CHAPTER 6

Open Methods

For the bracketing methods in the previous chapter, the root is located within an interval prescribed by a lower and an upper bound. Repeated application of these methods always results in closer estimates of the true value of the root. Such methods are said to be *convergent* because they move closer to the truth as the computation progresses (Fig. 6.1*a*).

In contrast, the *open methods* described in this chapter are based on formulas that require only a single starting value of x or two starting values that do not necessarily bracket

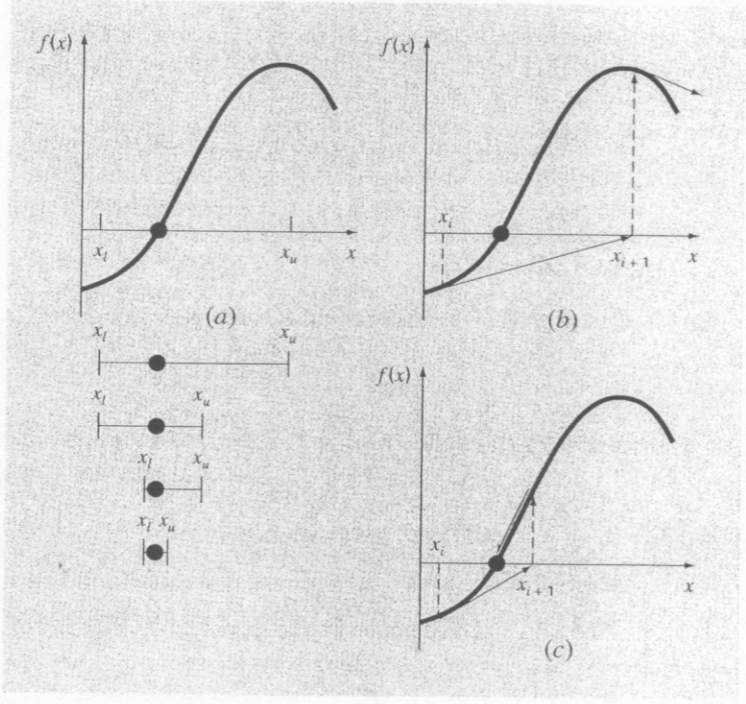


FIGURE 6.1
Graphical depiction of the fundamental difference between the (*a*) bracketing and (*b*) and (*c*) open methods for root location. In (*a*), which is the bisection method, the root is constrained within the interval prescribed by x_l and x_u. In contrast, for the open method depicted in (*b*) and (*c*), a formula is used to project from x_i to x_{i+1} in an iterative fashion. Thus, the method can either (*b*) diverge or (*c*) converge rapidly, depending on the value of the initial guess.

the root. As such, they sometimes *diverge* or move away from the true root as the computation progresses (Fig. 6.1*b*). However, when the open methods converge (Fig. 6.1*c*), they usually do so much more quickly than the bracketing methods. We will begin our discussion of open techniques with a simple version that is useful for illustrating their general form and also for demonstrating the concept of convergence.

6.1 SIMPLE FIXED-POINT ITERATION

As mentioned above, open methods employ a formula to predict the root. Such a formula can be developed for simple *fixed-point iteration* (or, as it is also called, one-point iteration or successive substitution) by rearranging the function $f(x) = 0$ so that x is on the left-hand side of the equation:

$$x = g(x) \tag{6.1}$$

This transformation can be accomplished either by algebraic manipulation or by simply adding x to both sides of the original equation. For example,

$$x^2 - 2x + 3 = 0$$

can be simply manipulated to yield

$$x = \frac{x^2 + 3}{2}$$

whereas $\sin x = 0$ could be put into the form of Eq. (6.1) by adding x to both sides to yield

$$x = \sin x + x.$$

The utility of Eq. (6.1) is that it provides a formula to predict a new value of x as a function of an old value of x. Thus, given an initial guess at the root x_i, Eq. (6.1) can be used to compute a new estimate x_{i+1} as expressed by the iterative formula

$$x_{i+1} = g(x_i) \tag{6.2}$$

As with other iterative formulas in this book, the approximate error for this equation can be determined using the error estimator [Eq. (3.5)]:

$$\varepsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| 100\%$$

EXAMPLE 6.1 Simple Fixed-Point Iteration

Problem Statement. Use simple fixed-point iteration to locate the root of $f(x) = e^{-x} - x$.

