4.3 FIXED-POINT METHODS

Two methods that normally converge more rapidly than bisection and *Regula Falsi* are Newton's method and the secant method. Although the Newton and secant methods have a simple geometric interpretation for "nice" functions (see, for instance, Figs. 4.4 and 4.8), they do not have the root-bracketing property, and do not guarantee convergence for all continuous functions as do the bisection and *Regula Falsi* methods. When they do converge, however, the Newton and secant methods are generally much faster. In order to explain these convergence properties, we shall derive these methods via a concept known as the *fixed-point problem* and illustrate them geometrically after they are derived. Another important reason for taking this approach is that it can easily be extended to solving systems of equations in several variables. Furthermore, we shall see that other problems such as the iterative methods of Chapter 2 and the predictor-corrector methods of Chapter 7 are special cases of fixed-point iterations and can be analyzed by the procedures of the next section.

To illustrate a specific fixed-point problem, we consider the geometric rationale for Newton's method as given in most calculus texts. This geometric interpretation is quite simple (see Fig. 4.4). Given an initial estimate x_0 to a root s of $f(x) = 0$, we first construct the tangent line to the curve $y = f(x)$ through the point $(x_0, f(x_0))$ and find that the equation of the tangent line is $y = f'(x_0)(x - x_0) + f(x_0)$. We then find the point x_1 where the tangent line intersects the x-axis, and x_1 is taken as the next approximation to s. The process is then repeated with x_1 playing the role of x_0; and a new approximation to s, x_2, is found. Since $x_1 = x_0 - f(x_0)/f'(x_0)$, $x_2 = x_1 - f(x_1)/f'(x_1)$, etc., we are generating the sequence

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \qquad n = 0, 1, \ldots .$$

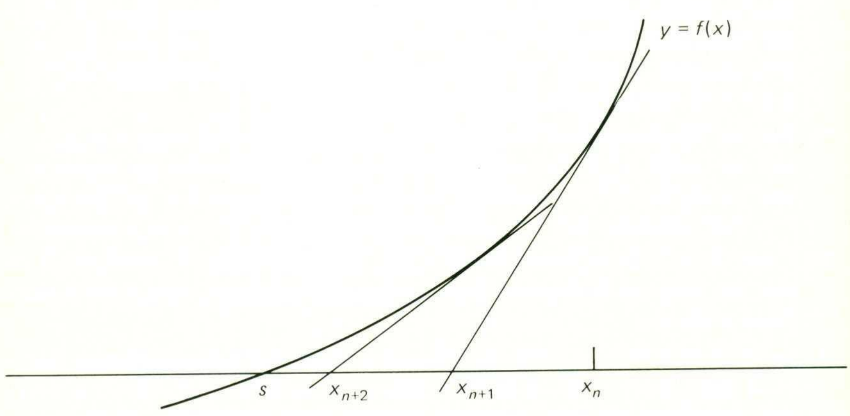

Figure 4.4 Newton's method.

Thus Newton's method is a special case of an iteration of the form $x_{n+1} = g(x_n)$ [where for the case of Newton's method, $g(x) = x - f(x)/f'(x)$]. The analysis of this general iteration, $x_{n+1} = g(x_n)$, is the topic of the next few sections.

4.3.1. The Fixed-Point Problem

Throughout this analysis let us be careful not to lose sight of our prime objective: given a function $f(x)$ where $a \le x \le b$, find values s such that $f(s) = 0$. Given such a function, $f(x)$, we now construct an auxiliary function, $g(x)$, such that $s = g(s)$ whenever $f(s) = 0$. The construction of $g(x)$ is not unique. For example, if $f(x) = x^3 - 13x + 18$, then possible choices for $g(x)$ might be (1) $g(x) = (x^3 + 18)/13$, (2) $g(x) = (13x - 18)^{1/3}$, (3) $g(x) = (13x - 18)/x^2$, and (4) $g(x) = x^3 - 12x + 18$, to list a few. In each of these cases, if $f(s) = 0$, then $s = g(s)$.

The problem of finding s such that $s = g(s)$ is known as the *fixed-point problem*, and s is said to be a *fixed point* of $g(x)$. Thus if we develop an efficient procedure for finding a fixed point for $g(x)$, $a \le x \le b$, then we automatically have an efficient procedure for finding a zero of $f(x)$, $a \le x \le b$. The fixed-point problem turns out to be quite simple, both theoretically and geometrically. It is immediate from Fig. 4.5 that $g(x)$ has a fixed point in the interval $[a, b]$ whenever the graph of $g(x)$ intersects the line $y = x$.

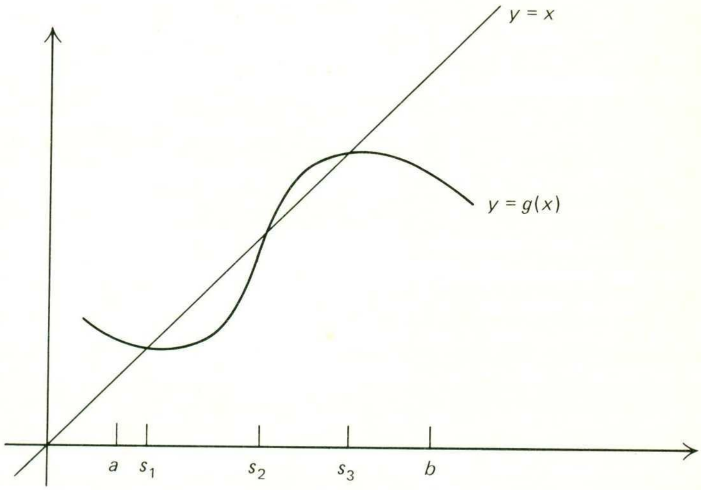

Figure 4.5 $s_i = g(s_i)$; $i = 1, 2, 3$.

