2.4 Error Analysis for Iterative Methods

In this section we investigate the order of convergence of functional iteration schemes and, as a means of obtaining rapid convergence, rediscover Newton's method. We also consider ways of accelerating the convergence of Newton's method in special circumstances. First, however, we need a new procedure for measuring how rapidly a sequence converges.

Order of Convergence

Definition 2.7 Suppose $\{p_n\}_{n=0}^{\infty}$ is a sequence that converges to p, with $p_n \neq p$ for all n. If positive constants λ and α exist with

$$\lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|^{\alpha}} = \lambda,$$

then $\{p_n\}_{n=0}^{\infty}$ **converges to p of order α, with asymptotic error constant λ.** ■

An iterative technique of the form $p_n = g(p_{n-1})$ is said to be of *order* α if the sequence $\{p_n\}_{n=0}^{\infty}$ converges to the solution $p = g(p)$ of order α.

In general, a sequence with a high order of convergence converges more rapidly than a sequence with a lower order. The asymptotic constant affects the speed of convergence but not to the extent of the order. Two cases of order are given special attention.

(i) If $\alpha = 1$ (and $\lambda < 1$), the sequence is **linearly convergent**.

(ii) If $\alpha = 2$, the sequence is **quadratically convergent**.

The next illustration compares a linearly convergent sequence to one that is quadratically convergent. It shows why we try to find methods that produce higher-order convergent sequences.

Illustration Suppose that $\{p_n\}_{n=0}^{\infty}$ is linearly convergent to 0 with

$$\lim_{n\to\infty} \frac{|p_{n+1}|}{|p_n|} = 0.5$$

and that $\{\tilde{p}_n\}_{n=0}^{\infty}$ is quadratically convergent to 0 with the same asymptotic error constant,

$$\lim_{n\to\infty} \frac{|\tilde{p}_{n+1}|}{|\tilde{p}_n|^2} = 0.5.$$

For simplicity we assume that for each n we have

$$\frac{|p_{n+1}|}{|p_n|} \approx 0.5 \quad \text{and} \quad \frac{|\tilde{p}_{n+1}|}{|\tilde{p}_n|^2} \approx 0.5.$$

For the linearly convergent scheme, this means that

$$|p_n - 0| = |p_n| \approx 0.5|p_{n-1}| \approx (0.5)^2|p_{n-2}| \approx \cdots \approx (0.5)^n|p_0|,$$

whereas the quadratically convergent procedure has

$$\begin{aligned} |\tilde{p}_n - 0| = |\tilde{p}_n| &\approx 0.5|\tilde{p}_{n-1}|^2 \approx (0.5)[0.5|\tilde{p}_{n-2}|^2]^2 = (0.5)^3|\tilde{p}_{n-2}|^4 \\ &\approx (0.5)^3[(0.5)|\tilde{p}_{n-3}|^2]^4 = (0.5)^7|\tilde{p}_{n-3}|^8 \\ &\approx \cdots \approx (0.5)^{2^n-1}|\tilde{p}_0|^{2^n}. \end{aligned}$$

Table 2.7 illustrates the relative speed of convergence of the sequences to 0 if $|p_0| = |\tilde{p}_0| = 1$.

Table 2.7

n	Linear Convergence Sequence $\{p_n\}_{n=0}^{\infty}$ $(0.5)^n$	Quadratic Convergence Sequence $\{\tilde{p}_n\}_{n=0}^{\infty}$ $(0.5)^{2^n-1}$
1	5.0000×10^{-1}	5.0000×10^{-1}
2	2.5000×10^{-1}	1.2500×10^{-1}
3	1.2500×10^{-1}	7.8125×10^{-3}
4	6.2500×10^{-2}	3.0518×10^{-5}
5	3.1250×10^{-2}	4.6566×10^{-10}
6	1.5625×10^{-2}	1.0842×10^{-19}
7	7.8125×10^{-3}	5.8775×10^{-39}

The quadratically convergent sequence is within 10^{-38} of 0 by the seventh term. At least 126 terms are needed to ensure this accuracy for the linearly convergent sequence. □

Quadratically convergent sequences are expected to converge much quicker than those that converge only linearly, but the next result implies that an arbitrary technique that generates a convergent sequences does so only linearly.

