Newton's method is very useful in problems in which $f'(x)$ is easily evaluated. [Such is the case where $f(x)$ is a polynomial as we shall see in Section 4.4.] We shall illustrate here a case of particular importance. Suppose we are given a constant $c > 0$ and wish to find the real, positive kth root of c. We then let $f(x) = x^k - c$, and the Newton iteration becomes

$$x_{n+1} = x_n - \frac{x_n^k - c}{kx_n^{k-1}} = \frac{(k-1)x_n + c/x_n^{k-1}}{k}. \tag{4.5}$$

EXAMPLE 4.4. In order to approximate $\sqrt{2}$, let $f(x) = x^2 - 2$ and $x_0 = 1$. Formula (4.5) reduces in this case to $x_{n+1} = (x_n + 2/x_n)/2$. Then to eight significant digits, $x_1 =$ 1.5000000, $x_2 = 1.4166667$, $x_3 = 1.4142156$, and $x_4 = 1.4142135$. In fact, $\sqrt{2} = 1.4142136$ (to eight places).

For practical computational purposes, some modifications of Newton's method are desirable. These modifications are based on the observation that although Newton's method converges rapidly for a starting value near a simple root of $f(x) = 0$, the method may diverge rapidly (or exhibit other erratic behavior) in the presence of a zero of $f'(x)$ or for a starting value somewhat removed from the root. In order to account for this fact in a general root-finding program, we might include a test of whether $|f(x_{n+1})| < |f(x_n)|$ at each step (such a test would determine whether it is profitable to continue the iteration using Newton's method). A somewhat more comprehensive program might include a combination of bisection and Newton's method. For example, suppose $f(a)f(b) < 0$ and $m = (a + b)/2$. If $f(m)f(b) < 0$, then there is a zero of $f(x)$ in (m, b). If Newton's method starting with $x_0 = b$ (or $x_0 = a$) does not produce an estimate x_1 in (m, b), then x_1 can be rejected and several steps of the bisection method can be executed before Newton's method is tried again. Similar modifications may also be made to other "fast" procedures, such as the secant method, which do not possess the root-bracketing property of bisection.

PROBLEMS, SECTION 4.3.3

1. Apply Newton's method to $f(x) = x^3 - 2x^2 + 2x - 1$; use $x_0 = 0$ and $x_0 = 10$. Terminate the iteration if $|f(x_n)| \le 10^{-6}$ or $|x_{n+1} - x_n| \le 10^{-6}$ or $n \ge 25$. Print each iterate x_n and $f(x_n)$. The root is $s = 1$; so $e_n = x_n - 1$. For each n, also print e_n and e_n^2, and verify that $e_{n+1} \simeq e_n^2$.
2. In Problem 8 it is shown that the errors in Newton's method satisfy $e_{n+1} \simeq Ke_n^2$ where $K = f''(s)/2f'(s)$ [under the assumption that $f(s) = 0$ and $f'(s) \neq 0$]. For $f(x)$ in Problem 1, verify that $K = 1$.
3. Repeat Problem 1 for $f(x) = x^4 - 4x^3 + 6x^2 - 4x + 1$; this time, print x_n, $f(x_n)$, e_n, and $.75\, e_n$ ($s = 1$ is a root). Note that $e_{n+1} \simeq .75\, e_n$. By Problem 9, $e_{n+1} \simeq Ke_n$ when s is a root of multiplicity p where $p \ge 2$ and $K = 1 - 1/p$. Verify that $s = 1$ is a root of multiplicity 4.
4. To see that the estimates from Newton's method may have to be monitored, consider $f(x) = \sin 15x - .5 \sin 14x$. By Problem 6, Section 4.2, $f(x)$ has zeros in $[k\pi/15,$

$(k + 1)\pi/15]$ for $1 \le k \le 13$. Try to find each of these 13 zeros; use $x_0 = k\pi/15$, $1 \le k \le 13$, and the termination criteria in Problem 1. Observe that many of the zeros found are not in the desired range.

5. Design a subroutine that incorporates bisection and Newton's method. The input should include an interval where $f(x)$ changes sign and should use two bisections when a Newton iterate strays outside the current interval. Test your program on the functions in Problems 1 and 4.

6. Use Theorem 4.4 and formula (4.1) to prove Theorem 4.6, with the additional assumption that $f'''(x)$ is continuous.

7. Prove that the tangent line to the graph of $y = f(x)$ at the point $(x_n, f(x_n))$ intersects the x-axis when $x = x_n - f(x_n)/f'(x_n)$.

8. Theorem 4.6 can be proved without the assumption about $f'''(x)$ in Problem 6. First, Theorem 4.4 implies there is an $\varepsilon > 0$ such that $\{x_i\} \to s$ whenever $|x_0 - s| < \varepsilon$ (why?). Now, given that $\{e_n\} \to 0$, show that

$$\lim_{n\to\infty} \frac{e_{n+1}}{e_n^2} = K$$

where $K = f''(s)/2f'(s)$. [Hint: Consider $x_{n+1} - s = x_n - s - f(x_n)/f'(x_n)$, and use the expansion $f(s) = f(x_n) + f'(x_n)(s - x_n) + f''(\theta_n)(s - x_n)^2/2!$ where θ_n is between x_n and s.]