It is also obvious that on any given interval, $I \equiv [a, b]$, $g(x)$ may have many fixed points or none at all. Thus, in order to ensure that $g(x)$ has a fixed point in I, certain restrictions must be placed on $g(x)$. First of all, let us assume for each $x \in I$, that $g(x) \in I$. This is plausible since, for $s \in I$, s cannot equal $g(s)$ if no

$g(x)$ belongs to I. [Hereafter this condition will be written as $g(I) \subseteq I$.] Even with this restriction, $g(x)$ may still not have a fixed point in I. For example if $g(x)$ is discontinuous, part of its graph may lie above $y = x$ and part may be below. However if we also require $g(x)$ to be continuous, we can prove that $g(x)$ must have a fixed point in I. To see this, suppose that $g(I) \subseteq I$ and $g(x)$ is continuous. Observe that $g(I) \subseteq I$ means $a \leq g(a) \leq b$ and $a \leq g(b) \leq b$. If either $a = g(a)$ or $b = g(b)$, then that endpoint is a fixed point. Let us assume that such is not the case so that $(g(a) - a) > 0$ and $(g(b) - b) < 0$. For $F(x) \equiv g(x) - x$, $F(x)$ is continuous and $F(a) > 0$ and $F(b) < 0$. Thus, by the intermediate value theorem, there exists at least one $s \in I$ such that $F(s) \equiv g(s) - s = 0$. Therefore we have established Theorem 4.1.

Theorem 4.1

If $g(I) \subseteq I$ and $g(x)$ is continuous, then $g(x)$ has at least one fixed point in I.

In order to ensure that $g(x)$ has a unique fixed point in I, we must not allow $g(x)$ to vary too rapidly. Thus we make the additional assumption that $g'(x)$ exists on I and that $|g'(x)| \leq L < 1$ for all $x \in I$. [Note that this condition implies that $g(x)$ is continuous on I.] Now let us assume that $s_1 \in I$, $s_2 \in I$, $s_1 \neq s_2$, and $s_1 = g(s_1)$ and $s_2 = g(s_2)$. Then by the mean-value theorem with ξ between s_1 and s_2,

$$|s_2 - s_1| = |g(s_2) - g(s_1)| = |g'(\xi)(s_2 - s_1)| \leq L|s_2 - s_1| < |s_2 - s_1|,$$

which is a contradiction. Thus we have proved Theorem 4.2.

Theorem 4.2

If $g(I) \subseteq I$ and $|g'(x)| \leq L < 1$ for all $x \in I$, then there exists exactly one $s \in I$ such that $g(s) = s$.

Now that we have established a condition for which $g(x)$ has a unique fixed point in I, there remains the problem of how to find it. The technique we shall employ is known as the fixed-point iteration, given by the following algorithm, and illustrated in Fig. 4.6.

Let x_0 be arbitrary in $I = [a, b]$, and let $x_{n+1} = g(x_n)$ for all $n \geq 0$.

Geometrically, this sequence can be pictured in the following way. Given any x_n of the above sequence, then $x_{n+1} = g(x_n)$ is the y-coordinate of the point $(x_n, g(x_n))$ on the graph of $y = g(x)$. Now consider the point $(x_{n+1}, x_{n+1}) = (x_{n+1}, g(x_n))$, which lies on the graph of $y = x$. The vertical projection from this point to the x-axis yields the point $(x_{n+1}, 0)$; so we know the position of x_{n+1} on the x-axis and are ready to repeat the process as illustrated in Fig. 4.6.

Note that if for any n, $x_n = s$, then $x_{n+1} = g(x_n) = g(s) = s = x_n$. Similarly, $x_m = s$, for all $m \geq n$, and the sequence stays "fixed" at s. We shall now show

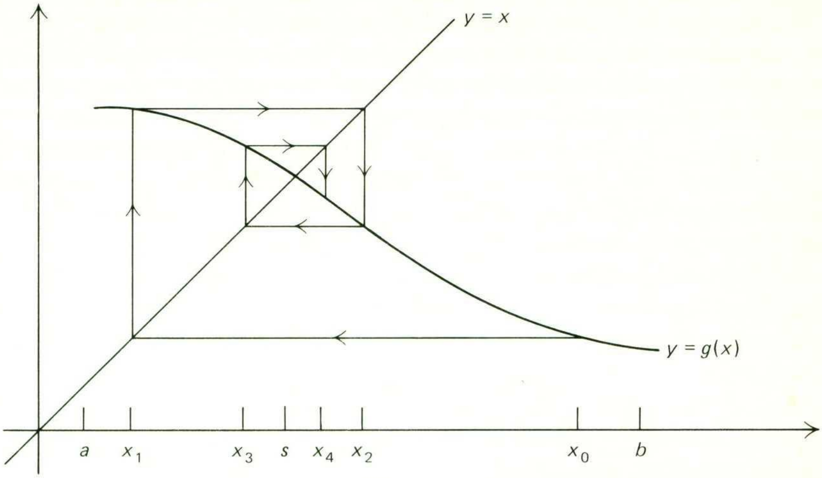

Figure 4.6 The fixed-point iteration.

that under the conditions of Theorem 4.2, the fixed-point iteration converges, and we shall give a bound on the error after n steps.