Solution. The function can be separated directly and expressed in the form of Eq. (6.2) as

$$x_{i+1} = e^{-x_i}$$

Starting with an initial guess of $x_0 = 0$, this iterative equation can be applied to compute

i	x_i	ε_a (%)	ε_t (%)
0	0		100.0
1	1.000000	100.0	76.3
2	0.367879	171.8	35.1
3	0.692201	46.9	22.1
4	0.500473	38.3	11.8
5	0.606244	17.4	6.89
6	0.545396	11.2	3.83
7	0.579612	5.90	2.20
8	0.560115	3.48	1.24
9	0.571143	1.93	0.705
10	0.564879	1.11	0.399

Thus, each iteration brings the estimate closer to the true value of the root: 0.56714329.

6.1.1 Convergence

Notice that the true percent relative error for each iteration of Example 6.1 is roughly proportional (by a factor of about 0.5 to 0.6) to the error from the previous iteration. This property, called *linear convergence,* is characteristic of fixed-point iteration.

Aside from the "rate" of convergence, we must comment at this point about the "possibility" of convergence. The concepts of convergence and divergence can be depicted graphically. Recall that in Sec. 5.1, we graphed a function to visualize its structure and behavior (Example 5.1). Such an approach is employed in Fig. 6.2*a* for the function $f(x) = e^{-x} - x$. An alternative graphical approach is to separate the equation into two component parts, as in

$$f_1(x) = f_2(x)$$

Then the two equations

$$y_1 = f_1(x) \tag{6.3}$$

and

$$y_2 = f_2(x) \tag{6.4}$$

can be plotted separately (Fig. 6.2*b*). The x values corresponding to the intersections of these functions represent the roots of $f(x) = 0$.

EXAMPLE 6.2 The Two-Curve Graphical Method

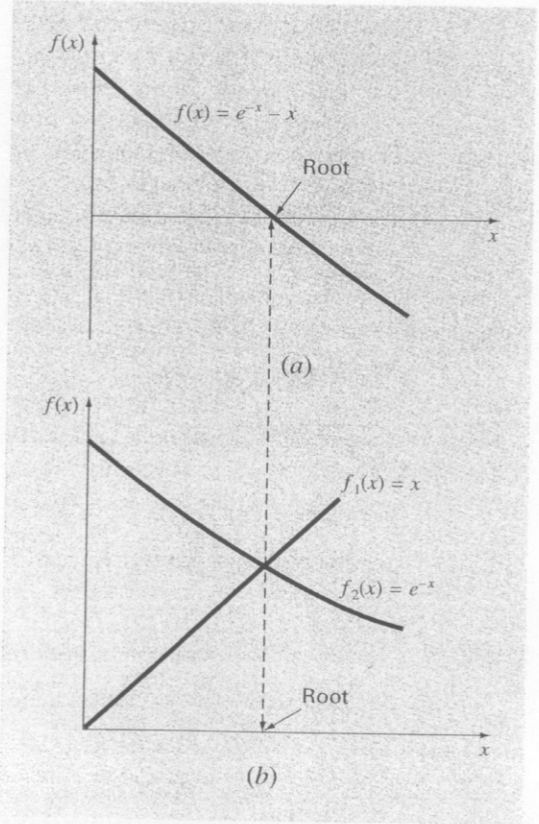
Problem Statement. Separate the equation $e^{-x} - x = 0$ into two parts and determine its root graphically.

Solution. Reformulate the equation as $y_1 = x$ and $y_2 = e^{-x}$. The following values can be computed:

x	y_1	y_2
0.0	0.0	1.000
0.2	0.2	0.819
0.4	0.4	0.670
0.6	0.6	0.549
0.8	0.8	0.449
1.0	1.0	0.368

These points are plotted in Fig. 6.2*b*. The intersection of the two curves indicates a root estimate of approximately $x = 0.57$, which corresponds to the point where the single curve in Fig. 6.2*a* crosses the x axis.

FIGURE 6.2
Two alternative graphical methods for determining the root of $f(x) = e^{-x} - x$. (*a*) Root at the point where it crosses the x axis; (*b*) root at the intersection of the component functions.



The two-curve method can now be used to illustrate the convergence and divergence of fixed-point iteration. First, Eq. (6.1) can be re-expressed as a pair of equations $y_1 = x$ and $y_2 = g(x)$. These two equations can then be plotted separately. As was the case with Eqs. (6.3) and (6.4), the roots of $f(x) = 0$ correspond to the abscissa value at the intersection of the two curves. The function $y_1 = x$ and four different shapes for $y_2 = g(x)$ are plotted in Fig. 6.3.