9. Assume that $f(s) = f'(s) = \cdots = f^{(p-1)}(s) = 0$, $f^{(p)}(x)$ is continuous, and $f^{(p)}(s) \neq 0$. Let $g(x) = x - f(x)/f'(x)$, and show that $g'(s) = 1 - 1/p$. [Hint: Let $h = x - s$, and expand both $f(x)$, and $f'(x)$ in a Taylor's expansion around s. Then let $h \to 0$.]

10. To illustrate the necessity of x_0 being "sufficiently close" to s for the convergence of the Newton iteration, we define

$$f(x) = \begin{cases} \sin x, & -\pi/2 \le x \le \pi/2 \\ 1, & x \ge \pi/2 \\ -1, & x \le -\pi/2. \end{cases}$$

Then $f'(x) = \begin{cases} \cos x, & -\pi/2 \le x \le \pi/2 \\ 0, & \text{otherwise.} \end{cases}$

Let t^*, $0 < t^* < \pi/2$, satisfy $\tan t^* = 2t^*$. (Since $\tan \pi/4 = 1 < \pi/2 = 2(\pi/4)$ and $\infty = \tan \pi/2 > \pi = 2(\pi/2)$, we know that such a t^* exists and $\pi/4 < t^* < \pi/2$.)

a) Assume that $x_0 = t^*$; then evaluate the rest of the Newton method iterates. Are they converging to $s = 0$? Are they diverging?

b) What happens to the Newton method iterates if $t^* < x_0 < \pi/2$?

c) What happens to the Newton method iterates if $0 < x_0 < t^*$?

11. Suppose $f(x) = (x - r_1)(x - r_2)\cdots(x - r_n)$ where $r_1 < r_2 < \cdots < r_n$. That is, $f(x)$ is an nth degree polynomial with n distinct real roots and with leading coefficient equal to 1. By a geometric argument, convince yourself that if $x_0 > r_n$, then the sequence $\{x_i\}$ generated by Newton's method satisfies

$$r_n < \cdots < x_{i+1} < x_i < \cdots < x_0 \qquad \text{for } i = 1, 2, \ldots .$$

Prove this mathematically, using Rolle's Theorem to observe that $f'(x) > 0$ for $x \ge r_n$.

12. As an extreme case of a function for which Newton's method is slowly convergent, consider $f(x) = (x - \alpha)^n$ for n some positive integer and α some real number. Show that Newton's method generates the sequence

$$x_{i+1} = (1 - 1/n)x_i + \alpha/n,$$

and then show that $x_{i+1} - \alpha = (1 - 1/n)(x_i - \alpha)$. This is a special case of Problem 9 above.

4.3.4. The Secant Method

In general Newton's method converges much faster than the bracketing methods, but it has serious disadvantages such as how close x_0 must be to s before convergence and the need to evaluate $f'(x_n)$, for each n. This derivative evaluation can be quite a cumbersome task. The secant method is, in a way, a compromise between Newton's method and the bracketing methods. The rate of convergence of the secant method is stronger than linear (called *superlinear*), but not quadratic. This fact, plus the fact that it does not require derivative evaluations, makes it a very attractive, practical method.

The secant method iteration comes directly from the Newton iteration by simply replacing $f'(x_n)$ by the difference quotient $(f(x_n) - f(x_{n-1}))/(x_n - x_{n-1})$. Note that when x_n and x_{n-1} are "close," then this difference quotient is an approximation to $f'(x_n)$. The secant method is represented by the following algorithm.

Given $f(x)$ such that $f(s) = 0$, let x_{-1} and x_0 be initial guesses for s. Then for $n \geq 0$,

$$x_{n+1} = x_n - \frac{f(x_n)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})} = \frac{f(x_n)x_{n-1} - f(x_{n-1})x_n}{f(x_n) - f(x_{n-1})}. \qquad (4.6)$$

This algorithm should remind the reader of the *Regula Falsi* method. In fact if $x_{-1} = a$ and $x_0 = b$ bracket s, then x_1 is generated by exactly the same formula that generates the first iterate of *Regula Falsi*. (See Problem 1.) However, x_2

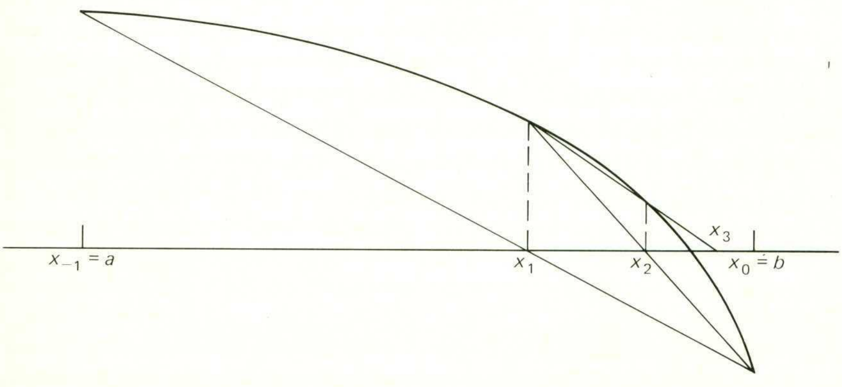

Figure 4.8 Secant method.