Theorem 4.3

Let $g(I) \subseteq I \equiv [a, b]$ and $|g'(x)| \leq L < 1$ for all $x \in I$. For $x_0 \in I$, the sequence $x_n = g(x_{n-1})$, $n = 1, 2, \ldots$ converges to the fixed-point s, and the nth error, $e_n \equiv x_n - s$, satisfies

$$|e_n| \leq \frac{L^n}{(1 - L)} |x_1 - x_0|.$$

Proof. By Theorem 4.2, we know there is precisely one fixed point s in I. Given any n, there exists a mean-value point ξ_n between x_{n-1} and s such that

$$|x_n - s| = |g(x_{n-1}) - g(s)| = |g'(\xi_n)|\,|x_{n-1} - s| \leq L|x_{n-1} - s|.$$

Successive repetition of this inequality yields $|x_n - s| \leq L^n|x_0 - s|$. Since $0 \leq L < 1$,

$$\lim_{n\to\infty} L^n = 0, \text{ and so } \lim_{n\to\infty} x_n = s.$$

Thus the method is convergent. To establish the error bound, note that

$$|x_0 - s| \leq |x_0 - x_1| + |x_1 - s| \leq |x_0 - x_1| + L|x_0 - s|.$$

Therefore, $(1 - L)|x_0 - s| \leq |x_1 - x_0|$; and since $|x_n - s| \leq L^n|x_0 - s|$, it follows that

$$|x_n - s| \leq L^n|x_1 - x_0|/(1 - L). \qquad \blacksquare$$

Theorem 4.3 bears a striking resemblance to Theorem 2.2 in Chapter 2, and the proofs are essentially the same. One important feature of Theorem 4.3 is that it provides an error estimate at each step and hence can be used as a test for terminating the iteration. Lacking an estimate such as the one provided by this theorem, we are left only with the possibly unattractive alternative of testing $|x_{n+1} - x_n|$ to determine whether or not to end the iteration.

Theorem 4.3 is called a "nonlocal" convergence theorem because it specifies a fixed, *known* interval, $I = [a, b]$, and displays convergence for any $x_0 \in I$. Often it is not possible to specify such an interval ahead of time, but we might still hope that the fixed-point iteration would converge if we could manage to make our initial guess, x_0, "sufficiently close" to the fixed point s. Any theorem that says, "If the initial guess is 'very close' to the solution, then the method will converge," is called a "local" convergence theorem because it does not specify beforehand precisely how close x_0 must be to s. The following is an example of a local convergence theorem.

Theorem 4.4

Let $g'(x)$ be continuous in some open interval containing s where s is a fixed point of $g(x)$. If $|g'(s)| < 1$, there exists an $\varepsilon > 0$ such that the fixed-point iteration is convergent whenever $|x_0 - s| < \varepsilon$.

Proof. Since $g'(x)$ is continuous in an open interval containing s and $|g'(s)| < 1$, then for any constant K satisfying $|g'(s)| < K < 1$, there exists an $\varepsilon > 0$ such that if $x \in [s - \varepsilon, s + \varepsilon] \equiv I_\varepsilon$, then $|g'(x)| \le K$. By the mean-value theorem, given any $x \in I_\varepsilon$, there exists an η between x and s such that $|g(x) - s| = |g(x) - g(s)| = |g'(\eta)|\,|x - s| \le K\varepsilon < \varepsilon$, and thus $g(I_\varepsilon) \subseteq I_\varepsilon$. Therefore by using I_ε in Theorem 4.3, our result is proved. ■

(Note that this theorem does not say what the value of ε is; the theorem merely assures us that there is an ε-neighborhood of s where the fixed-point iteration will converge.) Problem 7, gives a contrasting result, showing that if $|g'(s)| > 1$, then there is a neighborhood of s in which no initial guess (except $x_0 = s$) will work.

PROBLEMS, SECTION 4.3.1

1. The equation $x^3 - 13x + 18 = 0$ is equivalent to the fixed-point problem $x = g(x)$ for each of these choices:

   a) $g(x) = (x^3 + 18)/13$

   b) $g(x) = (13x - 18)^{\frac{1}{3}}$

   c) $g(x) = (13x - 18)/x^2$

   d) $g(x) = x^3 - 12x + 18$.

   Show by direct substitution that $s = 2$ is a fixed point in each case above. For which choices is $|g'(x)| < 1$?

2. The proof of Theorem 4.4 shows that if s is a fixed point of $g(x)$ and if $|g'(x)| \leq K < 1$ in $I = [s - \varepsilon, s + \varepsilon]$, then the fixed-point iteration will converge to s for any x_0 in I. For the appropriate choices in Problem 1, determine some value for ε. Having I, set $x_0 = s + \varepsilon$ and execute four steps of the fixed-point iteration.

3. Verify that the equation $x^2 - 5x + 6 = 0$ is equivalent to $x = g(x)$ for each of these choices:

   a) $g(x) = x^2 - 4x + 6$

   b) $g(x) = 5 - 6/x$

   c) $g(x) = (5x - 6)^{\frac{1}{2}}$

   d) $g(x) = (x^2 + 6)/5$.

   Find the roots of $x^2 - 5x + 6 = 0$ and repeat Problem 2 for each of the roots.

4. Verify that the equation $x^2 - c = 0$ $(c > 0)$ is equivalent to the fixed-point problem $x = (x^2 + c)/2x$. One fixed point is $s = \sqrt{c}$; verify that $0 < g'(x) < 1$ for $\sqrt{c} < x < \infty$. By Problem 5 below, the fixed-point iteration will converge for any x_0 in $(\sqrt{c}, \infty)$. Set $x_0 = c$ and execute six steps of the iteration for $c = 3, 5, 7$. Compare your estimates with the actual solution.

5. Suppose $g'(x)$ is continuous on $[s, b]$ where s is a fixed point of $g(x)$. Suppose also that $0 \leq g'(x) \leq K$ for x in $[s, b]$ where $K < 1$. Show that $[s, b]$ satisfies the hypotheses of Theorem 4.3. Also show that $s \leq \cdots \leq x_{n+1} \leq x_n \leq \cdots \leq x_1 \leq x_0$ when x_0 is in $[s, b]$.

