The easiest way to construct a fixed-point problem associated with a root-finding problem $f(x) = 0$ is to add or subtract a multiple of $f(x)$ from x. Consider the sequence

$$p_n = g(p_{n-1}), \quad \text{for } n \geq 1,$$

for g in the form

$$g(x) = x - \phi(x) f(x),$$

where ϕ is a differentiable function that will be chosen later.

For the iterative procedure derived from g to be quadratically convergent, we need to have $g'(p) = 0$ when $f(p) = 0$. Because

$$g'(x) = 1 - \phi'(x) f(x) - f'(x)\phi(x),$$

and $f(p) = 0$, we have

$$g'(p) = 1 - \phi'(p) f(p) - f'(p)\phi(p) = 1 - \phi'(p) \cdot 0 - f'(p)\phi(p) = 1 - f'(p)\phi(p),$$

and $g'(p) = 0$ if and only if $\phi(p) = 1/f'(p)$.

If we let $\phi(x) = 1/f'(x)$, then we will ensure that $\phi(p) = 1/f'(p)$ and produce the quadratically convergent procedure

$$p_n = g(p_{n-1}) = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}.$$

This, of course, is simply Newton's method. Hence

- If $f(p) = 0$ and $f'(p) \neq 0$, then for starting values sufficiently close to p, Newton's method will converge at least quadratically.

Multiple Roots

In the preceding discussion, the restriction was made that $f'(p) \neq 0$, where p is the solution to $f(x) = 0$. In particular, Newton's method and the Secant method will generally give problems if $f'(p) = 0$ when $f(p) = 0$. To examine these difficulties in more detail, we make the following definition.

Definition 2.10 A solution p of $f(x) = 0$ is a **zero of multiplicity** m of f if for $x \neq p$, we can write $f(x) = (x - p)^m q(x)$, where $\lim_{x \to p} q(x) \neq 0$. ■

For polynomials, p is a zero of multiplicity m of f if $f(x) = (x - p)^m q(x)$, where $q(p) \neq 0$.

In essence, $q(x)$ represents that portion of $f(x)$ that does not contribute to the zero of f. The following result gives a means to easily identify **simple** zeros of a function, those that have multiplicity one.

Theorem 2.11 The function $f \in C^1[a, b]$ has a simple zero at p in (a, b) if and only if $f(p) = 0$, but $f'(p) \neq 0$. ■

Proof If f has a simple zero at p, then $f(p) = 0$ and $f(x) = (x - p)q(x)$, where $\lim_{x \to p} q(x) \neq 0$. Since $f \in C^1[a, b]$,

$$f'(p) = \lim_{x \to p} f'(x) = \lim_{x \to p} [q(x) + (x - p)q'(x)] = \lim_{x \to p} q(x) \neq 0.$$

Conversely, if $f(p) = 0$, but $f'(p) \neq 0$, expand f in a zeroth Taylor polynomial about p. Then

$$f(x) = f(p) + f'(\xi(x))(x - p) = (x - p) f'(\xi(x)),$$

where $\xi(x)$ is between x and p. Since $f \in C^1[a,b]$,

$$\lim_{x\to p} f'(\xi(x)) = f'\left(\lim_{x\to p} \xi(x)\right) = f'(p) \neq 0.$$

Letting $q = f' \circ \xi$ gives $f(x) = (x-p)q(x)$, where $\lim_{x\to p} q(x) \neq 0$. Thus f has a simple zero at p. ■ ■ ■

The following generalization of Theorem 2.11 is considered in Exercise 12.

Theorem 2.12 The function $f \in C^m[a,b]$ has a zero of multiplicity m at p in (a,b) if and only if

$$0 = f(p) = f'(p) = f''(p) = \cdots = f^{(m-1)}(p), \quad \text{but} \quad f^{(m)}(p) \neq 0. \qquad ■$$

The result in Theorem 2.12 implies that an interval about p exists where Newton's method converges quadratically to p for any initial approximation $p_0 = p$, provided that p is a simple zero. The following example shows that quadratic convergence might not occur if the zero is not simple.

Example 1 Let $f(x) = e^x - x - 1$. **(a)** Show that f has a zero of multiplicity 2 at $x = 0$. **(b)** Show that Newton's method with $p_0 = 1$ converges to this zero but not quadratically.