will not (in general) be the second iterate of *Regula Falsi* since x_0 and x_1 will not necessarily bracket the root. This point is illustrated in Fig. 4.8, which has the same object function as Fig. 4.1. We further note that since x_{n+1} depends explicitly on x_{n-1} and x_n, the secant method is not a fixed-point iteration although directly derived from the Newton iteration, which is. The secant method does have the property, similar to the fixed-point iteration, that if $x_{n-1} \neq s$ but $x_n = s$, then $x_{n+1} = s$. For the secant iteration to be well defined, we must assume that $f(x_n) - f(x_{n-1}) \neq 0$.

EXAMPLE 4.5. The secant method was programmed in single precision for $f(x) = \cos(x) - x$ with $x_0 = 0$ and $x_1 = 1$. Note from Eq. (4.6) that there are two mathematically equivalent ways to generate the sequence $\{x_n\}$:

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

Form 2 $$x_{n+1} = \frac{f(x_n)x_{n-1} - f(x_{n-1})x_n}{f(x_n) - f(x_{n-1})}.$$

Most numerical analysts feel that Form 1 is preferable to Form 2 and is less subject to rounding error. This particular example was computed using Form 1. (See Table 4.5.)

TABLE 4.5

x_i	$f(x_i)$
0.0000000E 00	0.1000000E 01
0.1000000E 01	−0.4596977E 00
0.6850733E 00	0.8929920E−01
0.7362989E 00	0.4660129E−02
0.7391192E 00	−0.5722045E−04
0.7390850E 00	0.5960464E−07

To analyze the rate of convergence for the secant method, let us suppose that $f''(x)$ is continuous, $s \neq x_{n-1} \neq x_n$; and let us define $e_n = s - x_n$ for all n. Then after algebraic reduction,

$$\begin{aligned} e_{n+1} = s - x_{n+1} &= \frac{f(x_n)e_{n-1} - f(x_{n-1})e_n}{f(x_n) - f(x_{n-1})} \\ &= \frac{f(x_n)e_{n-1} - f(x_{n-1})e_n}{x_{n-1} - x_n} \cdot \frac{x_{n-1} - x_n}{f(x_n) - f(x_{n-1})}. \end{aligned} \tag{4.7}$$

Now,

$$\begin{aligned} \frac{f(x_n)e_{n-1} - f(x_{n-1})e_n}{x_{n-1} - x_n} &= e_n e_{n-1}\frac{f(x_n)/e_n - f(x_{n-1})/e_{n-1}}{x_{n-1} - x_n} \\ &= e_n e_{n-1}\left(\frac{\dfrac{f(x_n) - f(s)}{x_n - s} - \dfrac{f(x_{n-1}) - f(s)}{x_{n-1} - s}}{x_n - x_{n-1}}\right) \\ &\equiv e_n e_{n-1} f[x_n, s, x_{n-1}]. \end{aligned}$$

Let $G(x) = (f(x) - f(s))/(x - s)$; then by the mean-value theorem, $f[x_n, s, x_{n-1}] = (G(x_n) - G(x_{n-1}))/(x_n - x_{n-1}) = G'(\zeta_n)$. Now

$$G'(x) = \frac{f'(x)(x - s) + f(s) - f(x)}{(x - s)^2}$$

and

$$f(s) = f(x) + f'(x)(s - x) + \frac{f''(\eta)}{2}(s - x)^2$$

by Taylor's Theorem and the continuity of $f''(x)$. Putting these two equations together, we get

$$G'(x) = \frac{f''(\eta)}{2}, \qquad \text{or} \qquad f[x_n, s, x_{n-1}] = G'(\zeta_n) \equiv \frac{f''(\eta_n)}{2}. \tag{4.8}$$

Thus from Eqs. (4.7) and (4.8) and the mean-value theorem,

$$\begin{aligned} e_{n+1} &= e_n e_{n-1} f[x_n, s, x_{n-1}](x_{n-1} - x_n)/(f(x_n) - f(x_{n-1})) \\ &= e_n e_{n-1}\left(\frac{f''(\eta_n)}{2}\right)\left(\frac{-1}{f'(\xi_n)}\right) \end{aligned} \tag{4.9}$$

where both η_n and ξ_n lie in the smallest interval containing x_{n-1}, x_n, and s. With the aid of (4.9) we are able to prove the following local convergence theorem for the secant method.

Theorem 4.7

Let $f(s) = 0$, $f'(s) \neq 0$; and let $f''(x)$ be continuous in a neighborhood of s. Then there exists an $\varepsilon > 0$ such that if $x_{-1}, x_0 \in I_\varepsilon \equiv [s - \varepsilon, s + \varepsilon]$, then the secant method converges to s.