6. Evaluate: $s = \sqrt[3]{6 + \sqrt[3]{6 + \sqrt[3]{6 + \cdots}}}$. [Hint: Let $x_0 = 0$ and consider $g(x) = \sqrt[3]{6 + x}$.]

7. Suppose $g(s) = s$, $g(x)$ is continuously differentiable in an interval containing s, and $|g'(s)| > 1$. Show there is $\varepsilon > 0$ such that if $0 < |x_0 - s| < \varepsilon$, then $|x_0 - s| < |x_1 - s|$ (thus, no matter how close x_0 is to s, the next iterate is farther away).

8. Figure 4.6 illustrates the case where $-1 < g'(s) < 0$. Draw similar graphs illustrating these cases:

$$0 \leq g'(s) < 1, \qquad 1 < g'(s), \qquad g'(s) < -1.$$

9. Let $g(x) = x^2$. From a graph (as in Problem 8), deduce for what values x_0, $-\infty < x_0 < \infty$, the iteration $x_{i+1} = g(x_i)$ will converge to a fixed point of $g(x)$ and for what values x_0 will the iteration diverge.

10. For the equation $f(x) = 0$ with $f(x) = \cos(x) - x$ (as in Example 4.1), a natural associated fixed-point problem is $x = \cos(x)$. As in Problem 9, graph $g(x) = \cos(x)$ and convince yourself from the picture that the sequence $x_{i+1} = g(x_i)$ will converge for any $x_0 \in [0, 1]$. Program this iteration and test your program with $x_0 = 1$ and $x_0 = 0.1$. Use Theorem 4.3 to prove that the sequence converges for any $x_0 \in [0, 1]$, and print out both the theoretical error bounds and the actual errors at each step of the iteration.

11. Prove the following simple variation of Theorem 4.4. Suppose $g'(x)$ is continuous on $[a, b]$ and suppose $|g'(x)| \leq K < 1$ for all x in $[a, b]$. Suppose also that there is a fixed point s of $g(x)$ in $[a, b]$. Then for any x_0 in $[a, b]$, the fixed-point iteration converges to s. [Hint: as in the proof of Theorem 4.4, show that the hypotheses of Theorem 4.3 are satisfied.]

12. Show that uniqueness of the fixed point in $I = [a, b]$ can be established with the hypothesis that $g(x)$ is differentiable on I and $g'(x) \le L < 1$ (this hypothesis is weaker than the one employed in Theorem 4.2).

4.3.2. Rate of Convergence of the Fixed-point Algorithm

In this section, let s be a fixed point of $g(x)$ where $g(x)$ satisfies the hypotheses of Theorem 4.4 in an interval I. Let $x_0 \in I$; and for each k, let $e_k = x_k - s$. Further, let us suppose that the $(k + 1)$st derivative of $g(x)$ is continuous on I [hereafter written: $g \in C^{k+1}(I)$]. To determine how the errors decrease at each step of the iteration, we expand $g(x)$ in a Taylor's series about $x = s$. This expansion gives us

$$e_{n+1} = g(x_n) - g(s) = g'(s)e_n + \frac{g''(s)}{2!}e_n^2 + \cdots + \frac{g^{(k)}(s)}{k!}e_n^k + E_{k,n} \quad (4.1)$$

where

$$E_{k,n} = g^{(k+1)}(\alpha_n)e_n^{k+1}/(k + 1)!$$

(and where the mean-value point α_n is between x_n and s). Suppose first that $g'(x) \neq 0$ for all $x \in I$. From (4.1) with $k = 0$, we have

$$e_{n+1} = g'(\alpha_n)e_n \qquad \text{or} \qquad \frac{e_{n+1}}{e_n} = g'(\alpha_n).$$

By Theorem 4.4, we have $\lim_{n\to\infty} x_n = s$; so $\lim_{n\to\infty} \alpha_n = s$ as well. Using the continuity of $g'(x)$, we find

$$\lim_{n\to\infty} \frac{e_{n+1}}{e_n} = g'(s). \quad (4.1a)$$

The assumption that $g'(s) \neq 0$ means (for sufficiently large n) that $e_{n+1} \approx g'(s)e_n$. Such a rate of convergence is called *linear* or *first-order* convergence. By contrast, if $g'(s) = 0$ and $g''(x) \neq 0$ for all x in I, then [from (4.1) with $k = 1$] we obtain the stronger result

$$\lim_{n\to\infty} \frac{e_{n+1}}{e_n^2} = \frac{g''(s)}{2!}. \quad (4.1b)$$

This case, in which the $(n + 1)$st error is approximately proportional to the square of the nth error, is called *quadratic* or *second-order* convergence.

Similarly if $g'(s) = g''(s) = \cdots = g^{(k)}(s) = 0$ and $g^{(k+1)}(x)$ does not vanish on I, then we have "$(k + 1)$st order" convergence:

$$\lim_{n\to\infty} \frac{e_{n+1}}{e_n^{k+1}} = \frac{g^{(k+1)}(s)}{(k + 1)!}. \quad (4.1c)$$

Thus the more derivatives of $g(x)$ that vanish at $x = s$, the faster the rate of convergence of the fixed-point iteration. In the analysis above, we implicitly assumed that $e_n \neq 0$ for $n = 0, 1, 2, \ldots$. This assumption is always a valid one if $x_0 \neq s$ and if (as we required) $g^{(i)}(x) \neq 0$ for $x \in I$ when $g'(s) = \cdots = g^{(i-1)}(s) = 0$. For example, consider the linear case, in which $g'(s) \neq 0$. Let m be the first positive integer such that $e_m = 0$. Then

$$0 = e_m = g(x_{m-1}) - g(s) = g'(\alpha)(x_{m-1} - s) = g'(\alpha)e_{m-1}$$

where α is between x_{m-1} and s. As $g'(x) \neq 0$ for all x in I, then $e_{m-1} = 0$, which contradicts our choice of m. Thus if $e_0 \neq 0$, then $e_n \neq 0$ for $n = 1, 2, \ldots$.

