm defined by such an equation is called **functional iteration**. In Newton's method, the function F is given by

$$F(x) = x - \frac{f(x)}{f'(x)}$$