Proof. In this proof, we will let M_α denote an upper bound for $|f''(x)/f'(x')|$ where x and x' are any points in $[s - \alpha, s + \alpha]$. Since $f''(x)$ and $f'(x)$ are continuous at s and since $f'(s) \neq 0$, we see, for $\beta > 0$ but sufficiently small, that the inequality $|f''(x)/f'(x')| \leq M_\beta$ is valid for x and x' in $[s - \beta, s + \beta]$. Choose $\varepsilon > 0$ such that $\varepsilon M_\beta \equiv K < 1$ where $\varepsilon < \beta$ so that $M_\varepsilon \leq M_\beta$. Let $|x_{-1} - s| \leq \varepsilon$ and $|x_0 - s| \leq \varepsilon$; then $|e_1| \leq |e_{-1}e_0|M_\beta \leq \varepsilon^2 M_\beta = \varepsilon K < \varepsilon$. Also, $|e_2| \leq |e_0 e_1|M_\beta = |e_0|(|e_0|M_\beta) < (\varepsilon K)(\varepsilon M_\beta) < \varepsilon K^2$.

Now with the induction hypotheses that $e_i < \varepsilon K^i$ and $e_{i-1} < \varepsilon K^{i-1} < \varepsilon$, we can easily see that $|e_{i+1}| < \varepsilon K^{i+1}$ and that $x_{i+1} \in [s - \varepsilon, s + \varepsilon]$ for all i. Therefore $\lim_{i\to\infty} e_i = 0$, and we have convergence on I_ε. [The reader can easily see that the inequality on e_{i+1} can be sharpened (see below), but this process was not necessary for the proof of simple convergence.] ■

It is beyond the scope of this text to establish rigorously the exact rate of convergence of the secant method [for a thorough coverage, see Ostrowski (1966)]. We can, however, present a convincing intuitive argument. Let M_β be given as in the proof above, and let $d_n \equiv M_\beta e_n$. Then

$$d_{n+1} = M_\beta e_{n+1} \leq e_{n-1} e_n M_\beta^2 = d_n d_{n-1}.$$

Let $d \equiv \max\{d_{-1}, d_0\}$; then

$$d_1 \leq d_{-1} d_0 \leq d^2, \qquad d_2 \leq d_0 d_1 \leq d^3, \qquad d_3 \leq d_1 d_2 \leq d^5;$$

and clearly by induction we see that $d_n \leq d^{\alpha n}$ where $\alpha_{n+1} = \alpha_n + \alpha_{n-1}$, $\alpha_0 = 1$, $\alpha_1 = 2$. It is left (as Problem 3) for the reader to show that these integers, α_n, are given by

$$\alpha_n = \frac{3+\sqrt{5}}{2\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right)^n - \frac{3-\sqrt{5}}{2\sqrt{5}}\left(\frac{1-\sqrt{5}}{2}\right)^n,$$

which is the famous *Fibonacci sequence* with the so-called *golden ratio*,

$$r^* = \left(\frac{1+\sqrt{5}}{2}\right).$$

The rate of convergence as shown in Ostrowski is superlinear; and under the conditions of Theorem 4.7, $\lim_{n\to\infty} (e_{n+1}/e_n^{r^*})$ exists and is usually not zero so the order of convergence is r^*. (Note: $1 < r^* < 2$.)

4.3.5. Newton's Method in Two Variables

In this section, we will derive Newton's method for solving a system of nonlinear equations, particularly the system of two equations in two unknowns:

$$\begin{aligned} f(x, y) &= 0 \\ g(x, y) &= 0. \end{aligned} \tag{4.10}$$

In (4.10), $f(x, y)$ and $g(x, y)$ are real-valued functions of two variables. We will consider this problem in more detail in Section 4.5; we are content in this section to present an intuitive derivation. As we shall see in Section 4.4.2, Newton's method for the special case of the system, (4.10), can be used to find zeros of polynomials where the zeros may be either real or complex.

When solving (4.10), we are looking for a simultaneous solution, that is, numbers s and t such that

$$\begin{aligned} f(s, t) &= 0 \\ g(s, t) &= 0 \end{aligned}$$

In order to derive Newton's method, let us suppose that we have approximations x_0 and y_0 to s and t, respectively. Expanding $f(x, y)$ and $g(x, y)$ in a Taylor's expansion (in two variables) about the point (x_0, y_0), we find

$$\begin{aligned} f(x, y) &= f(x_0, y_0) + f_x(x_0, y_0)(x - x_0) + f_y(x_0, y_0)(y - y_0) + R_f(x, y) \\ g(x, y) &= g(x_0, y_0) + g_x(x_0, y_0)(x - x_0) + g_y(x_0, y_0)(y - y_0) + R_g(x, y) \end{aligned} \tag{4.11a}$$

where $f_x(x_0, y_0)$ denotes the partial derivative of $f(x, y)$ with respect to x evaluated at the point (x_0, y_0), and where $R_f(x, y)$ is given by

$$R_f(x, y) = \frac{[f_{xx}(\alpha, \beta)(x - x_0)^2 + 2f_{xy}(\alpha, \beta)(x - x_0)(y - y_0) + f_{yy}(\alpha, \beta)(y - y_0)^2]}{2}$$

with the mean-value point, (α, β), being somewhere on the line segment joining the points (x, y) and (x_0, y_0). If we substitute (s, t) for (x, y) in (4.11a), we find [since (s, t) is a solution of (4.10)] that

$$\begin{aligned} 0 &= f(x_0, y_0) + f_x(x_0, y_0)(s - x_0) + f_y(x_0, y_0)(t - y_0) + R_f(s, t) \\ 0 &= g(x_0, y_0) + g_x(x_0, y_0)(s - x_0) + g_y(x_0, y_0)(t - y_0) + R_g(s, t). \end{aligned} \tag{4.11b}$$