We shall be particularly interested in quadratic convergence since this leads to the derivation of Newton's method. For now, however, we pause to consider the slowest case, $g'(x) \neq 0$ for all $x \in I$; and we shall develop a way to speed up the convergence of these sequences. The technique we shall employ is called the *Aitken's Δ^2-method.*

We shall emphasize that Aitken's method can be used on sequences other than those generated by fixed-point iteration and that we can employ the Δ^2-method in different procedures in other chapters. [For example, we note by Problem 14 that the power-method sequence (see Chapter 3) can be accelerated by Aitken's method by virtue of Theorem 4.5.] Thus we present Aitken's method in a context completely divorced from the fixed-point iteration and in its full generality. This method is given in the following algorithm.

Let $\{t_n\}_{n=1}^{\infty}$ be any sequence that converges to t^*. Form a new sequence $\{t'_n\}_{n=1}^{\infty}$ by the formula

$$t'_n = t_n - \frac{(\Delta t_n)^2}{\Delta^2 t_n} \tag{4.2}$$

where $\Delta t_n = t_{n+1} - t_n$ and $\Delta^2 t_n = t_{n+2} - 2t_{n+1} + t_n$. The symbols Δ and Δ^2 are *forward differences,* but we will defer the theory of differences until later. Equation (4.2) is an "extrapolation" procedure that is suggested by considering sequences $\{x_n\}$, which are converging in a "fairly regular" fashion, such as the sequences generated by a linearly converging fixed-point iteration where

$$\lim_{n\to\infty} \frac{x_{n+1} - s}{x_n - s} = g'(s)$$

[that is, $x_{n+1} - s \approx g'(s)(x_n - s)$ when n is large]. If we knew, for example, that $x_{n+1} - s = B(x_n - s)$ and $x_{n+2} - s = B(x_{n+1} - s)$, then we could use these two equations (in the unknowns B and s) to solve for s and obtain

$$s = \frac{x_n - (x_{n+1} - x_n)^2}{x_{n+2} - 2x_{n+1} + x_n},$$

which is exactly analogous to Eq. (4.2) (see Problem 13).

In practice, we use the fact that whenever we have regularity of convergence, we can take three successive terms of a sequence and "extrapolate" to the limit. The manner in which Aitken's Δ^2-method speeds convergence is given by the following theorem, which also explains more precisely what we mean by "regular convergence."

Theorem 4.5

Let $\{t_n\}_{n=1}^{\infty}$ and $\{t'_n\}_{n=1}^{\infty}$ be as in Eq. (4.2) where $\lim_{n\to\infty} t_n = t^*$. Further assume for all n that $\varepsilon_n = t_n - t^*$ satisfies $\varepsilon_{n+1} = (B + \beta_n)\varepsilon_n$ where $\varepsilon_n \neq 0$, $|B| < 1$ and $\lim_{n\to\infty} \beta_n = 0$. Then, for n sufficiently large, t'_n is well defined and the new sequence converges to t^* faster than the old sequence in the sense that

$$\lim_{n\to\infty} \frac{t'_n - t^*}{t_n - t^*} = 0.$$

Proof. Observe that $\varepsilon_{n+2} = (B + \beta_{n+1})\varepsilon_{n+1} = (B + \beta_{n+1})(B + \beta_n)\varepsilon_n$. Therefore

$$\begin{aligned} \Delta^2 t_n &= \varepsilon_{n+2} - 2\varepsilon_{n+1} + \varepsilon_n \\ &= (B + \beta_{n+1})(B + \beta_n)\varepsilon_n - 2(B + \beta_n)\varepsilon_n + \varepsilon_n \\ &= [(B - 1)^2 + \beta'_n]\varepsilon_n \end{aligned}$$

where

$$\beta'_n = B(\beta_n + \beta_{n+1}) - 2\beta_n + \beta_n\beta_{n+1}.$$

Moreover, $\lim_{n\to\infty} \beta'_n = 0$ since $\beta_n \to 0$ as $n \to \infty$. Thus for n sufficiently large, $\Delta^2 t_n \neq 0$; and t'_n is well defined. Now setting

$$\Delta\varepsilon_n = \varepsilon_{n+1} - \varepsilon_n$$

and

$$\Delta^2\varepsilon_n = \varepsilon_{n+2} - 2\varepsilon_{n+1} + \varepsilon_n,$$

we have

$$\begin{aligned} t'_n - t^* = t_n - t^* - \frac{(\Delta t_n)^2}{\Delta^2 t_n} &= t_n - t^* - \frac{(\Delta\varepsilon_n)^2}{\Delta^2\varepsilon_n} \\ &= t_n - t^* - \frac{(B - 1 + \beta_n)^2\varepsilon_n^2}{[(B - 1)^2 + \beta'_n]\varepsilon_n}. \end{aligned}$$

Therefore

$$\lim_{n\to\infty} \frac{t'_n - t^*}{t_n - t^*} = \lim_{n\to\infty} \left\{1 - \frac{(B - 1)^2 + 2\beta_n(B - 1) + \beta_n^2}{(B - 1)^2 + \beta'_n}\right\} = 0. \quad ■$$

Corollary

Let $g(I) \subseteq I = [a, b]$ and $g'(x)$ be continuous on I where $0 < |g'(x)| \leq L < 1$. Then Theorem 4.5 may be applied to the fixed-point sequence, $\{x_n\}_{n=0}^{\infty}$, to speed its convergence.