Theorem 2.8 Let $g \in C[a, b]$ be such that $g(x) \in [a, b]$, for all $x \in [a, b]$. Suppose, in addition, that g' is continuous on (a, b) and a positive constant $k < 1$ exists with

$$|g'(x)| \leq k, \quad \text{for all } x \in (a, b).$$

If $g'(p) \neq 0$, then for any number $p_0 \neq p$ in $[a, b]$, the sequence

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

converges only linearly to the unique fixed point p in $[a, b]$. ■

Proof We know from the Fixed-Point Theorem 2.4 in Section 2.2 that the sequence converges to p. Since g' exists on (a, b), we can apply the Mean Value Theorem to g to show that for any n,

$$p_{n+1} - p = g(p_n) - g(p) = g'(\xi_n)(p_n - p),$$

where ξ_n is between p_n and p. Since $\{p_n\}_{n=0}^{\infty}$ converges to p, we also have $\{\xi_n\}_{n=0}^{\infty}$ converging to p. Since g' is continuous on (a, b), we have

$$\lim_{n\to\infty} g'(\xi_n) = g'(p).$$

Thus

$$\lim_{n\to\infty} \frac{p_{n+1} - p}{p_n - p} = \lim_{n\to\infty} g'(\xi_n) = g'(p) \quad \text{and} \quad \lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|} = |g'(p)|.$$

Hence, if $g'(p) \neq 0$, fixed-point iteration exhibits linear convergence with asymptotic error constant $|g'(p)|$. ■ ■ ■

Theorem 2.8 implies that higher-order convergence for fixed-point methods of the form $g(p) = p$ can occur only when $g'(p) = 0$. The next result describes additional conditions that ensure the quadratic convergence we seek.

Theorem 2.9 Let p be a solution of the equation $x = g(x)$. Suppose that $g'(p) = 0$ and g'' is continuous with $|g''(x)| < M$ on an open interval I containing p. Then there exists a $\delta > 0$ such that, for $p_0 \in [p - \delta, p + \delta]$, the sequence defined by $p_n = g(p_{n-1})$, when $n \geq 1$, converges at least quadratically to p. Moreover, for sufficiently large values of n,

$$|p_{n+1} - p| < \frac{M}{2}|p_n - p|^2.$$

■

Proof Choose k in $(0, 1)$ and $\delta > 0$ such that on the interval $[p-\delta, p+\delta]$, contained in I, we have $|g'(x)| \leq k$ and g'' continuous. Since $|g'(x)| \leq k < 1$, the argument used in the proof of Theorem 2.6 in Section 2.3 shows that the terms of the sequence $\{p_n\}_{n=0}^{\infty}$ are contained in $[p - \delta, p + \delta]$. Expanding $g(x)$ in a linear Taylor polynomial for $x \in [p - \delta, p + \delta]$ gives

$$g(x) = g(p) + g'(p)(x - p) + \frac{g''(\xi)}{2}(x - p)^2,$$

where ξ lies between x and p. The hypotheses $g(p) = p$ and $g'(p) = 0$ imply that

$$g(x) = p + \frac{g''(\xi)}{2}(x - p)^2.$$

In particular, when $x = p_n$,

$$p_{n+1} = g(p_n) = p + \frac{g''(\xi_n)}{2}(p_n - p)^2,$$

with ξ_n between p_n and p. Thus,

$$p_{n+1} - p = \frac{g''(\xi_n)}{2}(p_n - p)^2.$$

Since $|g'(x)| \leq k < 1$ on $[p - \delta, p + \delta]$ and g maps $[p - \delta, p + \delta]$ into itself, it follows from the Fixed-Point Theorem that $\{p_n\}_{n=0}^{\infty}$ converges to p. But ξ_n is between p and p_n for each n, so $\{\xi_n\}_{n=0}^{\infty}$ also converges to p, and

$$\lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|^2} = \frac{|g''(p)|}{2}.$$

This result implies that the sequence $\{p_n\}_{n=0}^{\infty}$ is quadratically convergent if $g''(p) \neq 0$ and of higher-order convergence if $g''(p) = 0$.

Because g'' is continuous and strictly bounded by M on the interval $[p - \delta, p + \delta]$, this also implies that, for sufficiently large values of n,

$$|p_{n+1} - p| < \frac{M}{2}|p_n - p|^2.$$

■ ■ ■

Theorems 2.8 and 2.9 tell us that our search for quadratically convergent fixed-point methods should point in the direction of functions whose derivatives are zero at the fixed point. That is:

- For a fixed point method to converge quadratically we need to have both $g(p) = p$, and $g'(p) = 0$.

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

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

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.