If we now suppose that the point (x_0, y_0) is close to (s, t), then the factors $(s - x_0)^2$, $(s - x_0)(t - y_0)$, and $(t - y_0)^2$, which appear in $R_f(s, t)$ and $R_g(s, t)$, are small with respect to the first-order terms, $(s - x_0)$ and $(t - y_0)$. Thus, we consider the *linear* system of equations, (4.11c), obtained by neglecting $R_f(s, t)$ and $R_g(s, t)$:

$$\begin{aligned} 0 &= f(x_0, y_0) + f_x(x_0, y_0)(s - x_0) + f_y(x_0, y_0)(t - y_0) \\ 0 &= g(x_0, y_0) + g_x(x_0, y_0)(s - x_0) + g_y(x_0, y_0)(t - y_0). \end{aligned} \tag{4.11c}$$

If we solve (4.11c) for s and t, the resulting approximation to the solution of (4.10) should be better than (x_0, y_0). Note, however, that a solution of (4.11c) will not be precisely the pair (s, t) since Eq. (4.11c) is not the same as Eq. (4.11b). If we let (x_1, y_1) denote the solution of (4.11c), then

$$\begin{aligned} f_x(x_0, y_0)(x_1 - x_0) + f_y(x_0, y_0)(y_1 - y_0) &= -f(x_0, y_0) \\ g_x(x_0, y_0)(x_1 - x_0) + g_y(x_0, y_0)(y_1 - y_0) &= -g(x_0, y_0). \end{aligned} \tag{4.11d}$$

It is convenient to write (4.11d) in matrix form as $J_0(\mathbf{x}_1 - \mathbf{x}_0) = -\mathbf{F}(\mathbf{x}_0)$ where

$$\mathbf{x}_0 = \begin{bmatrix} x_0 \\ y_0 \end{bmatrix}, \quad \mathbf{x}_1 = \begin{bmatrix} x_1 \\ y_1 \end{bmatrix}, \quad \mathbf{F}(\mathbf{x}_0) = \begin{bmatrix} f(x_0, y_0) \\ g(x_0, y_0) \end{bmatrix},$$

$$J_0 = \begin{bmatrix} f_x(x_0, y_0) & f_y(x_0, y_0) \\ g_x(x_0, y_0) & g_y(x_0, y_0) \end{bmatrix}.$$

If $\mathbf{c}_0 = \left[\begin{smallmatrix} u_0 \\ v_0 \end{smallmatrix}\right]$ is the solution of $J_0\mathbf{x} = -\mathbf{F}(\mathbf{x}_0)$, then $\mathbf{x}_1 = \mathbf{x}_0 + \mathbf{c}_0$ is an updated (or corrected) estimate to (s, t).

We note that (4.11c) is normally written in an equivalent form (obtained by multiplying by J_0^{-1}): $\mathbf{x}_1 = \mathbf{x}_0 - J_0^{-1}\mathbf{F}(\mathbf{x}_0)$. Having the new estimate, $\mathbf{x}_1$, to the solution, we repeat this correcting process, which leads to the iteration

$$\mathbf{x}_{i+1} = \mathbf{x}_i - J_i^{-1}\mathbf{F}(\mathbf{x}_i), \qquad i = 0, 1, \ldots . \tag{4.11e}$$

The algorithm described by (4.11e) is Newton's method in several variables. The matrix, J_i, of partial derivatives evaluated at $\mathbf{x}_i$ is called the *Jacobian* matrix and plays the role of a derivative (see Section 4.5). Thus the form of Newton's method displayed in (4.11e) is similar to Newton's method for a single function of one variable. This algorithm and variations of it are the basis for Bairstow's method (Section 4.4.2) and also can be effectively used in optimization problems (Appendix) and collocation methods for differential equations (Chapter 7) as well as in the problem of finding solutions to systems of nonlinear equations.

PROBLEMS, SECTION 4.3.5

1. If $x_{-1} = a$ and $x_0 = b$ where $f(a)f(b) < 0$, verify that the first iteration of the secant method is the same as for *Regula Falsi*.
2. Note that Eq. (4.9) can be rewritten as