Proof. In Theorem 4.5, identify $\{t_n\}_{n=0}^{\infty}$ with $\{x_n\}_{n=0}^{\infty}$ and t^* with s, the fixed point of $g(x)$. As noted previously, if $x_0 \neq s$, then $\varepsilon_n = t_n - t^* = x_n - s = e_n \neq 0$; and the theorem applies. ■

PROBLEMS, SECTION 4.3.2

1. Verify that $s = 1$ is a fixed point of $g(x) = (x^2 - 4x + 7)/4$. Using Problem 11, Section 4.3.1, show that the fixed-point iteration will converge to s for any x_0 satisfying $\varepsilon < x_0 < 4 - \varepsilon$ where $0 < \varepsilon < 1$. What is the rate of convergence?
2. If $x_{i+1} = g(x_i)$ is a fixed-point iteration converging linearly to s, then $e_{i+1} \simeq g'(s)e_i$, $i = 0, 1, \ldots$ For the iteration in Problem 1, print the values e_i and the ratios e_{i+1}/e_i for $i = 0, 1, \ldots, 10$; use $x_0 = 3.7$ and $x_0 = .1$ as starting values.
3. Code Aitken's Δ^2-method for the iteration in Problem 1; use $x_0 = 3.7$ and $x_0 = .1$ as starting values. Print the estimates x_i, x_i' and the ratio of the errors $(x_i' - s)/(x_i - s)$ for $i = 0, 1, \ldots, 10$.
4. Consider the fixed-point problem $x = g(x)$ where $g(x) = 5 - 6x^{-1}$. Verify that $s = 2$ and $s = 3$ are fixed points of $g(x)$. Using Problem 5, Section 4.3.1, show that the fixed point iteration will converge to $s = 3$ for any x_0 in $(3, \infty)$. Repeat Problems 2 and 3 for this function $g(x)$; choose $x_0 = 5$, $x_0 = 10$, and $x_0 = 1000$.
5. Let $g(x) = x^2 - 2x + 2$. What are the fixed points of $g(x)$? For each fixed point s, determine whether there is an $\varepsilon > 0$ such that if $|x_0 - s| < \varepsilon$, then the sequence $x_{i+1} = g(x_i)$ is convergent to s. What is the order of convergence of the iteration at those fixed points for which convergence occurs?
6. Let $\{t_n\}_{n=1}^{\infty} = \{(1/2)^n\}_{n=1}^{\infty}$ and $\{r_n\}_{n=1}^{\infty} = \{1/n^2\}_{n=1}^{\infty}$. Using Theorem 4.5, determine whether Aitken's Δ^2-method can be applied to either of these sequences.
7. Repeat Problem 6 for the sequence $\{t_n\}_{n=0}^{\infty}$ if
   a) $t_n = \dfrac{2n^2 + n - 3}{n^2 + 6}$
   b) $t_n = 1 - \left(\frac{7}{8}\right)^n$
8. The "geometric" series $\sum_{k=0}^{\infty} r^k$ converges for any value r in $(-1, 1)$, and the series converges to the value $1/(1 - r)$.
   a) Prove this statement by showing that if $S_n = 1 + r + r^2 + \cdots + r^n$, then $S_n = (1 - r^{n+1})/(1 - r)$. [Hint: Show that $(1 - r)(1 + r + r^2 + \cdots + r^n) = 1 - r^{n+1}$.]
   b) Complete the proof by calculating $\lim_{n \to \infty} S_n$.
9. Use Problem 8 and Theorem 4.5 to conclude that Aitken's Δ^2-method can be applied to the sequence of partial sums $\{S_n\}$ of the geometric series. For $r = .7$, calculate S_0, $S_1, \ldots, S_{20}$ and print these values. Next, apply the routine from Problem 3 to this sequence and note the improvement.
10. For $0 < x < 1$, the function $f(x) = 1/(1 - \sqrt{x})$ can be represented by a geometric series if we set $r = \sqrt{x}$. Repeat Problem 9 for this series representation for $f(x)$; use $x = .3$.
11. Using Problem 10, determine how you might estimate the integral
$$\int_{.04}^{.64} \frac{1}{1 - \sqrt{x}}\,dx.$$
12. In formula (4.1) assume that $x_0 \neq s$, $g'(s) = 0$, and that $g''(x)$ is continuous and nonzero on I. Show that $e_n \neq 0$ for all $n \geq 1$.

13. Suppose that $\{x_n\}$ is a sequence and $x_{i+1} - s = B(x_i - s)$ and $x_{i+2} - s = B(x_{i+1} - s)$ for some i. Under the assumption that $B \neq 1$, solve these two equations for s, and thus give an intuitive derivation for Aitken's Δ^2-method.

14. Consider the sequence $\{\beta_k\}$ generated by the power method as in formula (3.12). Use (3.12) to show that

$$\lim_{n\to\infty} \frac{\beta_{k+1} - \lambda_1}{\beta_k - \lambda_1} = r, \qquad |r| < 1.$$

Thus the sequence $\{\beta_k\}$ satisfies the conditions of Theorem 4.5, and can be accelerated by Aitken's method.