Solution **(a)** We have

$$f(x) = e^x - x - 1, \qquad f'(x) = e^x - 1 \qquad \text{and} \qquad f''(x) = e^x,$$

so

$$f(0) = e^0 - 0 - 1 = 0, \qquad f'(0) = e^0 - 1 = 0 \qquad \text{and} \qquad f''(0) = e^0 = 1.$$

Theorem 2.12 implies that f has a zero of multiplicity 2 at $x = 0$.

(b) The first two terms generated by Newton's method applied to f with $p_0 = 1$ are

$$p_1 = p_0 - \frac{f(p_0)}{f'(p_0)} = 1 - \frac{e-2}{e-1} \approx 0.58198,$$

and

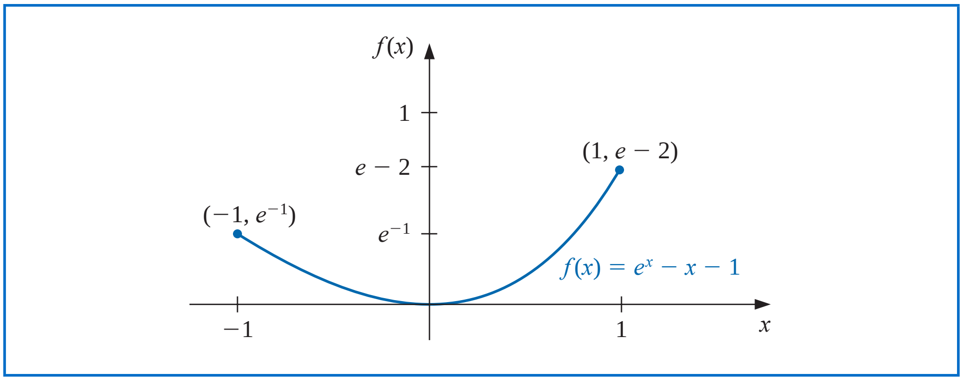
$$p_2 = p_1 - \frac{f(p_1)}{f'(p_1)} \approx 0.58198 - \frac{0.20760}{0.78957} \approx 0.31906.$$

The first sixteen terms of the sequence generated by Newton's method are shown in Table 2.8. The sequence is clearly converging to 0, but not quadratically. The graph of f is shown in Figure 2.12. ■

Table 2.8

n	p_n
0	1.0
1	0.58198
2	0.31906
3	0.16800
4	0.08635
5	0.04380
6	0.02206
7	0.01107
8	0.005545
9	2.7750×10^{-3}
10	1.3881×10^{-3}
11	6.9411×10^{-4}
12	3.4703×10^{-4}
13	1.7416×10^{-4}
14	8.8041×10^{-5}
15	4.2610×10^{-5}
16	1.9142×10^{-6}

Figure 2.12



One method of handling the problem of multiple roots of a function f is to define

$$\mu(x) = \frac{f(x)}{f'(x)}.$$

If p is a zero of f of multiplicity m with $f(x) = (x-p)^m q(x)$, then

$$\mu(x) = \frac{(x-p)^m q(x)}{m(x-p)^{m-1}q(x) + (x-p)^m q'(x)}$$
$$= (x-p)\frac{q(x)}{mq(x) + (x-p)q'(x)}$$

also has a zero at p. However, $q(p) \neq 0$, so

$$\frac{q(p)}{mq(p) + (p-p)q'(p)} = \frac{1}{m} \neq 0,$$

and p is a simple zero of $\mu(x)$. Newton's method can then be applied to $\mu(x)$ to give

$$g(x) = x - \frac{\mu(x)}{\mu'(x)} = x - \frac{f(x)/f'(x)}{\{[f'(x)]^2 - [f(x)][f''(x)]\}/[f'(x)]^2}$$

which simplifies to

$$g(x) = x - \frac{f(x)f'(x)}{[f'(x)]^2 - f(x)f''(x)}. \tag{2.13}$$

If g has the required continuity conditions, functional iteration applied to g will be quadratically convergent regardless of the multiplicity of the zero of f. Theoretically, the only drawback to this method is the additional calculation of $f''(x)$ and the more laborious procedure of calculating the iterates. In practice, however, multiple roots can cause serious round-off problems because the denominator of (2.13) consists of the difference of two numbers that are both close to 0.

