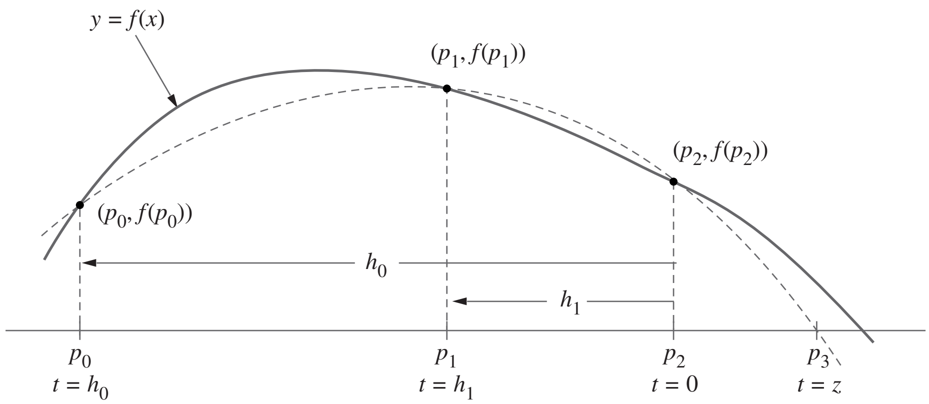

Figure 2.17 The starting approximations p_0, p_1, and p_2 for Muller's method, and the differences h_0 and h_1.

Muller's Method

Muller's method is a generalization of the secant method, in the sense that it does not require the derivative of the function. It is an iterative method that requires three starting points $(p_0, f(p_0))$, $(p_1, f(p_1))$, and $(p_2, f(p_2))$. A parabola is constructed that passes through the three points; then the quadratic formula is used to find a root of the quadratic for the next approximation. It has been proved that near a simple root Muller's method converges faster than the secant method and almost as fast as Newton's method. The method can be used to find real or complex zeros of a function and can be programmed to use complex arithmetic.

Without loss of generality, we assume that p_2 is the best approximation to the root and consider the parabola through the three starting values, shown in Figure 2.17. Make the change of variable

(9) $$t = x - p_2,$$

and use the differences

(10) $$h_0 = p_0 - p_2 \quad \text{and} \quad h_1 = p_1 - p_2.$$

Consider the quadratic polynomial involving the variable t:

(11) $$y = at^2 + bt + c.$$

Each point is used to obtain an equation involving a, b, and c:

$$\begin{aligned}
&\text{At } t = h_0: && ah_0^2 + bh_0 + c = f_0, \\
&\text{At } t = h_1: && ah_1^2 + bh_1 + c = f_1, \\
&\text{At } t = 0: && a0^2 + b0 \;\; + c = f_2.
\end{aligned} \tag{12}$$

From the third equation in (12), we see that

$$c = f_2. \tag{13}$$

Substituting (13) into the first two equations in (12) and using the definition $e_0 = f_0 - c$ and $e_1 = f_1 - c$ results in the linear system

$$\begin{aligned}
ah_0^2 + bh_0 &= f_0 - c = e_0, \\
ah_1^2 + bh_1 &= f_1 - c = e_1.
\end{aligned} \tag{14}$$

Solving the linear system for a and b results in

$$\begin{aligned}
a &= \frac{e_0 h_1 - e_1 h_0}{h_1 h_0^2 - h_0 h_1^2} \\
b &= \frac{e_1 h_0^2 - e_0 h_1^2}{h_1 h_0^2 - h_0 h_1^2}.
\end{aligned} \tag{15}$$

The quadratic formula is used to find the roots $t = z_1, z_2$ of (11):

$$z = \frac{-2c}{b \pm \sqrt{b^2 - 4ac}}. \tag{16}$$

Formula (16) is equivalent to the standard formula for the roots of a quadratic and is better in this case because we know that $c = f_2$.

To ensure the stability of the method, we choose the root in (16) that has the smallest absolute value. If $b > 0$, use the positive sign with the square root, and if $b < 0$, use the negative sign. Then p_3 is shown in Figure 2.17 and is given by

$$p_3 = p_2 + z. \tag{17}$$

To update the iterates, choose the new p_0 and the new p_1 to be the two values selected from among the old $\{p_0, p_1, p_3\}$ that lie closest to p_3 (i.e., throw out the one that is farthest away). Then take new p_2 to be old p_3. Although a lot of auxiliary calculations are done in Muller's method, it only requires one function evaluation per iteration.