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}

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

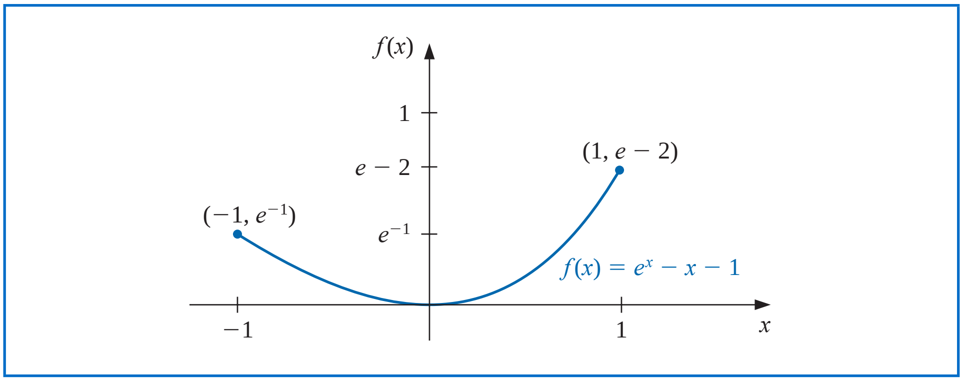
$$p_1 = p_0 - \frac{f(p_0)}{f'(p_0)} = 1 - \frac{e-2}{e-1} \approx 0.58198,$$

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. ■

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

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

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*])

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

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

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.** $x^2 - 2xe^{-x} + e^{-2x} = 0$, for $0 \le x \le 1$
   - **b.** $\cos(x + \sqrt{2}) + x(x/2 + \sqrt{2}) = 0$, for $-2 \le x \le -1$
   - **c.** $x^3 - 3x^2(2^{-x}) + 3x(4^{-x}) - 8^{-x} = 0$, for $0 \le x \le 1$
   - **d.** $e^{6x} + 3(\ln 2)^2 e^{2x} - (\ln 8)e^{4x} - (\ln 2)^3 = 0$, for $-1 \le x \le 0$
2. Use Newton's method to find solutions accurate to within 10^{-5} to the following problems.
   - **a.** $1 - 4x\cos x + 2x^2 + \cos 2x = 0$, for $0 \le x \le 1$
   - **b.** $x^2 + 6x^5 + 9x^4 - 2x^3 - 6x^2 + 1 = 0$, for $-3 \le x \le -2$
   - **c.** $\sin 3x + 3e^{-2x}\sin x - 3e^{-x}\sin 2x - e^{-3x} = 0$, for $3 \le x \le 4$
   - **d.** $e^{3x} - 27x^6 + 27x^4e^x - 9x^2e^{2x} = 0$, 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

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

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 $|p_n - p| \leq 5 \times 10^{-2}$?

a. $p_n = \dfrac{1}{n}, \quad n \geq 1$ **b.** $p_n = \dfrac{1}{n^2}, \quad n \geq 1$

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

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

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.

Aitken's Δ^2 Method

Alexander Aitken (1895-1967) used this technique in 1926 to accelerate the rate of convergence of a series in a paper on algebraic equations [Ai]. This process is similar to one used much earlier by the Japanese mathematician Takakazu Seki Kowa (1642-1708).

Suppose $\{p_n\}_{n=0}^{\infty}$ is a linearly convergent sequence with limit p. To motivate the construction of a sequence $\{\hat{p}_n\}_{n=0}^{\infty}$ that converges more rapidly to p than does $\{p_n\}_{n=0}^{\infty}$, let us first assume that the signs of $p_n - p$, $p_{n+1} - p$, and $p_{n+2} - p$ agree and that n is sufficiently large that

$$\frac{p_{n+1} - p}{p_n - p} \approx \frac{p_{n+2} - p}{p_{n+1} - p}.$$

Then

$$(p_{n+1} - p)^2 \approx (p_{n+2} - p)(p_n - p),$$

so

$$p_{n+1}^2 - 2p_{n+1}p + p^2 \approx p_{n+2}p_n - (p_n + p_{n+2})p + p^2$$

and

$$(p_{n+2} + p_n - 2p_{n+1})p \approx p_{n+2}p_n - p_{n+1}^2.$$

Solving for p gives

$$p \approx \frac{p_{n+2}p_n - p_{n+1}^2}{p_{n+2} - 2p_{n+1} + p_n}.$$

Adding and subtracting the terms p_n^2 and $2p_np_{n+1}$ in the numerator and grouping terms appropriately gives

$$\begin{aligned} p &\approx \frac{p_np_{n+2} - 2p_np_{n+1} + p_n^2 - p_{n+1}^2 + 2p_np_{n+1} - p_n^2}{p_{n+2} - 2p_{n+1} + p_n} \\ &= \frac{p_n(p_{n+2} - 2p_{n+1} + p_n) - (p_{n+1}^2 - 2p_np_{n+1} + p_n^2)}{p_{n+2} - 2p_{n+1} + p_n} \\ &= p_n - \frac{(p_{n+1} - p_n)^2}{p_{n+2} - 2p_{n+1} + p_n}. \end{aligned}$$

Aitken's Δ^2 method is based on the assumption that the sequence $\{\hat{p}_n\}_{n=0}^{\infty}$, defined by

$$\hat{p}_n = p_n - \frac{(p_{n+1} - p_n)^2}{p_{n+2} - 2p_{n+1} + p_n}, \tag{2.14}$$

converges more rapidly to p than does the original sequence $\{p_n\}_{n=0}^{\infty}$.