Example 2 In Example 1 it was shown that $f(x) = e^x - x - 1$ has a zero of multiplicity 2 at $x = 0$ and that Newton's method with $p_0 = 1$ converges to this zero but not quadratically. Show that the modification of Newton's method as given in Eq. (2.13) improves the rate of convergence.

Solution Modified Newton's method gives

$$p_1 = p_0 - \frac{f(p_0)f'(p_0)}{f'(p_0)^2 - f(p_0)f''(p_0)} = 1 - \frac{(e-2)(e-1)}{(e-1)^2 - (e-2)e} \approx -2.3421061 \times 10^{-1}.$$

This is considerably closer to 0 than the first term using Newton's method, which was 0.58918. Table 2.9 lists the first five approximations to the double zero at $x = 0$. The results were obtained using a system with ten digits of precision. The relative lack of improvement in the last two entries is due to the fact that using this system both the numerator and the denominator approach 0. Consequently there is a loss of significant digits of accuracy as the approximations approach 0. ■

Table 2.9

n	p_n
1	$-2.3421061 \times 10^{-1}$
2	$-8.4582788 \times 10^{-3}$
3	$-1.1889524 \times 10^{-5}$
4	$-6.8638230 \times 10^{-6}$
5	$-2.8085217 \times 10^{-7}$

The following illustrates that the modified Newton's method converges quadratically even when in the case of a simple zero.

Illustration In Section 2.2 we found that a zero of $f(x) = x^3 + 4x^2 - 10 = 0$ is $p = 1.36523001$. Here we will compare convergence for a simple zero using both Newton's method and the modified Newton's method listed in Eq. (2.13). Let

$$\textbf{(i)} \quad p_n = p_{n-1} - \frac{p_{n-1}^3 + 4p_{n-1}^2 - 10}{3p_{n-1}^2 + 8p_{n-1}}, \qquad \text{from Newton's method}$$

and, from the Modified Newton's method given by Eq. (2.13),

$$\textbf{(ii)} \quad p_n = p_{n-1} - \frac{(p_{n-1}^3 + 4p_{n-1}^2 - 10)(3p_{n-1}^2 + 8p_{n-1})}{(3p_{n-1}^2 + 8p_{n-1})^2 - (p_{n-1}^3 + 4p_{n-1}^2 - 10)(6p_{n-1} + 8)}.$$

With $p_0 = 1.5$, we have

Newton's method

$$p_1 = 1.37333333, \quad p_2 = 1.36526201, \quad \text{and} \quad p_3 = 1.36523001.$$

Modified Newton's method

$$p_1 = 1.35689898, \quad p_2 = 1.36519585, \quad \text{and} \quad p_3 = 1.36523001.$$

Both methods are rapidly convergent to the actual zero, which is given by both methods as p_3. Note, however, that in the case of a simple zero the original Newton's method requires substantially less computation. □

Maple contains Modified Newton's method as described in Eq. (2.13) in its *NumericalAnalysis* package. The options for this command are the same as those for the Bisection method. To obtain results similar to those in Table 2.9 we can use

with(*Student*[*NumericalAnalysis*])

$f := e^x - x - 1$

$\mathit{ModifiedNewton}\left(f, x = 1.0, \mathit{tolerance} = 10^{-10}, \mathit{output} = \mathit{sequence}, \mathit{maxiterations} = 20\right)$

Remember that there is sensitivity to round-off error in these calculations, so you might need to reset *Digits* in Maple to get the exact values in Table 2.9.

