When complex roots are possible, the bracketing methods cannot be used because of the obvious problem that the criterion for defining a bracket (that is, sign change) does not translate to complex guesses.

Of the open methods, the conventional Newton-Raphson method would provide a viable approach. In particular, concise code including deflation can be developed. If a language that accommodates complex variables (like Fortran) is used, such an algorithm will locate both real and complex roots. However, as might be expected, it would be susceptible to convergence problems. For this reason, special methods have been developed to find the real and complex roots of polynomials. We describe two—the Müller and Bairstow methods—in the following sections. As you will see, both are related to the more conventional open approaches described in Chap. 6.

7.4 MÜLLER'S METHOD

Recall that the secant method obtains a root estimate by projecting a straight line to the x axis through two function values (Fig. 7.3*a*). Müller's method takes a similar approach, but projects a parabola through three points (Fig. 7.3*b*).

The method consists of deriving the coefficients of the parabola that goes through the three points. These coefficients can then be substituted into the quadratic formula to obtain the point where the parabola intercepts the x axis—that is, the root estimate. The approach is facilitated by writing the parabolic equation in a convenient form,

$$f_2(x) = a(x - x_2)^2 + b(x - x_2) + c \tag{7.17}$$

We want this parabola to intersect the three points $[x_0, f(x_0)]$, $[x_1, f(x_1)]$, and $[x_2, f(x_2)]$. The coefficients of Eq. (7.17) can be evaluated by substituting each of the three points to give

$$f(x_0) = a(x_0 - x_2)^2 + b(x_0 - x_2) + c \tag{7.18}$$

$$f(x_1) = a(x_1 - x_2)^2 + b(x_1 - x_2) + c \tag{7.19}$$

$$f(x_2) = a(x_2 - x_2)^2 + b(x_2 - x_2) + c \tag{7.20}$$

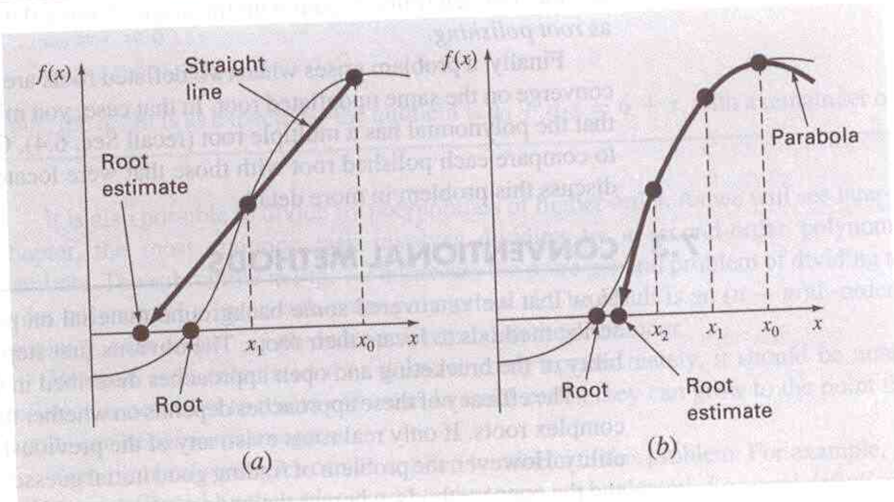

FIGURE 7.3
A comparison of two related approaches for locating roots: (*a*) the secant method and (*b*) Müller's method.

Note that we have dropped the subscript "2" from the function for conciseness. Because we have three equations, we can solve for the three unknown coefficients, a, b, and c. Because two of the terms in Eq. (7.20) are zero, it can be immediately solved for $c = f(x_2)$. Thus, the coefficient c is merely equal to the function value evaluated at the third guess, x_2. This result can then be substituted into Eqs. (7.18) and (7.19) to yield two equations with two unknowns:

$$f(x_0) - f(x_2) = a(x_0 - x_2)^2 + b(x_0 - x_2) \tag{7.21}$$

$$f(x_1) - f(x_2) = a(x_1 - x_2)^2 + b(x_1 - x_2) \tag{7.22}$$

Algebraic manipulation can then be used to solve for the remaining coefficients, a and b. One way to do this involves defining a number of differences,

$$h_0 = x_1 - x_0 \qquad h_1 = x_2 - x_1$$
$$\delta_0 = \frac{f(x_1) - f(x_0)}{x_1 - x_0} \qquad \delta_1 = \frac{f(x_2) - f(x_1)}{x_2 - x_1} \tag{7.23}$$