For the first case (Fig. 6.3*a*), the initial guess of x_0 is used to determine the corresponding point on the y_2 curve $[x_0, g(x_0)]$. The point (x_1, x_1) is located by moving left horizontally to the y_1 curve. These movements are equivalent to the first iteration in the fixed-point method:

$$x_1 = g(x_0)$$

Thus, in both the equation and in the plot, a starting value of x_0 is used to obtain an estimate of x_1. The next iteration consists of moving to $[x_1, g(x_1)]$ and then to (x_2, x_2). This iteration

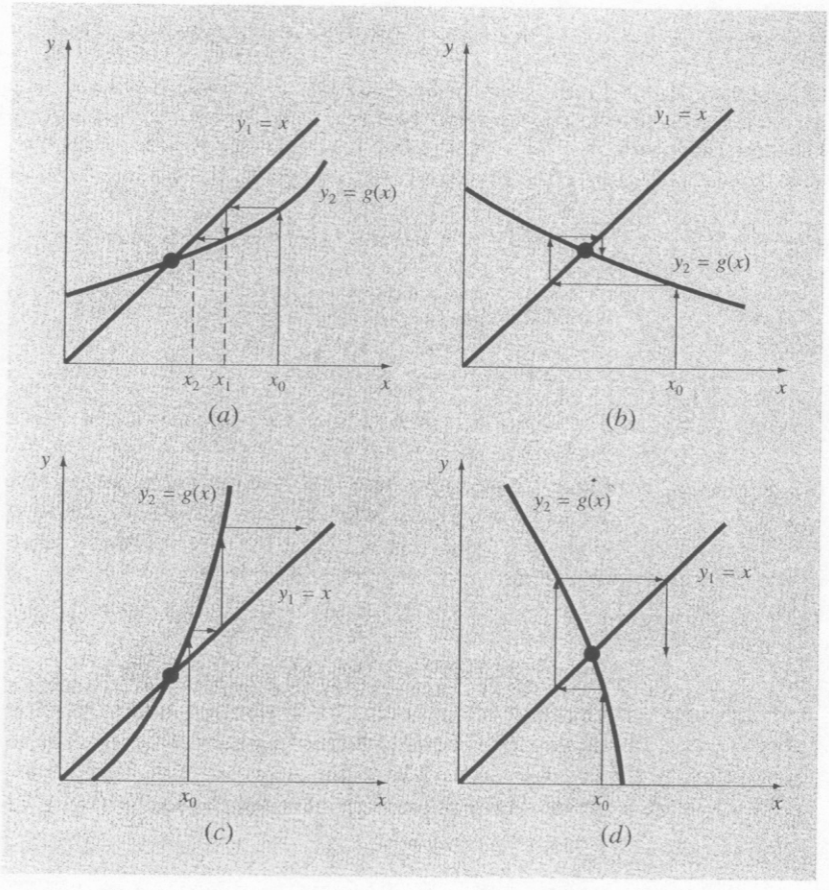


FIGURE 6.3
Graphical depiction of (*a*) and (*b*) convergence and (*c*) and (*d*) divergence of simple fixed-point iteration. Graphs (*a*) and (*c*) are called monotone patterns, whereas (*b*) and (*d*) are called oscillating or spiral patterns. Note that convergence occurs when $|g'(x)| < 1$.

Box 6.1 Convergence of Fixed-Point Iteration

From studying Fig. 6.3, it should be clear that fixed-point iteration converges if, in the region of interest, $|g'(x)| < 1$. In other words, convergence occurs if the magnitude of the slope of $g(x)$ is less than the slope of the line $f(x) = x$. This observation can be demonstrated theoretically. Recall that the iterative equation is

$$x_{i+1} = g(x_i)$$

Suppose that the true solution is

$$x_r = g(x_r)$$

Subtracting these equations yields

$$x_r - x_{i+1} = g(x_r) - g(x_i) \tag{B6.1.1}$$

The *derivative mean-value theorem* (recall Sec. 4.1.1) states that if a function $g(x)$ and its first derivative are continuous over an interval $a \le x \le b$, then there exists at least one value of $x = \xi$ within the interval such that

$$g'(\xi) = \frac{g(b) - g(a)}{b - a} \tag{B6.1.2}$$

The right-hand side of this equation is the slope of the line joining $g(a)$ and $g(b)$. Thus, the mean-value theorem states that there is at least one point between a and b that has a slope, designated by $g'(\xi)$, which is parallel to the line joining $g(a)$ and $g(b)$ (recall Fig. 4.3).

