

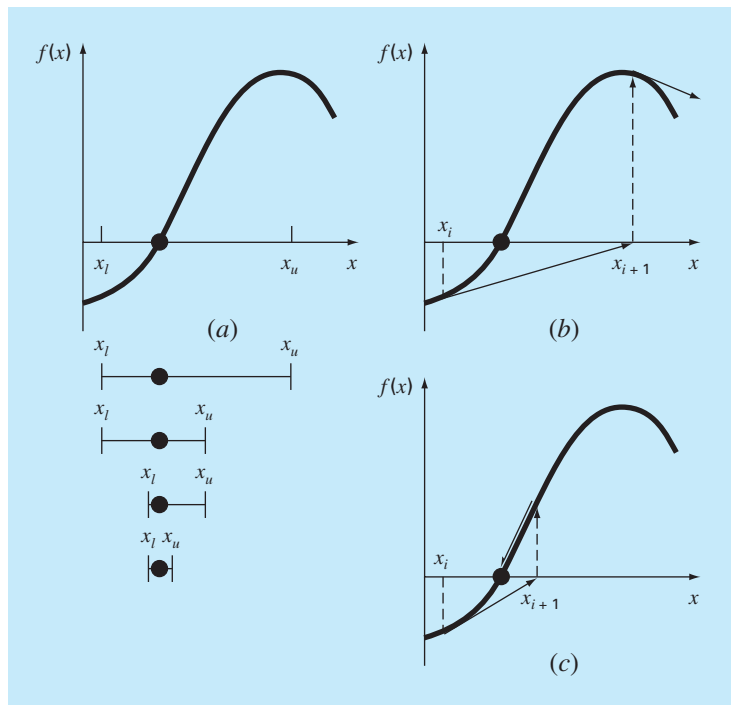
Open Methods

For the bracketing methods in Chap. 5, 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. 6.1a).

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

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.



necessarily bracket 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. 6.2a 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. 6.2b). 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.

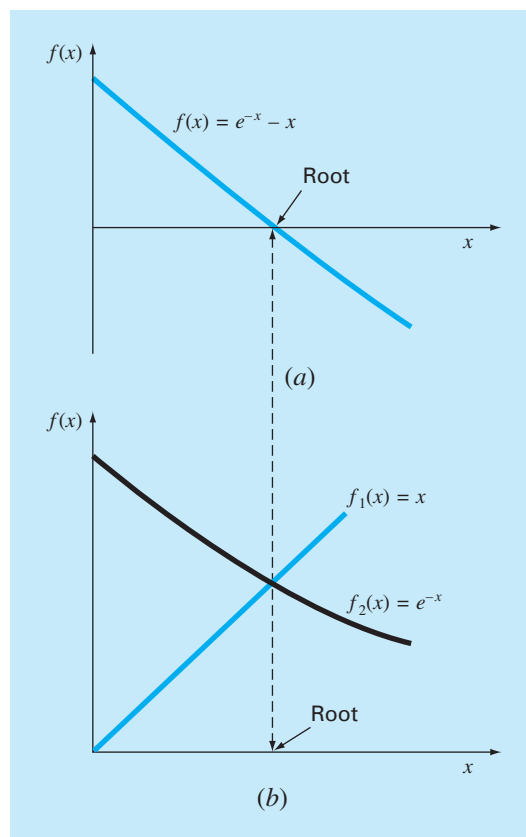
Solution. Reformulate the equation as $y_1 = x$ and $y_2 = e^{-x}$. The following values can be computed:

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 reexpressed 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. 6.3a), 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:

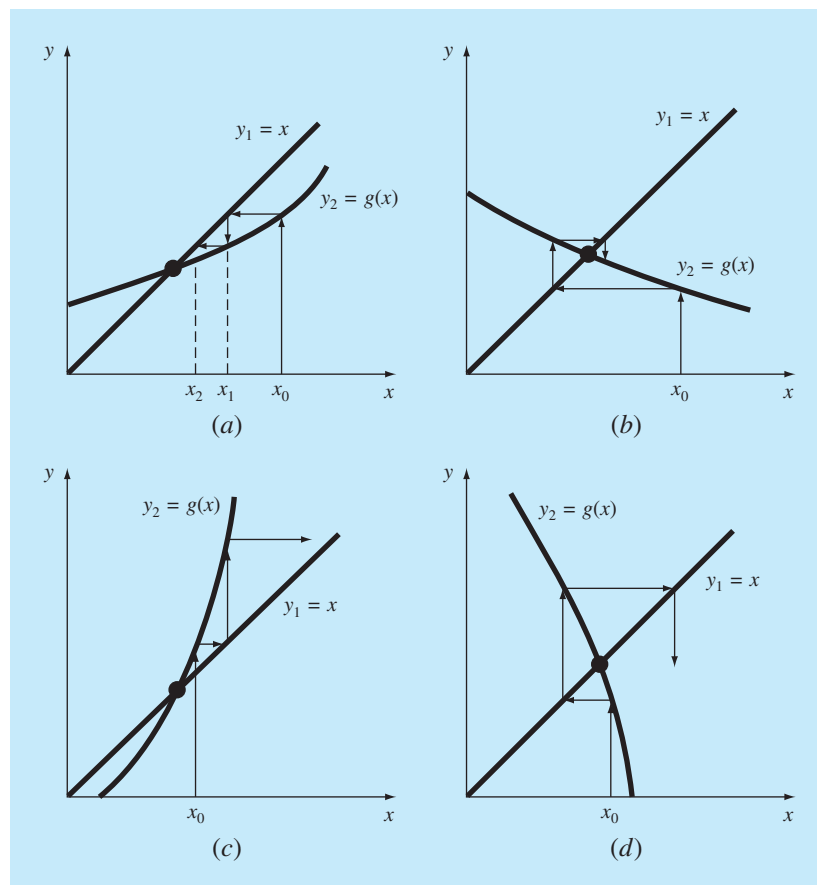
$$x_1 = g(x_0)$$

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 is equivalent to the equation

$$x_2 = g(x_1)$$

FIGURE 6.3

Iteration cobwebs depicting convergence (a and b) and divergence (c and d) 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

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

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 $a \leq x \leq b$, then there exists at least one value of $x = \xi$ within the interval such that

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

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

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

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. 6.3a and c). If the derivative is negative, the errors will oscillate (Fig. 6.3b 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*.

The solution in Fig. 6.3a is *convergent* because the estimates of x move closer to the root with each iteration. The same is true for Fig. 6.3b. However, this is not the case for Fig. 6.3c 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.

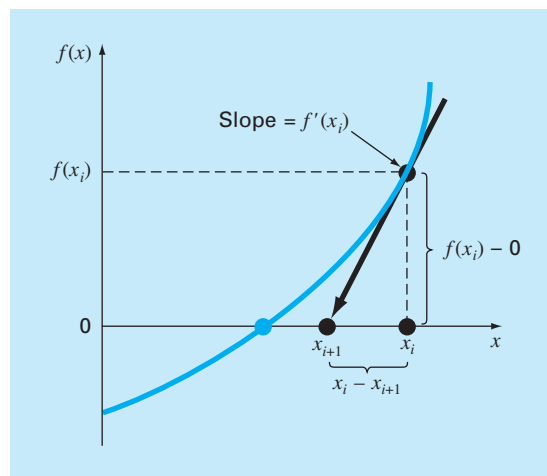
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FUNCTION Fixpt(x0, es, imax, iter, ea)
  xr = x0
  iter = 0
  DO
    xrold = xr
    xr = g(xrold)
    iter = iter + 1
    IF xr ≠ 0 THEN
      ea =  $\left| \frac{xr - xrold}{xr} \right| \cdot 100$ 
    END IF
    IF ea < es OR iter ≥ imax EXIT
  END 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} .