Table 2.10

n	p_n	$\hat{p}_n$
1	0.54030	0.96178
2	0.87758	0.98213
3	0.94496	0.98979
4	0.96891	0.99342
5	0.98007	0.99541
6	0.98614	
7	0.98981	

Example 1 The sequence $\{p_n\}_{n=1}^{\infty}$, where $p_n = \cos(1/n)$, converges linearly to $p = 1$. Determine the first five terms of the sequence given by Aitken's Δ^2 method.

Solution In order to determine a term $\hat{p}_n$ of the Aitken's Δ^2 method sequence we need to have the terms p_n, p_{n+1}, and p_{n+2} of the original sequence. So to determine $\hat{p}_5$ we need the first 7 terms of $\{p_n\}$. These are given in Table 2.10. It certainly appears that $\{\hat{p}_n\}_{n=1}^{\infty}$ converges more rapidly to $p = 1$ than does $\{p_n\}_{n=1}^{\infty}$. ■

The Δ notation associated with this technique has its origin in the following definition.

Definition 2.13 For a given sequence $\{p_n\}_{n=0}^{\infty}$, the **forward difference** Δp_n (read "delta p_n") is defined by

$$\Delta p_n = p_{n+1} - p_n, \quad \text{for } n \geq 0.$$

Higher powers of the operator Δ are defined recursively by

$$\Delta^k p_n = \Delta(\Delta^{k-1} p_n), \quad \text{for } k \geq 2.$$ ▪

The definition implies that

$$\Delta^2 p_n = \Delta(p_{n+1} - p_n) = \Delta p_{n+1} - \Delta p_n = (p_{n+2} - p_{n+1}) - (p_{n+1} - p_n).$$

So $\Delta^2 p_n = p_{n+2} - 2p_{n+1} + p_n$, and the formula for $\hat{p}_n$ given in Eq. (2.14) can be written as

$$\hat{p}_n = p_n - \frac{(\Delta p_n)^2}{\Delta^2 p_n}, \quad \text{for } n \geq 0. \tag{2.15}$$

To this point in our discussion of Aitken's Δ^2 method, we have stated that the sequence $\{\hat{p}_n\}_{n=0}^{\infty}$, converges to p more rapidly than does the original sequence $\{p_n\}_{n=0}^{\infty}$, but we have not said what is meant by the term "more rapid" convergence. Theorem 2.14 explains and justifies this terminology. The proof of this theorem is considered in Exercise 16.

Theorem 2.14 Suppose that $\{p_n\}_{n=0}^{\infty}$ is a sequence that converges linearly to the limit p and that

$$\lim_{n\to\infty} \frac{p_{n+1} - p}{p_n - p} < 1.$$

Then the Aitken's Δ^2 sequence $\{\hat{p}_n\}_{n=0}^{\infty}$ converges to p faster than $\{p_n\}_{n=0}^{\infty}$ in the sense that

$$\lim_{n\to\infty} \frac{\hat{p}_n - p}{p_n - p} = 0.$$ ▪

Steffensen's Method

Johan Frederik Steffensen (1873–1961) wrote an influential book entitled *Interpolation* in 1927.

By applying a modification of Aitken's Δ^2 method to a linearly convergent sequence obtained from fixed-point iteration, we can accelerate the convergence to quadratic. This procedure is known as Steffensen's method and differs slightly from applying Aitken's Δ^2 method directly to the linearly convergent fixed-point iteration sequence. Aitken's Δ^2 method constructs the terms in order:

$$p_0, \quad p_1 = g(p_0), \quad p_2 = g(p_1), \quad \hat{p}_0 = \{\Delta^2\}(p_0),$$
$$p_3 = g(p_2), \quad \hat{p}_1 = \{\Delta^2\}(p_1), \ldots,$$

where $\{\Delta^2\}$ indicates that Eq. (2.15) is used. Steffensen's method constructs the same first four terms, p_0, p_1, p_2, and $\hat{p}_0$. However, at this step we assume that $\hat{p}_0$ is a better approximation to p than is p_2 and apply fixed-point iteration to $\hat{p}_0$ instead of p_2. Using this notation, the sequence is

$$p_0^{(0)}, \quad p_1^{(0)} = g(p_0^{(0)}), \quad p_2^{(0)} = g(p_1^{(0)}), \quad p_0^{(1)} = \{\Delta^2\}(p_0^{(0)}), \quad p_1^{(1)} = g(p_0^{(1)}), \ldots.$$

Every third term of the Steffensen sequence is generated by Eq. (2.15); the others use fixed-point iteration on the previous term. The process is described in Algorithm 2.6.