These can be substituted into Eqs. (7.21) and (7.22) to give

$$(h_0 + h_1)b - (h_0 + h_1)^2 a = h_0\delta_0 + h_1\delta_1$$
$$h_1 \quad b - \quad h_1^2 \quad a = \quad h_1\delta_1$$

which can be solved for a and b. The results can be summarized as

$$a = \frac{\delta_1 - \delta_0}{h_1 + h_0} \tag{7.24}$$

$$b = ah_1 + \delta_1 \tag{7.25}$$

$$c = f(x_2) \tag{7.26}$$

To find the root, we apply the quadratic formula to Eq. (7.17). However, because of potential round-off error, rather than using the conventional form, we use the alternative formulation [Eq. (3.13)] to yield

$$x_3 - x_2 = \frac{-2c}{b \pm \sqrt{b^2 - 4ac}} \tag{7.27a}$$

or isolating the unknown x_3 on the left side of the equal sign,

$$x_3 = x_2 + \frac{-2c}{b \pm \sqrt{b^2 - 4ac}} \tag{7.27b}$$

Note that the use of the quadratic formula means that both real and complex roots can be located. This is a major benefit of the method.

In addition, Eq. (7.27a) provides a neat means to determine the approximate error. Because the left side represents the difference between the present (x_3) and the previous (x_2) root estimate, the error can be calculated as

$$\varepsilon_a = \left|\frac{x_3 - x_2}{x_3}\right| 100\%$$

Now, a problem with Eq. (7.27*a*) is that it yields two roots, corresponding to the ± term in the denominator. In Müller's method, the sign is chosen to agree with the sign of b. This choice will result in the largest denominator, and hence, will give the root estimate that is closest to x_2.

Once x_3 is determined, the process is repeated. This brings up the issue of which point is discarded. Two general strategies are typically used:

1. If only real roots are being located, we choose the two original points that are nearest the new root estimate, x_3.
2. If both real and complex roots are being evaluated, a sequential approach is employed. That is, just like the secant method, x_1, x_2, and x_3 take the place of x_0, x_1, and x_2.

EXAMPLE 7.2 Müller's Method

Problem Statement. Use Müller's method with guesses of x_0, x_1, and $x_2 = 4.5$, 5.5, and 5 to determine a root of the equation

$$f(x) = x^3 - 13x - 12$$

Note that the roots of this equation are −3, −1, and 4.

Solution. First, we evaluate the function at the guesses

$$f(4.5) = 20.625 \qquad f(5.5) = 82.875 \qquad f(5) = 48$$

which can be used to calculate

$$h_0 = 5.5 - 4.5 = 1 \qquad h_1 = 5 - 5.5 = -0.5$$

$$\delta_0 = \frac{82.875 - 20.625}{5.5 - 4.5} = 62.25 \qquad \delta_1 = \frac{48 - 82.875}{5 - 5.5} = 69.75$$

These values in turn can be substituted into Eqs. (7.24) through (7.26) to compute

$$a = \frac{69.75 - 62.25}{-0.5 + 1} = 15 \qquad b = 15(-0.5) + 69.75 = 62.25 \qquad c = 48$$

The square root of the discriminant can be evaluated as

$$\sqrt{62.25^2 - 4(15)48} = 31.54461$$

Then, because $|62.25 + 31.54451| > |62.25 - 31.54451|$, a positive sign is employed in the denominator of Eq. (7.27*b*), and the new root estimate can be determined as

$$x_3 = 5 + \frac{-2(48)}{62.25 + 31.54451} = 3.976487$$

and develop the error estimate

$$\varepsilon_a = \left|\frac{-1.023513}{3.976487}\right| 100\% = 25.74\%$$

Because the error is large, new guesses are assigned; x_0 is replaced by x_1, x_1 is replaced by x_2, and x_2 is replaced by x_3. Therefore, for the new iteration,

$$x_0 = 5.5 \qquad x_1 = 5 \qquad x_2 = 3.976487$$

and the calculation is repeated. The results, tabulated below, show that the method converges rapidly on the root, $x_r = 4$:

i	x_r	ε_a(%)
0	5	
1	3.976487	25.74
2	4.00105	0.6139
3	4	0.0262
4	4	0.0000119

Pseudocode to implement Müller's method for real roots is presented in Fig. 7.4. Notice that this routine is set up to take a single initial nonzero guess that is then perturbed to