$$s - \alpha = -(s - a)(s - b)\frac{f''(\eta)}{2f'(\xi)} \tag{4.9a}$$

where α is the point where the line segment through $(a, f(a))$ and $(b, f(b))$ crosses the x-axis. Thus (4.9) can be used for an analysis of *Regula Falsi*. Suppose x_0 and x_1 are such that $f(x_0) > 0 > f(x_1)$, and suppose $f''(x)f'(x) > 0$ for $x_0 \le x \le x_1$ (see Fig. 4.1). If $x_2, x_3, \ldots, x_n, \ldots$ are the iterates of *Regula Falsi*, and if $f(s) = 0$, then
   a) show $s > x_i$ for $i = 2, 3, \ldots$;
   b) let $s - x_i = e_i$ and show (in the notation of Theorem 4.7) that $e_{i+1} \le M_\beta e_i e_0$;
   c) for $\varepsilon = \text{Max}\{|e_0|, |e_1|\}$, show $e_{i+1} \le \lambda^i \varepsilon$ where $\lambda = \varepsilon M_\beta$ (see Section 2).
3. Consider the sequence, $\{\alpha_n\}_{n=0}^{\infty}$, such that $\alpha_{n+1} = \alpha_n + \alpha_{n-1}$, $\alpha_0 = 1$, $\alpha_1 = 2$. Find the only two values of γ (γ_1 and γ_2) that satisfy $\gamma^{n+1} = \gamma^n + \gamma^{n-1}$ for *all* integers $n \ge 0$. Verify that $c_1\gamma_1^n + c_2\gamma_2^n \equiv \alpha_n$ satisfies the equation $\alpha_{n+1} = \alpha_n + \alpha_{n-1}$ for any two values of c_1 and c_2. Verify that for $\alpha_0 = 1$ and $\alpha_1 = 2$, $c_1 = (3 + \sqrt{5})/2\sqrt{5}$ and $c_2 = -(3 - \sqrt{5})/2\sqrt{5}$.
4. Let $f(x) = x^2 - 2$ and $[a, b] \equiv [1, 3]$. Compute the first four iterates of both the secant method and *Regula Falsi*; note how they differ.
5. Program the secant method and test your program on the function $f(x) = \cos(x) - x$.
6. Program Newton's method for two variables and test your program on the system

$$x^2 + y^2 - 9 = 0$$

$$x + y - 1 = 0.$$

(This sytem has two solutions where a solution represents the intersection of the line and the circle described by the equations.)
7. Let $p(x) = x^3 - x^2 - x - 2$ and let u and v be any real numbers.
   a) Verify that $p(x) = (x^2 - ux - v)(x + u - 1) + f_1(u, v)(x - u) + f_2(u, v)$ where

$$f_1(u, v) = u^2 - u + v - 1 \qquad \text{and} \qquad f_2(u, v) = u^3 - u^2 + 2uv - u - v - 2.$$

Obviously, $p(x) = (x^2 - u^*x - v^*)(x + u^* - 1)$ if and only if u^* and v^* are solutions of $f_1(u^*, v^*) = 0 = f_2(u^*, v^*)$ (see Section 4.4.2). Thus if we know u^* and v^*, we can find two zeros of $p(x)$ by merely applying the quadratic formula to find the two zeros of $x^2 - u^*x - v^*$. Note that even if these two zeros are complex, we need not use any complex arithmetic in finding them.

b) Let $\mathbf{x}_0 \equiv (u_0, v_0) \equiv (0, 0)$, and apply Newton's method for four iterations to find approximations u_4 and v_4 for u^* and v^*, respectively. Apply the quadratic formula to $x^2 - u_4x - v_4 = 0$ to obtain approximations for two zeros of $p(x)$. [The true answers are $(u^*, v^*) = (-1, -1)$, and the resulting zeros are $\frac{1}{2}(-1 \pm \sqrt{3}i)$. This problem presents the basic idea of Bairstow's method, which is presented in Section 4.4.2.]

4.4 ZEROS OF POLYNOMIALS

In Section 4.3, it was noted that a disadvantage of Newton's method was that the derivative of the object function, $f(x)$, had to be calculated at each iterate. For many functions, the calculation of $f'(x)$ is a formidable task. Such is not true, however, if the function is an nth degree polynomial,

$$p(x) = a_0x^n + a_1x^{n-1} + \cdots + a_{n-1}x + a_n, \qquad a_0 \neq 0. \tag{4.12}$$

Finding the zeros of an nth degree polynomial is one of the oldest and most studied problems in mathematics, and is also one of the more important problems in applied mathematics and has extensive practical applications. For $n = 1$, the only zero of $p(x)$ is given by $r = -a_1/a_0$. If $n = 2$, it is well known that the zeros are given by the quadratic formula,

$$r = \frac{-a_1 \pm \sqrt{a_1^2 - 4a_0a_2}}{2a_0}. \tag{4.13}$$

There are similar, but more cumbersome formulas for $n = 3$ and $n = 4$. What makes the problem so difficult in general is that for $n \geq 5$ there is *no* algebraic formula such as (4.13) that gives the zeros of $p(x)$ in terms of the coefficients. Thus we are forced to develop numerical procedures to approximate the zeros of $p(x)$. There are numerous such numerical procedures in the literature; but because of space and time considerations, we shall concentrate on just three—the Newton, Bairstow, and inverse power methods. (There is no reason, however, why the other methods we have discussed, such as the secant method, cannot be used for polynomials.) We shall also limit ourselves to the case in which all of the coefficients a_i in (4.12) are real.

Before proceeding further, we shall develop some basic and well-known theory about polynomials that is necessary for understanding and utilizing numerical root-finding techniques. The most basic result, which we recall from Chapter 1, is the *Fundamental Theorem of Algebra*.