ALGORITHM 2.6

Steffensen's

To find a solution to $p = g(p)$ given an initial approximation p_0:

INPUT initial approximation p_0; tolerance TOL; maximum number of iterations N_0.

OUTPUT approximate solution p or message of failure.

Step 1 Set $i = 1$.

Step 2 While $i \le N_0$ do Steps 3–6.

Step 3 Set $p_1 = g(p_0)$; (*Compute* $p_1^{(i-1)}$.)
$p_2 = g(p_1)$; (*Compute* $p_2^{(i-1)}$.)
$p = p_0 - (p_1 - p_0)^2/(p_2 - 2p_1 + p_0)$. (*Compute* $p_0^{(i)}$.)

Step 4 If $|p - p_0| < TOL$ then
OUTPUT (p); (*Procedure completed successfully.*)
STOP.

Step 5 Set $i = i + 1$.

Step 6 Set $p_0 = p$. (*Update* p_0.)

Step 7 OUTPUT ('Method failed after N_0 iterations, N_0 =', N_0);
(*Procedure completed unsuccessfully.*)
STOP. ■

Note that $\Delta^2 p_n$ might be 0, which would introduce a 0 in the denominator of the next iterate. If this occurs, we terminate the sequence and select $p_2^{(n-1)}$ as the best approximation.

Illustration To solve $x^3 + 4x^2 - 10 = 0$ using Steffensen's method, let $x^3 + 4x^2 = 10$, divide by $x + 4$, and solve for x. This procedure produces the fixed-point method

$$g(x) = \left(\frac{10}{x+4}\right)^{1/2}.$$

We considered this fixed-point method in Table 2.2 column **(d)** of Section 2.2.

Applying Steffensen's procedure with $p_0 = 1.5$ gives the values in Table 2.11. The iterate $p_0^{(2)} = 1.365230013$ is accurate to the ninth decimal place. In this example, Steffensen's method gave about the same accuracy as Newton's method applied to this polynomial. These results can be seen in the Illustration at the end of Section 2.4. □

Table 2.11

k	$p_0^{(k)}$	$p_1^{(k)}$	$p_2^{(k)}$
0	1.5	1.348399725	1.367376372
1	1.365265224	1.365225534	1.365230583
2	1.365230013		

From the Illustration, it appears that Steffensen's method gives quadratic convergence without evaluating a derivative, and Theorem 2.14 states that this is the case. The proof of this theorem can be found in [He2], pp. 90–92, or [IK], pp. 103–107.

Theorem 2.15 Suppose that $x = g(x)$ has the solution p with $g'(p) \neq 1$. If there exists a $\delta > 0$ such that $g \in C^3[p-\delta, p+\delta]$, then Steffensen's method gives quadratic convergence for any $p_0 \in [p-\delta, p+\delta]$. ■

Steffensen's method can be implemented in Maple with the *NumericalAnalysis* package. For example, after entering the function

$$g := \sqrt{\frac{10}{x+4}}$$

the Maple command

Steffensen(*fixedpointiterator* $= g, x = 1.5$, *tolerance* $= 10^{-8}$, *output* = *information*, *maxiterations* $= 20$)

produces the results in Table 2.11, as well as an indication that the final approximation has a relative error of approximately 7.32×10^{-10}.