EXERCISE SET 2.4

1. Use Newton's method to find solutions accurate to within 10^{-5} to the following problems.
   a. $x^2 - 2xe^{-x} + e^{-2x} = 0, \quad \text{for } 0 \le x \le 1$
   b. $\cos(x + \sqrt{2}) + x(x/2 + \sqrt{2}) = 0, \quad \text{for } -2 \le x \le -1$
   c. $x^3 - 3x^2(2^{-x}) + 3x(4^{-x}) - 8^{-x} = 0, \quad \text{for } 0 \le x \le 1$
   d. $e^{6x} + 3(\ln 2)^2 e^{2x} - (\ln 8)e^{4x} - (\ln 2)^3 = 0, \quad \text{for } -1 \le x \le 0$
2. Use Newton's method to find solutions accurate to within 10^{-5} to the following problems.
   a. $1 - 4x\cos x + 2x^2 + \cos 2x = 0, \quad \text{for } 0 \le x \le 1$
   b. $x^2 + 6x^5 + 9x^4 - 2x^3 - 6x^2 + 1 = 0, \quad \text{for } -3 \le x \le -2$
   c. $\sin 3x + 3e^{-2x}\sin x - 3e^{-x}\sin 2x - e^{-3x} = 0, \quad \text{for } 3 \le x \le 4$
   d. $e^{3x} - 27x^6 + 27x^4e^x - 9x^2e^{2x} = 0, \quad \text{for } 3 \le x \le 5$
3. Repeat Exercise 1 using the modified Newton's method described in Eq. (2.13). Is there an improvement in speed or accuracy over Exercise 1?

4. Repeat Exercise 2 using the modified Newton's method described in Eq. (2.13). Is there an improvement in speed or accuracy over Exercise 2?

5. Use Newton's method and the modified Newton's method described in Eq. (2.13) to find a solution accurate to within 10^{-5} to the problem

$$e^{6x} + 1.441e^{2x} - 2.079e^{4x} - 0.3330 = 0, \quad \text{for } -1 \le x \le 0.$$

This is the same problem as 1(d) with the coefficients replaced by their four-digit approximations. Compare the solutions to the results in 1(d) and 2(d).

6. Show that the following sequences converge linearly to $p = 0$. How large must n be before $|p_n - p| \le 5 \times 10^{-2}$?

a. $p_n = \dfrac{1}{n}, \quad n \ge 1$

b. $p_n = \dfrac{1}{n^2}, \quad n \ge 1$

7. **a.** Show that for any positive integer k, the sequence defined by $p_n = 1/n^k$ converges linearly to $p = 0$.

b. For each pair of integers k and m, determine a number N for which $1/N^k < 10^{-m}$.

8. **a.** Show that the sequence $p_n = 10^{-2^n}$ converges quadratically to 0.

b. Show that the sequence $p_n = 10^{-n^k}$ does not converge to 0 quadratically, regardless of the size of the exponent $k > 1$.

9. **a.** Construct a sequence that converges to 0 of order 3.

b. Suppose $\alpha > 1$. Construct a sequence that converges to 0 zero of order α.

10. Suppose p is a zero of multiplicity m of f, where $f^{(m)}$ is continuous on an open interval containing p. Show that the following fixed-point method has $g'(p) = 0$:

$$g(x) = x - \frac{mf(x)}{f'(x)}.$$

11. Show that the Bisection Algorithm 2.1 gives a sequence with an error bound that converges linearly to 0.

12. Suppose that f has m continuous derivatives. Modify the proof of Theorem 2.11 to show that f has a zero of multiplicity m at p if and only if

$$0 = f(p) = f'(p) = \cdots = f^{(m-1)}(p), \quad \text{but } f^{(m)}(p) \ne 0.$$

13. The iterative method to solve $f(x) = 0$, given by the fixed-point method $g(x) = x$, where

$$p_n = g(p_{n-1}) = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})} - \frac{f''(p_{n-1})}{2f'(p_{n-1})}\left[\frac{f(p_{n-1})}{f'(p_{n-1})}\right]^2, \quad \text{for } n = 1, 2, 3, \ldots,$$

has $g'(p) = g''(p) = 0$. This will generally yield cubic ($\alpha = 3$) convergence. Expand the analysis of Example 1 to compare quadratic and cubic convergence.

14. It can be shown (see, for example, [DaB], pp. 228–229) that if $\{p_n\}_{n=0}^{\infty}$ are convergent Secant method approximations to p, the solution to $f(x) = 0$, then a constant C exists with $|p_{n+1} - p| \approx C\,|p_n - p|\,|p_{n-1} - p|$ for sufficiently large values of n. Assume $\{p_n\}$ converges to p of order α, and show that $\alpha = (1 + \sqrt{5})/2$. (*Note:* This implies that the order of convergence of the Secant method is approximately 1.62).

2.5 Accelerating Convergence

Theorem 2.8 indicates that it is rare to have the luxury of quadratic convergence. We now consider a technique called **Aitken's Δ^2 method** that can be used to accelerate the convergence of a sequence that is linearly convergent, regardless of its origin or application.