Muller's Method

Recall that the secant method obtains a root estimate by projecting a straight line to the x axis through two function values . Müller's method takes a similar approach, but projects a parabola through three points (Fig. 1). 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,

$$f(x) = a(x - x_0)^2 + b(x - x_0) + c \tag{1}$$

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. (1) can be evaluated by substituting each of the three points to give

$$f_0 = f(x_0) = a(x_0 - x_0)^2 + b(x_0 - x_0) + c \tag{2}$$

$$f_1 = f(x_1) = a(x_1 - x_0)^2 + b(x_1 - x_0) + c \tag{3}$$

$$f_2 = f(x_2) = a(x_2 - x_0)^2 + b(x_2 - x_0) + c \tag{4}$$

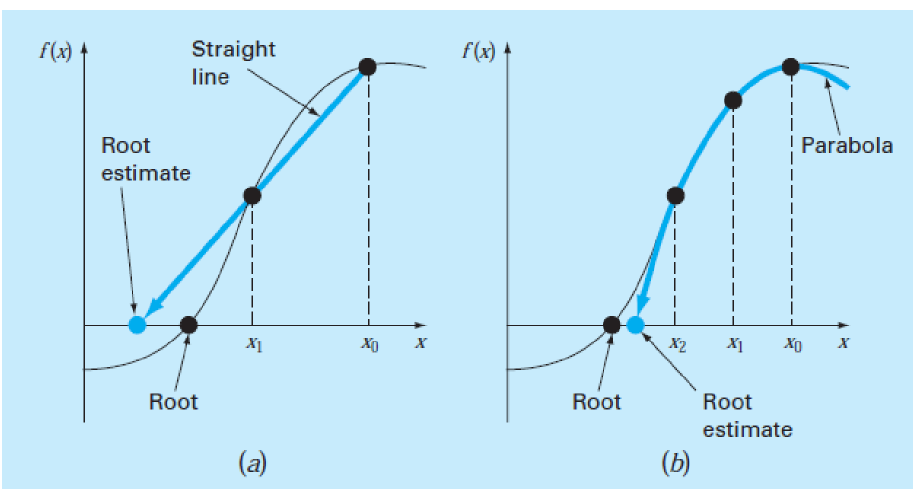

Figure 1: A comparison of two related approaches for locating roots: (a)Secant mehtod (b)Muller method

we can solve for the three unknown coefficients, a, b, and c. Because two of the terms in Eq. (2) are zero, it can be immediately solved for

$$c = f_0 = f(x_0) \tag{5}$$

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. (3) and (4) to yield two equations with two unknowns:

$$f_1 - f_0 = a(x_1 - x_0)^2 + b(x_1 - x_0) \tag{6}$$

$$f_2 - f_0 = a(x_2 - x_0)^2 + b(x_2 - x_0) \tag{7}$$

Algebraic manipulation can then be used to solve for the remaining coefficients, a and b. From Eq.(6)

$$\frac{f_1 - f_0}{x_1 - x_0} = a\left(x_1 - x_0\right) + b \tag{8}$$

$$\frac{f_2 - f_0}{x_2 - x_0} = a\left(x_2 - x_0\right) + b \tag{9}$$

Let $h_1 = x_1 - x_0$ and $h_2 = x_0 - x_2$ then equations (8) and (9) become

$$\frac{f_1 - f_0}{h_1} = ah_1 + b \tag{10}$$

$$-\frac{f_2 - f_0}{h_2} = -ah_2 + b \tag{11}$$

$$\Rightarrow \frac{f_2 - f_0}{h_2} = ah_2 - b \tag{12}$$

adding (10) and (12)

$$\frac{f_1 - f_0}{h_1} + \frac{f_2 - f_0}{h_2} = ah_1 + ah_2$$

$$\Rightarrow \frac{h_2\left(f_1 - f_0\right) + h_1\left(f_2 - f_0\right)}{h_1 h_2} = a\left(h_1 + h_2\right)$$

$$\Rightarrow \frac{h_2 f_1 - h_2 f_0 + h_1 f_2 - h_1 f_0}{h_1 h_2\left(h_1 + h_2\right)} = a$$

$$\Rightarrow \frac{h_2 f_1 - \left(h_2 + h_1\right) f_0 + h_1 f_2}{h_1 h_2\left(h_1 + h_2\right)} = a \tag{13}$$

from equation (10) we get

$$\frac{f_1 - f_0}{h_1} - ah_1 = b$$

$$\frac{f_1 - f_0 - ah_1^2}{h_1} = b \tag{14}$$

To find the root, we apply the quadratic formula to Eq.(1). However, because of potential round-off error, rather than using the conventional form, we use the alternative formulation to yield

$$x = x_0 - \frac{2c}{b \pm \sqrt{b^2 - 4ac}} \tag{15}$$

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.

Now, a problem with Eq. (15) is that it yields two roots, corresponding to the $\pm$ 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_0.

Once x 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.

(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.