Now, if we let $a = x_i$ and $b = x_r$, the right-hand side of Eq. (B6.1.1) can be expressed as

$$g(x_r) - g(x_i) = (x_r - x_i)g'(\xi)$$

where ξ is somewhere between x_i and x_r. This result can then be substituted into Eq. (B6.1.1) to yield

$$x_r - x_{i+1} = (x_r - x_i)g'(\xi) \tag{B6.1.3}$$

If the true error for iteration i is defined as

$$E_{t,i} = x_r - x_i$$

then Eq. (B6.1.3) becomes

$$E_{t,i+1} = g'(\xi)E_{t,i}$$

Consequently, if $|g'(x)| < 1$, the errors decrease with each iteration. For $|g'(x)| > 1$, the errors grow. Notice also that if the derivative is positive, the errors will be positive, and hence, the iterative solution will be monotonic (Fig. 6.3*a* and *c*). If the derivative is negative, the errors will oscillate (Fig. 6.3*b* and *d*).

An offshoot of the analysis is that it also demonstrates that when the method converges, the error is roughly proportional to and less than the error of the previous step. For this reason, simple fixed-point iteration is said to be *linearly convergent*.

is equivalent to the equation

$$x_2 = g(x_1)$$

The solution in Fig. 6.3*a* is *convergent* because the estimates of x move closer to the root with each iteration. The same is true for Fig. 6.3*b*. However, this is not the case for Fig. 6.3*c* and *d*, where the iterations diverge from the root. Notice that convergence seems to occur only when the absolute value of the slope of $y_2 = g(x)$ is less than the slope of $y_1 = x$, that is, when $|g'(x)| < 1$. Box 6.1 provides a theoretical derivation of this result.

6.1.2 Algorithm for Fixed-Point Iteration

The computer algorithm for fixed-point iteration is extremely simple. It consists of a loop to iteratively compute new estimates until the termination criterion has been met. Figure 6.4 presents pseudocode for the algorithm. Other open methods can be programmed in a similar way, the major modification being to change the iterative formula that is used to compute the new root estimate.

```
FUNCTION Fixpt(x0, es, imax, iter, ea)
  xr = x0
  iter = 0
  DO
    xrold = xr
    xr = g(xrold)
    iter = iter + 1
    IF xr ≠ 0 THEN
      ea = |(xr - xrold)/xr| · 100
    END IF
    IF ea < es OR iter ≥ imax EXIT
  END DO
  Fixpt = xr
END Fixpt
```

FIGURE 6.4
Pseudocode for fixed-point iteration. Note that other open methods can be cast in this general format.

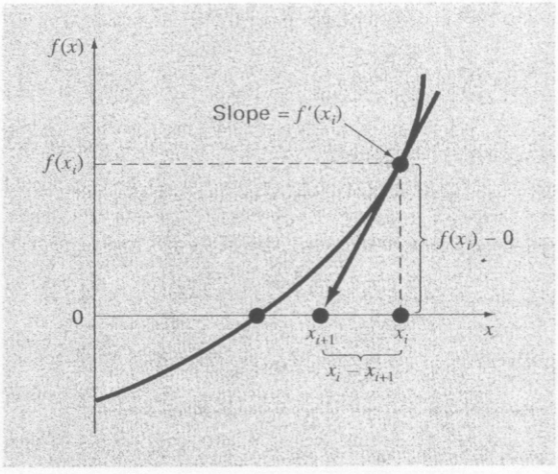


FIGURE 6.5
Graphical depiction of the Newton-Raphson method. A tangent to the function of x_i [that is, $f'(x_i)$] is extrapolated down to the x axis to provide an estimate of the root at x_{i+1}.

6.2 THE NEWTON-RAPHSON METHOD

Perhaps the most widely used of all root-locating formulas is the Newton-Raphson equation (Fig. 6.5). If the initial guess at the root is x_i, a tangent can be extended from the point $[x_i, f(x_i)]$. The point where this tangent crosses the x axis usually represents an improved estimate of the root.