15. (Steffensen's method). Consider the fixed-point problem, $x = g(x)$, with an initial guess $x_0 = t_0$ and solution $s = g(s)$. Let $x_1 = g(x_0)$ and $x_2 = g(x_1) = g(g(x_0))$. Now apply the Aitken formula (4.2) to obtain

$$t_1 = x_0 - \frac{(\Delta x_0)^2}{\Delta^2 x_0} = x_0 - \frac{(x_1 - x_0)^2}{x_2 - 2x_1 + x_0}.$$

Now repeat the process; that is, let $x_0' = t_1$, $x_1' = g(t_1)$, $x_2' = g(x_1') = g(g(t_1))$, and $t_2 = t_1 - (g(t_1) - t_1)^2/[g(g(t_1)) - 2g(t_1) + t_1]$. Thus we see we are generating a sequence $\{t_k\}$ where each t_k is obtained by three steps of a fixed-point iteration and then an Aitken's method correction. We formalize this procedure by defining $R(x) = g(g(x)) - 2g(x) + x$; let $G(x) = x - (g(x) - x)^2/R(x)$ if $R(x) \neq 0$; and let $G(x) = x$ if $R(x) = 0$. Thus with t_0 given, the sequence $\{t_k\}$ is generated by the fixed-point formula: $t_{k+1} = G(t_k)$, $k \geq 0$.

a) Let $g(x) = \sqrt[3]{6 + x}$ and $x_0 = t_0 = 3$. Write a program that generates *both* the fixed-point sequence $x_{k+1} = g(x_k)$ and the Steffensen sequence $t_{k+1} = G(t_k)$. Compare the rates of convergence. [Obviously $s = 2$ satisfies $s = g(s)$.]

*b) Assume that an arbitrary $g(x)$ satisfies $g'(s) \neq 1$ and $g''(x)$ is continuous: Prove that $G'(s) = 0$, and thus Steffensen's method is quadratically convergent by (4.1) and (4.1b).

4.3.3. Newton's Method

We are now ready to apply the fixed-point analysis above to our principal problem of finding the zeros of a given function $f(x)$. One natural choice of the fixed-point function would be $g(x) = x + cf(x)$ where c is a nonzero constant. Then $f(s) = 0$ if and only if $s = g(s)$. From Section 4.3.2, we see that the fixed-point iteration is accelerated by making as many derivatives of $g(x)$ at $x = s$ equal to zero as possible. Now, $g'(s) = 1 + cf'(s)$; thus $g'(s) \neq 0$ unless $c = -(1/f'(s))$. Unfortunately since we do not know the value of s, it is impossible to make an *a priori* choice for c.

Thus we are led to make a different choice for $g(x)$. This time we let $g(x) = x + h(x)f(x)$, and try to select $h(x)$ such that $g'(s) = 0$. Now, $g'(s) = 1 + h'(s)f(s) + h(s)f'(s) = 1 + h(s)f'(s)$. Thus for $g'(s) = 0$, we must select $h(x)$ such that $h(s) = -(1/f'(s))$. Immediately we see that $h(x) \equiv -(1/f'(x))$ has this property, and furthermore we need not know the value of s to make this choice. Therefore, we select $g(x) \equiv x - f(x)/f'(x)$, and the fixed-point algorithm yields the following iteration, known as Newton's method. Given the function $f(x)$, let x_0 be an initial guess for s where $f(s) = 0$. Then let

$$x_{n+1} = x_n - f(x_n)/f'(x_n), \qquad n = 0, 1, \ldots . \tag{4.3}$$

The analysis above along with Theorem 4.4 yields the following local convergence theorem for Newton's method. (The proof is left to the reader.)

$g(x) = x - \frac{f(x)}{f'(x)}$, $f(s) = 0 \Leftrightarrow g(s) = s$, $g'(s) = 0$

Theorem 4.6

Let $f''(x)$ be continuous and $f'(x) \neq 0$ in some open interval containing s where $f(s) = 0$. Then there exists an $\varepsilon > 0$ such that Newton's method is quadratically convergent whenever $|x_0 - s| < \varepsilon$.

Subroutine NEWTON (Fig. 4.7) employs Newton's method to find an approximate root of the equation $f(x) = 0$. Programming a root-finding procedure that does not possess the bracketing property of the bisection method or *Regula Falsi* presents one difficulty: selecting an appropriate test for terminating the iteration. When it is not practical to use a guaranteed error bound, such as that displayed in Theorem 4.3, we are left with the alternatives of prescribing either a tolerance $\varepsilon > 0$ or a tolerance $\delta > 0$, and stopping the iteration when $|x_{n+1} - x_n| < \delta$ or when $|f(x_n)| < \varepsilon$. Subroutine NEWTON uses both of these criteria and an upper bound on the number of iterations to be executed as well.

```
      SUBROUTINE NEWTON(XO,XTERM,FTERM,N,ITERM)
C
C     THIS SUBROUTINE USES NEWTON'S METHOD TO FIND A ROOT OF F(X)=0.  THE
C     CALLING PROGRAM MUST SUPPLY AN INITIAL GUESS, XO, AND 3 TERMINATION
C     CRITERIA, XTERM, FTERM AND N.  THE SUBROUTINE RETURNS AN APPROXIMATE
C     ROOT IN XO WHEN ONE OF THE TERMINATION REQUIREMENTS IS MET.  A FLAG,
C     ITERM, IS SET TO 1 WHEN THE ABSOLUTE VALUE OF F(XO) IS LESS THAN
C     FTERM; ITERM IS SET TO 2 WHEN 2 SUCESSIVE ITERATES DIFFER BY LESS
C     THAN XTERM AND ITERM IS SET TO 3 WHEN THE MAXIMUM NUMBER OF
C     ITERATIONS, N, IS REACHED.  TWO FUNCTION SUBPROGRAMS NAMED F(X)
C     AND FPRIM(X) MUST BE SUPPLIED TO CALCULATE F(X) AND THE DERIVATIVE
C     OF F(X).
C
      DO 1 I=1,N
      FO=F(XO)
      IF(ABS(FO).LT.FTERM)   GO TO 2
      FPO=FPRIM(XO)
      CORREC=FO/FPO
      IF(ABS(CORREC).LT.XTERM)    GO TO 3
    1 XO=XO-CORREC
      ITERM=3
      RETURN
    2 ITERM=1
      RETURN
    3 ITERM=2
      XO=XO-CORREC
      RETURN
      END
```

Figure 4.7 Subroutine NEWTON.