Theorem 4.8

Given $p(x)$ as in (4.12) with $n \geq 1$, there exists at least one value r (possibly complex) such that $p(r) = 0$.

Given an r_1 such that $p(r_1) = 0$, it is then easily shown (Problem 1) that $p(x)$ can be written as $p(x) = (x - r_1)q_1(x)$ where $q_1(x)$ is an $(n - 1)$st degree polynomial. Applying Theorem 4.8 to $q(x)$, we obtain a value r_2 (not necessarily distinct from r_1) such that $q_1(r_2) = 0$. Thus there exists an $(n - 2)$nd degree polynomial $q_2(x)$ such that $q_1(x) = (x - r_2)q_2(x)$; so $p(x) = (x - r_1)(x - r_2)q_2(x)$. Repeating this process, we finally arrive at n values $r_1, r_2, \ldots, r_n$ such that $p(r_i) = 0, 1 \leq i \leq n$. Furthermore it can be shown that this set of roots is unique, and so $p(x)$ can be written as

$$p(x) = a_0(x - r_1)(x - r_2)\cdots(x - r_n). \tag{4.14}$$

This argument also shows that an nth degree polynomial can have no more than n zeros. As noted above, the r_j's need not all be distinct. If any r_j appears in (4.14) exactly m times, r_j is said to have "multiplicity m." The reader may easily verify that if r_j is a root of a multiplicity m, then $p(r_j) = p'(r_j) = \cdots = p^{(m-1)}(r_j) = 0$ and $p^{(m)}(r_j) \neq 0$. Note that this statement agrees with our earlier definition of "multiplicity m" for a zero of an arbitrary function.

The example, $p(x) = x^2 + 1 = (x + i)(x - i)$, demonstrates that even though the coefficients a_i are real, the zeros $\{r_j\}_{j=1}^{n}$ may be complex. It is well known that complex zeros of a polynomial with real coefficients occur in conjugate pairs. To be more precise, if $r = a + ib$, $b \neq 0$, is a complex number, then $\bar{r}$ (called the *conjugate* of r) is defined by $\bar{r} = a - ib$. If z_1 and z_2 are two complex numbers, then an elementary result is that $\overline{z_1 + z_2} = \overline{z_1} + \overline{z_2}$ and $\overline{z_1 z_2} = \overline{z_1}\,\overline{z_2}$. By induction, it is easy to show that $\overline{z_1 + z_2 + \cdots + z_n} = \overline{z_1} + \overline{z_2} + \cdots + \overline{z_n}$ and $\overline{(r^k)} = (\bar{r})^k$. Finally, for any real number a, we have $\bar{a} = a$. Combining these properties for a polynomial $p(x)$ with real coefficients, we find that $\overline{p(r)} = p(\bar{r})$ for any complex number r. Thus if $p(r) = 0$, then

$$p(r) = 0 = \overline{0} = \overline{p(r)} = p(\bar{r}), \tag{4.15}$$

which shows that if r is a zero of $p(x)$, then so is $\bar{r}$. If r is a complex zero of $p(x)$ of multiplicity m, then $\bar{r}$ is also a zero of $p(x)$ of multiplicity m. This result follows since $p^{(i)}(x)$ is a polynomial with real coefficients for $i = 1, 2, \ldots, m - 1$; and therefore if $p^{(i)}(r) = 0$, then $p^{(i)}(\bar{r}) = 0$. Note that this equation implies that if n is odd, $p(x)$ must have at least one real zero. The last fundamental result we shall need here is the well-known *division algorithm*.

Theorem 4.9

Let $P(x)$ and $Q(x)$ be polynomials of degree n and m, respectively, where $1 \leq m \leq n$. Then there exists a unique polynomial $S(x)$ of degree $n - m$ and a unique polynomial $R(x)$ of degree $m - 1$ or less such that

$$P(x) = Q(x)S(x) + R(x). \tag{4.16}$$

In this formula, a polynomial of degree 0 is a constant. Thus if $Q(x)$ is a linear polynomial, the result of dividing $P(x)$ by $Q(x)$ is a quotient $S(x)$ and a remainder $R(x)$ where $R(x)$ is a constant.