If Muller's method is used to find the real roots of $f(x) = 0$, it is possible that one may encounter complex approximations, because the roots of the quadratic in (16) might be complex (nonzero imaginary components). In these cases the imaginary components will have a small magnitude and can be set equal to zero so that the calculations proceed with real numbers.

Table 2.12 Comparison of Convergences near a Simple Root

k	Secant method	Muller's method	Newton's method	Steffensen with Newton
0	−2.600000000	−2.600000000	−2.400000000	−2.400000000
1	−2.400000000	−2.500000000	−2.076190476	−2.076190476
2	−2.106598985	−2.400000000	−2.003596011	−2.003596011
3	−2.022641412	−1.985275287	−2.000008589	−1.982618143
4	−2.001511098	−2.000334062	−2.000000000	−2.000204982
5	−2.000022537	−2.000000218		−2.000000028
6	−2.000000022	−2.000000000		−2.000002389
7	−2.000000000			−2.000000000

Comparison of Methods

Steffensen's method can be used together with the Newton-Raphson fixed-point function $g(x) = x - f(x)/f'(x)$. In the next two examples we look at the roots of the polynomial $f(x) = x^3 - 3x + 2$. The Newton-Raphson function is $g(x) = (2x^3 - 2)/(3x^2 - 3)$. When this function is used in Program 2.7, we get the calculations under the heading Steffensen with Newton in Tables 2.12 and 2.13. For example, starting with $p_0 = -2.4$, we would compute

$$p_1 = g(p_0) = -2.076190476, \tag{18}$$

and

$$p_2 = g(p_1) = -2.003596011. \tag{19}$$

Then Aitken's improvement will give $p_3 = -1.982618143$.

Example 2.19 (Convergence near a Simple Root). This is a comparison of methods for the function $f(x) = x^3 - 3x + 2$ near the simple root $p = -2$.

Newton's method and the secant method for this function were given in Examples 2.14 and 2.16, respectively. Table 2.12 provides a summary of calculations for the methods. ■

Example 2.20 (Convergence near a Double Root). This is a comparison of the methods for the function $f(x) = x^3 - 3x + 2$ near the double root $p = 1$. Table 2.13 provides a summary of calculations. ■

Newton's method is the best choice for finding a simple root (see Table 2.12). At a double root, either Muller's method or Steffensen's method with the Newton-Raphson formula is a good choice (see Table 2.13). Note in the Aitken's acceleration formula (4) that division by zero can occur as the sequence $\{p_k\}$ converges. In this case, the last calculated approximation to zero should be used as the approximation to the zero of f.

Table 2.13 Comparison of Convergence Near a Double Root

k	Secant method	Muller's method	Newton's method	Steffensen with Newton
0	1.400000000	1.400000000	1.200000000	1.200000000
1	1.200000000	1.300000000	1.103030303	1.103030303
2	1.138461538	1.200000000	1.052356417	1.052356417
3	1.083873738	1.003076923	1.026400814	0.996890433
4	1.053093854	1.003838922	1.013257734	0.998446023
5	1.032853156	1.000027140	1.006643418	0.999223213
6	1.020429426	0.999997914	1.003325375	0.999999193
7	1.012648627	0.999999747	1.001663607	0.999999597
8	1.007832124	1.000000000	1.000832034	0.999999798
9	1.004844757		1.000416075	0.999999999
	$\vdots$		$\vdots$	

In the following program the sequence $\{p_k\}$, generated by Steffensen's method with the Newton-Raphson formula, is stored in a matrix $\boldsymbol{Q}$ that has `max1` rows and three columns. The first column of $\boldsymbol{Q}$ contains the initial approximation to the root, p_0, and the terms $p_3, p_6, \ldots, p_{3k}, \ldots$ generated by Aitken's acceleration method (4). The second and third columns of $\boldsymbol{Q}$ contain the terms generated by Newton's method. The stopping criteria in the program are based on the difference between consecutive terms from the first column of $\boldsymbol{Q}$.

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