EXAMPLE 4.2. Let $f(x)$ be the simple function of Example 4.1, $f(x) = \cos(x) - x$. Starting with $x_0 = 0$, the following sequence of iterates was generated by Subroutine NEWTON. (See Table 4.2.) For this example, convergence is quite rapid.

TABLE 4.2 Newton's method.

x_i	$f(x_i)$
0.0000000E 00	0.1000000E 01
0.1000000E 01	−0.4596977E 00
0.7503638E 00	−0.1892304E−01
0.7391128E 00	−0.4643201E−04
0.7390850E 00	0.5960464E−07

We note that although quite simple, the geometric derivation illustrated in Figure 4.4 says nothing about quadratic convergence, sufficient conditions on $f(x)$ to ensure convergence, and the question of convergence when $f'(s) = 0$. Recall that we say the root s has *multiplicity* p if $f(s) = f'(s) = \cdots = f^{(p-1)}(s) = 0$, but $f^{(p)}(s) \neq 0$. We shall consider the case in which s has multiplicity 2, that is, s is a *double root* of $f(x)$, and consider higher multiplicities in the problems.

Let us assume that $f(s) = f'(s) = 0$ and $f^{(4)}(x)$ is continuous. Again let $g(x) = x - f(x)/f'(x)$; so $g'(x) = 1 - (f'(x)^2 - f(x)f''(x))/f'(x)^2$, or $g'(x) = f(x)f''(x)/f'(x)^2$. We easily verify by l'Hôpital's rule that $g'(s) = 1/2$. Since $|g'(s)| < 1$, and the rest of the hypotheses of Theorem 4.4 are satisfied, we see that Newton's method still converges locally to s. The convergence, however, is not quadratic. Instead we get only linear convergence where $\lim_{n\to\infty} (e_{n+1}/e_n) = g'(s) = 1/2$.

In the analysis above, however, if we choose $g(x) = x - 2f(x)/f'(x)$, then $g'(s) = 0$. Thus if we know *a priori* that the multiplicity of s is 2, then the sequence

$$x_{n+1} = x_n - 2f(x_n)/f'(x_n)$$

will converge to s quadratically for x_0 sufficiently close to s.

In general, if s has multiplicity p, then we can show (Problem 9) that if $g(x) = x - f(x)/f'(x)$, then $g'(s) = 1 - 1/p$; and if $g(x) = x - pf(x)/f'(x)$, then $g'(s) = 0$. Thus for x_0 sufficiently close to s, the sequence

$$x_{n+1} = x_n - pf(x_n)/f'(x_n) \tag{4.4}$$

is quadratically convergent to s. The formula (4.4) is of little practical use, however, since we rarely know the multiplicity of a root in advance.

EXAMPLE 4.3. In this example we illustrate the behavior of Newton's method near a point s where $f(s) = f'(s) = 0$. For $f(x) = x^3 + x^2 - 5x + 3$, we have $f(x) = (x-1)^2(x+3)$ so that $f(1) = f'(1) = 0$ and $f(-3) = 0$. Newton's method was run with an initial guess of $x_0 = 4$. Convergence to $s = 1$ is seen to be quite slow. As the iterates near 1, they exhibit an oscillatory behavior that is typical when the limits of machine accuracy are approached. The same program was run with an initial guess of $x_0 = -6$, with rapid convergence to $s = -3$. (See Table 4.3.) The same program run in double precision with $x_0 = 4$ yields results (Table 4.4) that are in agreement with geometric intuition (see Problem 9 of this section).

TABLE 4.3.

x_i	$f(x_i)$	x_i	$f(x_i)$
0.4000000E 01	0.6300000E 02	−0.6000000E 01	−0.1470000E 03
0.2764706E 01	0.1795237E 02	−0.4384615E 01	−0.4014566E 02
0.1999479E 01	0.4994273E 01	−0.3470246E 01	−0.9396978E 01
0.1545152E 01	0.1350779E 01	−0.3081737E 01	−0.1361792E 01
0.1287998E 01	0.3556594E 00	−0.3003147E 01	−0.5043125E−01
0.1148676E 01	0.9170532E−01	−0.3000004E 01	−0.7629394E−04
0.1075647E 01	0.2332305E−01	−0.3000000E 01	0.0000000E 00
0.1038170E 01	0.5883216E−02		
0.1019176E 01	0.1478195E−02		
0.1009609E 01	0.3700256E−03		
0.1004812E 01	0.9250640E−04		
0.1002412E 01	0.2384185E−04		
0.1001178E 01	0.5722045E−05		
0.1000572E 01	0.1907348E−05		
0.1000155E 01	0.9536743E−06		
0.9993886E 00	0.1907348E−05		
0.9997784E 00	0.9536743E−06		
0.1000315E 01	0.9536743E−06		
0.9999380E 00	0.0000000E 00		

TABLE 4.4

x_i	$f(x_i)$
0.40000000D 01	0.63000000D 02
0.27647059D 01	0.17952371D 02
0.19994794D 01	0.49942757D 01
0.15451534D 01	0.13507843D 01
0.12879985D 01	0.35566004D 00
0.11486779D 01	0.91707018D−01
0.10756476D 01	0.23323111D−01
0.10381716D 01	0.58838948D−02
0.10191756D 01	0.14778606D−02
0.10096106D 01	0.37034232D−03
0.10048111D 01	0.92696274D−04
0.10024070D 01	0.23187972D−04
0.10012038D 01	0.57987349D−05
0.10006020D 01	0.14499018D−05
0.10003010D 01	0.36250271D−06
0.10001505D 01	0.90629086D−07
0.10000753D 01	0.22657698D−07
0.10000376D 01	0.56644780D−08
0.10000188D 01	0.14161259D−08
0.10000094D 01	0.35403258D−09