The Newton-Raphson method can be derived on the basis of this geometrical interpretation (an alternative method based on the Taylor series is described in Box 6.2). As in Fig. 6.5, the first derivative at x is equivalent to the slope:

$$f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}} \tag{6.5}$$

which can be rearranged to yield

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \tag{6.6}$$

which is called the *Newton-Raphson formula.*

EXAMPLE 6.3 Newton-Raphson Method

Problem Statement. Use the Newton-Raphson method to estimate the root of $f(x) = e^{-x} - x$, employing an initial guess of $x_0 = 0$.

Solution. The first derivative of the function can be evaluated as

$$f'(x) = -e^{-x} - 1$$

which can be substituted along with the original function into Eq. (6.6) to give

$$x_{i+1} = x_i - \frac{e^{-x_i} - x_i}{-e^{-x_i} - 1}$$

Starting with an initial guess of $x_0 = 0$, this iterative equation can be applied to compute

i	x_i	ε_t (%)
0	0	100
1	0.500000000	11.8
2	0.566311003	0.147
3	0.567143165	0.0000220
4	0.567143290	$< 10^{-8}$

Thus, the approach rapidly converges on the true root. Notice that the true percent relative error at each iteration decreases much faster than it does in simple fixed-point iteration (compare with Example 6.1).

6.2.1 Termination Criteria and Error Estimates

As with other root-location methods, Eq. (3.5) can be used as a termination criterion. In addition, however, the Taylor series derivation of the method (Box 6.2) provides theoretical insight regarding the rate of convergence as expressed by $E_{i+1} = O(E_i^2)$. Thus the error should be roughly proportional to the square of the previous error. In other words, the

Box 6.2 Derivation and Error Analysis of the Newton-Raphson Method

Aside from the geometric derivation [Eqs. (6.5) and (6.6)], the Newton-Raphson method may also be developed from the Taylor series expansion. This alternative derivation is useful in that it also provides insight into the rate of convergence of the method.

Recall from Chap. 4 that the Taylor series expansion can be represented as

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(\xi)}{2!}(x_{i+1} - x_i)^2 \tag{B6.2.1}$$

where ξ lies somewhere in the interval from x_i to x_{i+1}. An approximate version is obtainable by truncating the series after the first derivative term:

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

At the intersection with the x axis, $f(x_{i+1})$ would be equal to zero, or

$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i) \tag{B6.2.2}$$

which can be solved for

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

which is identical to Eq. (6.6). Thus, we have derived the Newton-Raphson formula using a Taylor series.

Aside from the derivation, the Taylor series can also be used to estimate the error of the formula. This can be done by realizing that if the complete Taylor series were employed, an exact result would be obtained. For this situation $x_{i+1} = x_r$, where x is the true value of the root. Substituting this value along with $f(x_r) = 0$ into Eq. (B6.2.1) yields

$$0 = f(x_i) + f'(x_i)(x_r - x_i) + \frac{f''(\xi)}{2!}(x_r - x_i)^2 \tag{B6.2.3}$$

Equation (B6.2.2) can be subtracted from Eq. (B6.2.3) to give

$$0 = f'(x_i)(x_r - x_{i+1}) + \frac{f''(\xi)}{2!}(x_r - x_i)^2 \tag{B6.2.4}$$

Now, realize that the error is equal to the discrepancy between x_{i+1} and the true value x_r, as in

$$E_{t,i+1} = x_r - x_{i+1}$$

and Eq. (B6.2.4) can be expressed as

$$0 = f'(x_i)E_{t,i+1} + \frac{f''(\xi)}{2!}E_{t,i}^2 \tag{B6.2.5}$$

If we assume convergence, both x_i and ξ should eventually be approximated by the root x_r, and Eq. (B6.2.5) can be rearranged to yield

$$E_{t,i+1} = \frac{-f''(x_r)}{2f'(x_r)}E_{t,i}^2 \tag{B6.2.6}$$

According to Eq. (B6.2.6), the error is roughly proportional to the square of the previous error. This means that the number of correct decimal places approximately doubles with each iteration. Such behavior is referred to as *quadratic convergence*. Example 6.4 manifests this property.

number of significant figures of accuracy approximately doubles with each iteration. This behavior is examined in the following example.

EXAMPLE 6.4 Error Analysis of Newton-Raphson Method

Problem Statement. As derived in Box 6.2, the Newton-Raphson method is quadratically convergent. That is, the error is roughly proportional to the square of the previous error, as in

$$E_{t,i+1} \cong \frac{-f''(x_r)}{2f'(x_r)}E_{t,i}^2 \tag{E6.4.1}$$

Examine this formula and see if it applies to the results of Example 6.3.