FIGURE 7.4
Pseudocode for Müller's method.

```
SUB Muller(xr, h, eps, maxit)
x2 = xr
x1 = xr + h*xr
x0 = xr - h*xr
DO
  iter = iter + 1
  h0 = x1 - x0
  h1 = x2 - x1
  d0 = (f(x1) - f(x0)) / h0
  d1 = (f(x2) - f(x1)) / h1
  a = (d1 - d0) / (h1 + h0)
  b = a*h1 + d1
  c = f(x2)
  rad = SQRT(b*b - 4*a*c)
  If |b+rad| > |b-rad| THEN
    den = b + rad
  ELSE
    den = b - rad
  END IF
  dxr = -2*c / den
  xr = x2 + dxr
  PRINT iter, xr
  IF (|dxr| < eps*xr  OR  iter > maxit) EXIT
  x0 = x1
  x1 = x2
  x2 = xr
END DO
END Müller
```

develop the other two guesses. Of course, the algorithm can also be programmed to accommodate three guesses. For languages like Fortran, the code will find complex roots if the proper variables are declared as complex.

7.5 BAIRSTOW'S METHOD

Bairstow's method is an iterative approach related loosely to both the Müller and Newton-Raphson methods. Before launching into a mathematical description of the technique, recall the factored form of the polynomial,

$$f_5(x) = (x+1)(x-4)(x-5)(x+3)(x-2) \tag{7.28}$$

If we divided by a factor that is not a root (for example, $x + 6$), the quotient would be a fourth-order polynomial. However, for this case, a remainder would result.

On the basis of the above, we can elaborate on an algorithm for determining a root of a polynomial: (1) guess a value for the root $x = t$, (2) divide the polynomial by the factor $x - t$, and (3) determine whether there is a remainder. If not, the guess was perfect and the root is equal to t. If there is a remainder, the guess can be systematically adjusted and the procedure repeated until the remainder disappears and a root is located. After this is accomplished, the entire procedure can be repeated for the quotient to locate another root.

Bairstow's method is generally based on this approach. Consequently, it hinges on the mathematical process of dividing a polynomial by a factor. Recall from our discussion of polynomial deflation (Sec. 7.2.2) that synthetic division involves dividing a polynomial by a factor $x - t$. For example, the general polynomial [Eq. (7.1)]

$$f_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n \tag{7.29}$$

can be divided by the factor $x - t$ to yield a second polynomial that is one order lower,

$$f_{n-1}(x) = b_1 + b_2 x + b_3 x^2 + \cdots + b_n x^{n-1} \tag{7.30}$$

with a remainder $R = b_0$, where the coefficients can be calculated by the recurrence relationship

$$b_n = a_n$$
$$b_i = a_i + b_{i+1} t \qquad \text{for } i = n-1 \text{ to } 0$$

Note that if t were a root of the original polynomial, the remainder b_0 would equal zero.

To permit the evaluation of complex roots, Bairstow's method divides the polynomial by a quadratic factor $x^2 - rx - s$. If this is done to Eq. (7.29), the result is a new polynomial

$$f_{n-2}(x) = b_2 + b_3 x + \cdots + b_{n-1} x^{n-3} + b_n x^{n-2}$$

with a remainder

$$R = b_1(x - r) + b_0 \tag{7.31}$$

As with normal synthetic division, a simple recurrence relationship can be used to perform the division by the quadratic factor:

$$b_n = a_n \tag{7.32a}$$

$$b_{n-1} = a_{n-1} + rb_n \tag{7.32b}$$

$$b_i = a_i + rb_{i+1} + sb_{i+2} \qquad \text{for } i = n-2 \text{ to } 0 \tag{7.32c}$$

The quadratic factor is introduced to allow the determination of complex roots. This relates to the fact that, if the coefficients of the original polynomial are real, the complex roots occur in conjugate pairs. If $x^2 - rx - s$ is an exact divisor of the polynomial, complex roots can be determined by the quadratic formula. Thus, the method reduces to determining the values of r and s that make the quadratic factor an exact divisor. In other words, we seek the values that make the remainder term equal to zero.