EXERCISE SET 2.5

1. The following sequences are linearly convergent. Generate the first five terms of the sequence $\{\hat{p}_n\}$ using Aitken's Δ^2 method.
   a. $p_0 = 0.5, \quad p_n = (2 - e^{p_{n-1}} + p_{n-1}^2)/3, \quad n \geq 1$
   b. $p_0 = 0.75, \quad p_n = (e^{p_{n-1}}/3)^{1/2}, \quad n \geq 1$
   c. $p_0 = 0.5, \quad p_n = 3^{-p_{n-1}}, \quad n \geq 1$
   d. $p_0 = 0.5, \quad p_n = \cos p_{n-1}, \quad n \geq 1$
2. Consider the function $f(x) = e^{6x} + 3(\ln 2)^2 e^{2x} - (\ln 8)e^{4x} - (\ln 2)^3$. Use Newton's method with $p_0 = 0$ to approximate a zero of f. Generate terms until $|p_{n+1} - p_n| < 0.0002$. Construct the sequence $\{\hat{p}_n\}$. Is the convergence improved?
3. Let $g(x) = \cos(x-1)$ and $p_0^{(0)} = 2$. Use Steffensen's method to find $p_0^{(1)}$.
4. Let $g(x) = 1 + (\sin x)^2$ and $p_0^{(0)} = 1$. Use Steffensen's method to find $p_0^{(1)}$ and $p_0^{(2)}$.
5. Steffensen's method is applied to a function $g(x)$ using $p_0^{(0)} = 1$ and $p_2^{(0)} = 3$ to obtain $p_0^{(1)} = 0.75$. What is $p_1^{(0)}$?
6. Steffensen's method is applied to a function $g(x)$ using $p_0^{(0)} = 1$ and $p_1^{(0)} = \sqrt{2}$ to obtain $p_0^{(1)} = 2.7802$. What is $p_2^{(0)}$?
7. Use Steffensen's method to find, to an accuracy of 10^{-4}, the root of $x^3 - x - 1 = 0$ that lies in $[1, 2]$, and compare this to the results of Exercise 6 of Section 2.2.
8. Use Steffensen's method to find, to an accuracy of 10^{-4}, the root of $x - 2^{-x} = 0$ that lies in $[0, 1]$, and compare this to the results of Exercise 8 of Section 2.2.
9. Use Steffensen's method with $p_0 = 2$ to compute an approximation to $\sqrt{3}$ accurate to within 10^{-4}. Compare this result with those obtained in Exercise 9 of Section 2.2 and Exercise 12 of Section 2.1.
10. Use Steffensen's method with $p_0 = 3$ to compute an approximation to $\sqrt[3]{25}$ accurate to within 10^{-4}. Compare this result with those obtained in Exercise 10 of Section 2.2 and Exercise 13 of Section 2.1.
11. Use Steffensen's method to approximate the solutions of the following equations to within 10^{-5}.
    a. $x = (2 - e^x + x^2)/3$, where g is the function in Exercise 11(a) of Section 2.2.
    b. $x = 0.5(\sin x + \cos x)$, where g is the function in Exercise 11(f) of Section 2.2.
    c. $x = (e^x/3)^{1/2}$, where g is the function in Exercise 11(c) of Section 2.2.
    d. $x = 5^{-x}$, where g is the function in Exercise 11(d) of Section 2.2.
12. Use Steffensen's method to approximate the solutions of the following equations to within 10^{-5}.
    a. $2 + \sin x - x = 0$, where g is the function in Exercise 12(a) of Section 2.2.
    b. $x^3 - 2x - 5 = 0$, where g is the function in Exercise 12(b) of Section 2.2.

c. $3x^2 - e^x = 0$, where g is the function in Exercise 12(c) of Section 2.2.

d. $x - \cos x = 0$, where g is the function in Exercise 12(d) of Section 2.2.

13. The following sequences converge to 0. Use Aitken's Δ^2 method to generate $\{\hat{p}_n\}$ until $|\hat{p}_n| \le 5\times 10^{-2}$:

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

14. A sequence $\{p_n\}$ is said to be **superlinearly convergent** to p if

$$\lim_{n\to\infty} \frac{|p_{n+1} - p|}{|p_n - p|} = 0.$$

a. Show that if $p_n \to p$ of order α for $\alpha > 1$, then $\{p_n\}$ is superlinearly convergent to p.

b. Show that $p_n = \frac{1}{n^n}$ is superlinearly convergent to 0 but does not converge to 0 of order α for any $\alpha > 1$.

15. Suppose that $\{p_n\}$ is superlinearly convergent to p. Show that

$$\lim_{n\to\infty} \frac{|p_{n+1} - p_n|}{|p_n - p|} = 1.$$

16. Prove Theorem 2.14. [*Hint:* Let $\delta_n = (p_{n+1} - p)/(p_n - p) - \lambda$, and show that $\lim_{n\to\infty} \delta_n = 0$. Then express $(\hat{p}_{n+1} - p)/(p_n - p)$ in terms of δ_n, δ_{n+1}, and λ.]

17. Let $P_n(x)$ be the nth Taylor polynomial for $f(x) = e^x$ expanded about $x_0 = 0$.

a. For fixed x, show that $p_n = P_n(x)$ satisfies the hypotheses of Theorem 2.14.

b. Let $x = 1$, and use Aitken's Δ^2 method to generate the sequence $\hat{p}_0, \dots, \hat{p}_8$.

c. Does Aitken's method accelerate convergence in this situation?

2.6 Zeros of Polynomials and Müller's Method

A *polynomial of degree n* has the form

$$P(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0,$$

where the a_i's, called the *coefficients* of P, are constants and $a_n \ne 0$. The zero function, $P(x) = 0$ for all values of x, is considered a polynomial but is assigned no degree.