Solution. The first derivative of $f(x) = e^{-x} - x$ is

$$f'(x) = -e^{-x} - 1$$

which can be evaluated at $x_r = 0.56714329$ as $f'(0.56714329) = -1.56714329$. The second derivative is

$$f''(x) = e^{-x}$$

which can be evaluated as $f''(0.56714329) = 0.56714329$. These results can be substituted into Eq. (E6.4.1) to yield

$$E_{t,i+1} \cong -\frac{0.56714329}{2(-1.56714329)} E_{t,i}^2 = 0.18095 E_{t,i}^2$$

From Example 6.3, the initial error was $E_{t,0} = 0.56714329$, which can be substituted into the error equation to predict

$$E_{t,1} \cong 0.18095(0.56714329)^2 = 0.0582$$

which is close to the true error of 0.06714329. For the next iteration,

$$E_{t,2} \cong 0.18095(0.06714329)^2 = 0.0008158$$

which also compares favorably with the true error of 0.0008323. For the third iteration,

$$E_{t,3} \cong 0.18095(0.0008323)^2 = 0.000000125$$

which is the error obtained in Example 6.3. The error estimate improves in this manner because, as we come closer to the root, x and ξ are better approximated by x_r [recall our assumption in going from Eq. (B6.2.5) to Eq. (B6.2.6) in Box 6.2]. Finally,

$$E_{t,4} \cong 0.18095(0.000000125)^2 = 2.83 \times 10^{-15}.$$

Thus, this example illustrates that the error of the Newton-Raphson method for this case is, in fact, roughly proportional (by a factor of 0.18095) to the square of the error of the previous iteration.

6.2.2 Pitfalls of the Newton-Raphson Method

Although the Newton-Raphson method is often very efficient, there are situations where it performs poorly. A special case—multiple roots—will be addressed later in this chapter. However, even when dealing with simple roots, difficulties can also arise, as in the following example.

EXAMPLE 6.5 Example of a Slowly Converging Function with Newton-Raphson

Problem Statement. Determine the positive root of $f(x) = x^{10} - 1$ using the Newton-Raphson method and an initial guess of $x = 0.5$.

Solution. The Newton-Raphson formula for this case is

$$x_{i+1} = x_i - \frac{x_i^{10} - 1}{10x_i^9}$$

which can be used to compute

Iteration	x
0	0.5
1	51.65
2	46.485
3	41.8365
4	37.65285
5	33.887565
.	
.	
.	
∞	1.0000000

Thus, after the first poor prediction, the technique is converging on the true root of 1, but at a very slow rate.

Aside from slow convergence due to the nature of the function, other difficulties can arise, as illustrated in Fig. 6.6. For example, Fig. 6.6*a* depicts the case where an inflection point [that is, $f''(x) = 0$] occurs in the vicinity of a root. Notice that iterations beginning at x_0 progressively diverge from the root. Figure 6.6*b* illustrates the tendency of the Newton-Raphson technique to oscillate around a local maximum or minimum. Such oscillations may persist, or as in Fig. 6.6*b*, a near-zero slope is reached, whereupon the solution is sent far from the area of interest. Figure 6.6*c* shows how an initial guess that is close to one root can jump to a location several roots away. This tendency to move away from the area of interest is because near-zero slopes are encountered. Obviously, a zero slope [$f'(x) = 0$] is truly a disaster because it causes division by zero in the Newton-Raphson formula [Eq. (6.6)]. Graphically (see Fig 6.6*d*), it means that the solution shoots off horizontally and never hits the x axis.

Thus, there is no general convergence criterion for Newton-Raphson. Its convergence depends on the nature of the function and on the accuracy of the initial guess. The only remedy is to have an initial guess that is "sufficiently" close to the root. And for some functions, no guess will work! Good guesses are usually predicated on knowledge of the physical problem setting or on devices such as graphs that provide insight into the behavior of the solution. The lack of a general convergence criterion also suggests that good computer software should be designed to recognize slow convergence or divergence. The next section addresses some of these issues.

6.2.3 Algorithm for Newton-Raphson

An algorithm for the Newton-Raphson method is readily obtained by substituting Eq. (6.6) for the predictive formula [Eq. (6.2)] in Fig. 6.4. Note, however, that the program must also be modified to compute the first derivative. This can be simply accomplished by the inclusion of a user-defined function.