Inspection of Eq. (7.31) leads us to conclude that for the remainder to be zero, b_0 and b_1 must be zero. Because it is unlikely that our initial guesses at the values of r and s will lead to this result, we must determine a systematic way to modify our guesses so that b_0 and b_1 approach zero. To do this, Bairstow's method uses a strategy similar to the Newton-Raphson approach. Because both b_0 and b_1 are functions of both r and s, they can be expanded using a Taylor series, as in [recall Eq. (4.26)]

$$\begin{aligned} b_1(r + \Delta r, s + \Delta s) &= b_1 + \frac{\partial b_1}{\partial r}\Delta r + \frac{\partial b_1}{\partial s}\Delta s \\ b_0(r + \Delta r, s + \Delta s) &= b_0 + \frac{\partial b_0}{\partial r}\Delta r + \frac{\partial b_0}{\partial s}\Delta s \end{aligned} \tag{7.33}$$

where the values on the right-hand side are all evaluated at r and s. Notice that second- and higher-order terms have been neglected. This represents an implicit assumption that $-r$ and $-s$ are small enough that the higher-order terms are negligible. Another way of expressing this assumption is to say that the initial guesses are adequately close to the values of r and s at the roots.

The changes, Δr and Δs, needed to improve our guesses can be estimated by setting Eq. (7.33) equal to zero to give

$$\frac{\partial b_1}{\partial r}\Delta r + \frac{\partial b_1}{\partial s}\Delta s = -b_1 \tag{7.34}$$

$$\frac{\partial b_0}{\partial r}\Delta r + \frac{\partial b_0}{\partial s}\Delta s = -b_0 \tag{7.35}$$

If the partial derivatives of the b's can be determined, these are a system of two equations that can be solved simultaneously for the two unknowns, Δr and Δs. Bairstow showed that the partial derivatives can be obtained by a synthetic division of the b's in a fashion similar to the way in which the b's themselves were derived:

$$c_n = b_n \tag{7.36a}$$

$$c_{n-1} = b_{n-1} + rc_n \tag{7.36b}$$

$$c_i = b_i + rc_{i+1} + sc_{i+2} \qquad \text{for } i = n-2 \text{ to } 1 \tag{7.36c}$$

where $\partial b_0/\partial r = c_1$, $\partial b_0/\partial s = \partial b_1/\partial r = c_2$, and $\partial b_1/\partial s = c_3$. Thus, the partial derivatives are obtained by synthetic division of the b's. Then the partial derivatives can be substituted into Eqs. (7.34) and (7.35) along with the b's to give

$$c_2\Delta r + c_3\Delta s = -b_1$$
$$c_1\Delta r + c_2\Delta s = -b_0$$

These equations can be solved for Δr and Δs, which can in turn be employed to improve the initial guesses of r and s. At each step, an approximate error in r and s can be estimated, as in

$$|\varepsilon_{a,r}| = \left|\frac{\Delta r}{r}\right| 100\% \tag{7.37}$$

and

$$|\varepsilon_{a,s}| = \left|\frac{\Delta s}{s}\right| 100\% \tag{7.38}$$

When both of these error estimates fall below a prespecified stopping criterion ε_s, the values of the roots can be determined by

$$x = \frac{r \pm \sqrt{r^2 + 4s}}{2} \tag{7.39}$$

At this point, three possibilities exist:

1. *The quotient is a third-order polynomial or greater.* For this case, Bairstow's method would be applied to the quotient to evaluate new values for r and s. The previous values of r and s can serve as the starting guesses for this application.
2. *The quotient is a quadratic.* For this case, the remaining two roots could be evaluated directly with Eq. (7.39).
3. *The quotient is a first-order polynomial.* For this case, the remaining single root can be evaluated simply as

$$x = -\frac{s}{r} \tag{7.40}$$

EXAMPLE 7.3 Bairstow's Method

Problem Statement. Employ Bairstow's method to determine the roots of the polynomial

$$f_5(x) = x^5 - 3.5x^4 + 2.75x^3 + 2.125x^2 - 3.875x + 1.25$$

Use initial guesses of $r = s = -1$ and iterate to a level of $\varepsilon_s = 1\%$.