PROBLEMS, SECTION 4.4

1. Let $p(x)$ be given by (4.12) and let r be a value such that $p(r) = 0$. Show that there exists a polynomial $q(x)$ of degree $n - 1$ such that $p(x) = (x - r)q(x)$. [Hint: Consider (4.16) with $Q(x) = (x - r)$.]
2. In (4.12), let $n = 4$ and $a_0 = 2$, and assume that $r_1 = 2 - 3i$ and $r_2 = -2 - 3i$ are zeros of $p(x)$. Find a_4, a_3, a_2, and a_1.
3. What are the relationships between the coefficients of (4.12) and the derivatives of p evaluated at zero. [Consider a Maclaurin expansion for $p(x)$.]
4. Using (4.16), show that if $P(r) = P'(r) = 0$, then $P(x) = (x - r)^2Q(x)$. Thus from the remarks following (4.14), r is a zero of multiplicity 2 of $P(x)$ if and only if $P(r) = P'(r) = 0$, $P''(r) \neq 0$. It should be clear that this statement extends to zeros of multiplicity $m > 2$.
5. Establish the special case of (4.16) when $Q(x)$ is the linear polynomial $Q(x) = x - \alpha$. To establish this case, let $P(x)$ be a given polynomial: $P(x) = a_0x^n + a_1x^{n-1} + \cdots + a_{n-1}x + a_n$. Set $S(x) = b_0x^{n-1} + b_1x^{n-2} + \cdots + b_{n-2}x + b_{n-1}$ where $b_0 = a_0$ and $b_j = \alpha b_{j-1} + a_j$ for $j = 1, 2, \ldots, n$. By comparing like powers in (4.16), establish the identity $P(x) = (x - \alpha)S(x) + b_n$.
6. Establish (4.16) for $Q(x) = (x - \alpha)(x - \beta)$ as follows. By Problem 5, there is $S(x)$ such that $P(x) = (x - \alpha)S(x) + R(x)$. Now by Problem 5 there is $T(x)$ such that $S(x) = (x - \beta)T(x) + R_1(x)$.
7. Apply the ideas in Problems 5 and 6 to find the quotient and remainder in (4.16) for $P(x) = x^5 - 3x^4 + 2x^2 + x - 1$ and for
   a) $Q(x) = x + 2$
   b) $Q(x) = x - 1$
   c) $Q(x) = x^2 - 5x + 6$
8. Using the ideas in Problems 5 and 6, prove Theorem 4.9.

4.4.1. Efficient Evaluation of a Polynomial and Its Derivatives

In order to use Newton's method on a polynomial $p(x)$ as given in Eq. (4.12), we must be able to evaluate $p(\alpha)$ and $p'(\alpha)$ for any α. Direct substitution of α into $p(x)$ and $p'(x)$, however, is far from the most efficient way to meet this objective. Furthermore as we have noted before, if the initial iterate x_0 of

Newton's method is not "close" to a zero, the Newton iteration may not converge. [This is obviously the case if all of the zeros of $p(x)$ are complex and x_0 is real.] Thus we need some means of "localizing" a zero, r, of $p(x)$ in order to choose x_0 "close" to r. Many of these "localization techniques" (see Section 4.4.3) require that we make a change of variable, $t = x - \alpha$, and write $p(x)$ as

$$p(x) = \beta_0(x - \alpha)^n + \beta_1(x - \alpha)^{n-1} + \cdots + \beta_{n-1}(x - \alpha) + \beta_n \quad (4.17)$$

instead of in its original form, (4.12). By a Taylor's expansion, we can write

$$p(x) = p(\alpha) + p'(\alpha)(x - \alpha) + \frac{p''(\alpha)}{2!}(x - \alpha)^2 + \cdots + \frac{p^{(n)}(\alpha)}{n!}(x - \alpha)^n. \quad (4.18)$$

Equating (4.17) and (4.18), we see that

$$\beta_j = p^{(n-j)}(\alpha)/(n - j)! \qquad \text{for } 0 \le j \le n. \quad (4.19)$$

This equation shows that it will be useful to have an efficient way of evaluating not only $p(\alpha)$ and $p'(\alpha)$, but $p^{(j)}(\alpha)$, $2 \le j \le n$, as well.

The technique we shall employ is known as *nested multiplication* or *synthetic division* and is based on the division algorithm (4.16). We first note that there is an alternative way of writing $p(x)$. For example with $n = 4$, we can write (4.12) as

$$p(x) = x(x(x(a_0x + a_1) + a_2) + a_3) + a_4. \quad (4.20)$$

We see that $p(x)$ in (4.20) can be evaluated at $x = \alpha$ by only four multiplications and four additions whereas (Problem 2) direct substitution of α into (4.12) for $n = 4$ requires at least seven multiplications and four additions (if there is no $a_i = 0$). We can easily see that Eq. (4.20) can be extended for any value of n, and this extension is given by the following algorithm.

Let $p(x)$ be given by (4.12) and let α be any constant. Let $b_0 = a_0$, and generate $\{b_j\}_{j=1}^{n}$ by

$$b_j = \alpha b_{j-1} + a_j, \qquad 1 \le j \le n;$$

then $p(\alpha) = b_n$.

This algorithm is known as synthetic division and is exactly analogous to (4.20) where $b_n = p(\alpha)$. A less intuitive but more rigorous development of synthetic division is given in Problem 3. Note that the synthetic division algorithm requires only n multiplications to form $b_n = p(\alpha)$. This method is an efficient means of evaluating $p(\alpha)$, and moreover the iteration scheme can also be used to evaluate *all* derivatives, $p^{(m)}(\alpha)$, $0 \le m \le n$.

To see this point, we consider the division algorithm (4.16) and write $p(x)$ in the form

$$p(x) = (x - \alpha)q_{n-1}(x) + r_0(x). \quad (4.21)$$

In (4.12), $a_0 \ne 0$; so $q_{n-1}(x)$ has degree $n - 1$ and its leading coefficient is a_0. Further, $r_0(x)$ is the constant $p(\alpha)$ as can be seen by setting $x = \alpha$ in (4.21).