Additionally, in light of the foregoing discussion of potential problems of the Newton-Raphson method, the program would be improved by incorporating several additional features:

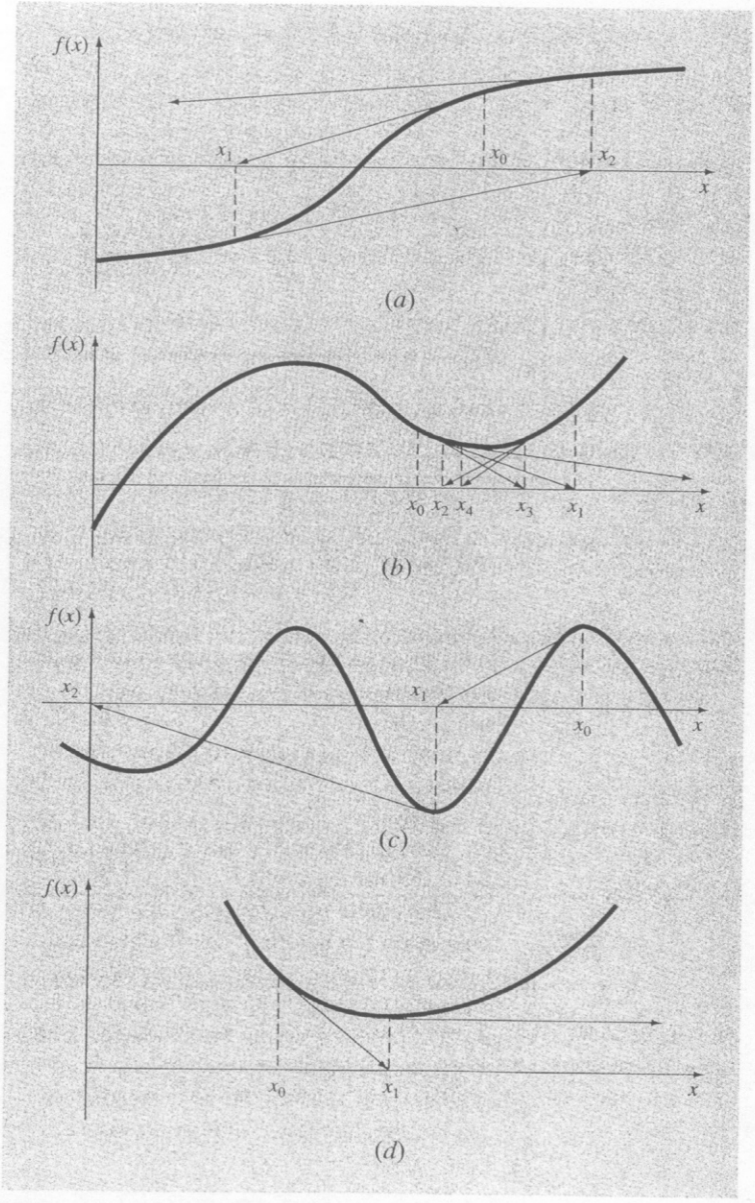


FIGURE 6.6
Four cases where the Newton-Raphson method exhibits poor convergence.

1. A plotting routine should be included in the program.
2. At the end of the computation, the final root estimate should always be substituted into the original function to compute whether the result is close to zero. This check partially guards against those cases where slow or oscillating convergence may lead to a small value of ε_a while the solution is still far from a root.
3. The program should always include an upper limit on the number of iterations to guard against oscillating, slowly convergent, or divergent solutions that could persist interminably.
4. The program should alert the user and take account of the possibility that $f'(x)$ might equal zero at any time during the computation.

6.3 THE SECANT METHOD

A potential problem in implementing the Newton-Raphson method is the evaluation of the derivative. Although this is not inconvenient for polynomials and many other functions, there are certain functions whose derivatives may be extremely difficult or inconvenient to evaluate. For these cases, the derivative can be approximated by a backward finite divided difference, as in (Fig. 6.7)

$$f'(x_i) \cong \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i}$$

FIGURE 6.7
Graphical depiction of the secant method. This technique is similar to the Newton-Raphson technique (Fig. 6.5) in the sense that an estimate of the root is predicted by extrapolating a tangent of the function to the x axis. However, the secant method uses a difference rather than a derivative to estimate the slope.