Solution. Equations (7.32) and (7.36) can be applied to compute

$$b_5 = 1 \quad b_4 = -4.5 \quad b_3 = 6.25 \quad b_2 = 0.375 \quad b_1 = -10.5$$
$$b_0 = 11.375$$
$$c_5 = 1 \quad c_4 = -5.5 \quad c_3 = 10.75 \quad c_2 = -4.875 \quad c_1 = -16.375$$

Thus, the simultaneous equations to solve for Δr and Δs are

$$-4.875\Delta r + 10.75\Delta s = 10.5$$
$$-16.375\Delta r - 4.875\Delta s = -11.375$$

which can be solved for $\Delta r = 0.3558$ and $\Delta s = 1.1381$. Therefore, our original guesses can be corrected to

$$r = -1 + 0.3558 = -0.6442$$
$$s = -1 + 1.1381 = 0.1381$$

and the approximate errors can be evaluated by Eqs. (7.37) and (7.38),

$$|\varepsilon_{a,r}| = \left|\frac{0.3558}{-0.6442}\right|100\% = 55.23\% \qquad |\varepsilon_{a,s}| = \left|\frac{1.1381}{0.1381}\right|100\% = 824.1\%$$

Next, the computation is repeated using the revised values for r and s. Applying Eqs. (7.32) and (7.36) yields

$$b_5 = 1 \quad b_4 = -4.1442 \quad b_3 = 5.5578 \quad b_2 = -2.0276 \quad b_1 = -1.8013$$
$$b_0 = 2.1304$$
$$c_5 = 1 \quad c_4 = -4.7884 \quad c_3 = 8.7806 \quad c_2 = -8.3454 \quad c_1 = 4.7874$$

Therefore, we must solve

$$-8.3454\Delta r + 8.7806\Delta s = 1.8013$$
$$4.7874\Delta r - 8.3454\Delta s = -2.1304$$

for $\Delta r = 0.1331$ and $\Delta s = 0.3316$, which can be used to correct the root estimates as

$$r = -0.6442 + 0.1331 = -0.5111 \qquad |\varepsilon_{a,r}| = 26.0\%$$
$$s = 0.1381 + 0.3316 = 0.4697 \qquad |\varepsilon_{a,s}| = 70.6\%$$

The computation can be continued, with the result that after four iterations the method converges on values of $r = -0.5$ ($|\varepsilon_{a,r}| = 0.063\%$) and $s = 0.5$ ($|\varepsilon_{a,s}| = 0.040\%$). Equation (7.39) can then be employed to evaluate the roots as

$$x = \frac{-0.5 \pm \sqrt{(-0.5)^2 + 4(0.5)}}{2} = 0.5, -1.0$$

At this point, the quotient is the cubic equation

$$f(x) = x^3 - 4x^2 + 5.25x - 2.5$$

Bairstow's method can be applied to this polynomial using the results of the previous step, $r = -0.5$ and $s = 0.5$, as starting guesses. Five iterations yield estimates of $r = 2$ and $s = -1.249$, which can be used to compute

$$x = \frac{2 \pm \sqrt{2^2 + 4(-1.249)}}{2} = 1 \pm 0.499i$$

At this point, the quotient is a first-order polynomial that can be directly evaluated by Eq. (7.40) to determine the fifth root: 2.

Note that the heart of Bairstow's method is the evaluation of the b's and c's via Eqs. (7.32) and (7.36). One of the primary strengths of the method is the concise way in which these recurrence relationships can be programmed.

Figure 7.5 lists pseudocode to implement Bairstow's method. The heart of the algorithm consists of the loop to evaluate the b's and c's. Also notice that the code to solve the simultaneous equations checks to prevent division by zero. If this is the case, the values of r and s are perturbed slightly and the procedure is begun again. In addition, the algorithm