Algebraic Polynomials

Theorem 2.16 **(Fundamental Theorem of Algebra)**

If $P(x)$ is a polynomial of degree $n \ge 1$ with real or complex coefficients, then $P(x) = 0$ has at least one (possibly complex) root. ■

Although the Fundamental Theorem of Algebra is basic to any study of elementary functions, the usual proof requires techniques from the study of complex function theory. The reader is referred to [SaS], p. 155, for the culmination of a systematic development of the topics needed to prove the Theorem.

Example 1 Determine all the zeros of the polynomial $P(x) = x^3 - 5x^2 + 17x - 13$.

Solution It is easily verified that $P(1) = 1 - 5 + 17 - 13 = 0$. so $x = 1$ is a zero of P and $(x - 1)$ is a factor of the polynomial. Dividing $P(x)$ by $x - 1$ gives

$$P(x) = (x - 1)(x^2 - 4x + 13).$$

Carl Friedrich Gauss (1777–1855), one of the greatest mathematicians of all time, proved the Fundamental Theorem of Algebra in his doctoral dissertation and published it in 1799. He published different proofs of this result throughout his lifetime, in 1815, 1816, and as late as 1848. The result had been stated, without proof, by Albert Girard (1595–1632), and partial proofs had been given by Jean d'Alembert (1717–1783), Euler, and Lagrange.

To determine the zeros of $x^2 - 4x + 13$ we use the quadratic formula in its standard form, which gives the complex zeros

$$\frac{-(-4) \pm \sqrt{(-4)^2 - 4(1)(13)}}{2(1)} = \frac{4 \pm \sqrt{-36}}{2} = 2 \pm 3i.$$

Hence the third-degree polynomial $P(x)$ has three zeros, $x_1 = 1$, $x_2 = 2 - 3i$, and $x_2 = 2 + 3i$. ■

In the preceding example we found that the third-degree polynomial had three distinct zeros. An important consequence of the Fundamental Theorem of Algebra is the following corollary. It states that this is always the case, provided that when the zeros are not distinct we count the number of zeros according to their multiplicities.

Corollary 2.17 If $P(x)$ is a polynomial of degree $n \geq 1$ with real or complex coefficients, then there exist unique constants $x_1, x_2, \ldots, x_k$, possibly complex, and unique positive integers $m_1, m_2, \ldots, m_k$, such that $\sum_{i=1}^{k} m_i = n$ and

$$P(x) = a_n(x - x_1)^{m_1}(x - x_2)^{m_2} \cdots (x - x_k)^{m_k}.$$ ■

By Corollary 2.17 the collection of zeros of a polynomial is unique and, if each zero x_i is counted as many times as its multiplicity m_i, a polynomial of degree n has exactly n zeros.

The following corollary of the Fundamental Theorem of Algebra is used often in this section and in later chapters.

Corollary 2.18 Let $P(x)$ and $Q(x)$ be polynomials of degree at most n. If $x_1, x_2, \ldots, x_k$, with $k > n$, are distinct numbers with $P(x_i) = Q(x_i)$ for $i = 1, 2, \ldots, k$, then $P(x) = Q(x)$ for all values of x. ■

This result implies that to show that two polynomials of degree less than or equal to n are the same, we only need to show that they agree at $n + 1$ values. This will be frequently used, particularly in Chapters 3 and 8.

Horner's Method

William Horner (1786–1837) was a child prodigy who became headmaster of a school in Bristol at age 18. Horner's method for solving algebraic equations was published in 1819 in the Philosophical Transactions of the Royal Society.

To use Newton's method to locate approximate zeros of a polynomial $P(x)$, we need to evaluate $P(x)$ and $P'(x)$ at specified values. Since $P(x)$ and $P'(x)$ are both polynomials, computational efficiency requires that the evaluation of these functions be done in the nested manner discussed in Section 1.2. Horner's method incorporates this nesting technique, and, as a consequence, requires only n multiplications and n additions to evaluate an arbitrary nth-degree polynomial.

Theorem 2.19 **(Horner's Method)**

Let

$$P(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0.$$

Define $b_n = a_n$ and

$$b_k = a_k + b_{k+1}x_0, \quad \text{for } k = n-1, n-2, \ldots, 1, 0.$$

Then $b_0 = P(x_0)$. Moreover, if

$$Q(x) = b_n x^{n-1} + b_{n-1}x^{n-2} + \cdots + b_2 x + b_1,$$

then

$$P(x) = (x - x_0)Q(x) + b_0. \qquad \blacksquare$$

Paolo Ruffini (1765–1822) had described a similar method which won him the gold medal from the Italian Mathematical Society for Science. Neither Ruffini nor Horner was the first to discover this method; it was known in China at least 500 years earlier.

Proof By the definition of $Q(x)$,

$$\begin{aligned}(x - x_0)Q(x) + b_0 &= (x - x_0)(b_n x^{n-1} + \cdots + b_2 x + b_1) + b_0\\ &= (b_n x^n + b_{n-1}x^{n-1} + \cdots + b_2 x^2 + b_1 x)\\ &\quad - (b_n x_0 x^{n-1} + \cdots + b_2 x_0 x + b_1 x_0) + b_0\\ &= b_n x^n + (b_{n-1} - b_n x_0)x^{n-1} + \cdots + (b_1 - b_2 x_0)x + (b_0 - b_1 x_0).\end{aligned}$$

By the hypothesis, $b_n = a_n$ and $b_k - b_{k+1}x_0 = a_k$, so

$$(x - x_0)Q(x) + b_0 = P(x) \quad \text{and} \quad b_0 = P(x_0). \qquad \blacksquare\ \blacksquare\ \blacksquare$$

Example 2 Use Horner's method to evaluate $P(x) = 2x^4 - 3x^2 + 3x - 4$ at $x_0 = -2$.

Solution When we use hand calculation in Horner's method, we first construct a table, which suggests the *synthetic division* name that is often applied to the technique. For this problem, the table appears as follows:

	Coefficient of x^4	Coefficient of x^3	Coefficient of x^2	Coefficient of x	Constant term
$x_0 = -2$	$a_4 = 2$	$a_3 = 0$	$a_2 = -3$	$a_1 = 3$	$a_0 = -4$
		$b_4 x_0 = -4$	$b_3 x_0 = 8$	$b_2 x_0 = -10$	$b_1 x_0 = 14$
	$b_4 = 2$	$b_3 = -4$	$b_2 = 5$	$b_1 = -7$	$b_0 = 10$

So,

$$P(x) = (x + 2)(2x^3 - 4x^2 + 5x - 7) + 10. \qquad \blacksquare$$

The word synthetic has its roots in various languages. In standard English it generally provides the sense of something that is "false" or "substituted". But in mathematics it takes the form of something that is "grouped together". Synthetic geometry treats shapes as whole, rather than as individual objects, which is the style in analytic geometry. In synthetic division of polynomials, the various powers of the variables are not explicitly given but kept grouped together.

An additional advantage of using the Horner (or synthetic-division) procedure is that, since

$$P(x) = (x - x_0)Q(x) + b_0,$$

where

$$Q(x) = b_n x^{n-1} + b_{n-1}x^{n-2} + \cdots + b_2 x + b_1,$$

differentiating with respect to x gives

$$P'(x) = Q(x) + (x - x_0)Q'(x) \quad \text{and} \quad P'(x_0) = Q(x_0). \tag{2.16}$$

When the Newton-Raphson method is being used to find an approximate zero of a polynomial, $P(x)$ and $P'(x)$ can be evaluated in the same manner.

Example 3 Find an approximation to a zero of

$$P(x) = 2x^4 - 3x^2 + 3x - 4,$$

using Newton's method with $x_0 = -2$ and synthetic division to evaluate $P(x_n)$ and $P'(x_n)$ for each iterate x_n.

Solution With $x_0 = -2$ as an initial approximation, we obtained $P(-2)$ in Example 1 by

$x_0 = -2$	2	0	−3	3	−4	
		−4	8	−10	14	
	2	−4	5	−7	10	$= P(-2)$.

Using Theorem 2.19 and Eq. (2.16),

$$Q(x) = 2x^3 - 4x^2 + 5x - 7 \quad \text{and} \quad P'(-2) = Q(-2),$$

so $P'(-2)$ can be found by evaluating $Q(-2)$ in a similar manner:

$x_0 = -2$	2	−4	5	−7	
		−4	16	−42	
	2	−8	21	−49	$= Q(-2) = P'(-2)$

and

$$x_1 = x_0 - \frac{P(x_0)}{P'(x_0)} = x_0 - \frac{P(x_0)}{Q(x_0)} = -2 - \frac{10}{-49} \approx -1.796.$$

Repeating the procedure to find x_2 gives

−1.796	2	0	−3	3	−4	
		−3.592	6.451	−6.197	5.742	
	2	−3.592	3.451	−3.197	1.742	$= P(x_1)$
		−3.592	12.902	−29.368		
	2	−7.184	16.353	−32.565	$= Q(x_1)$	$= P'(x_1)$.

So $P(-1.796) = 1.742$, $P'(-1.796) = Q(-1.796) = -32.565$, and

$$x_2 = -1.796 - \frac{1.742}{-32.565} \approx -1.7425.$$

In a similar manner, $x_3 = -1.73897$, and an actual zero to five decimal places is −1.73896.

Note that the polynomial $Q(x)$ depends on the approximation being used and changes from iterate to iterate. ■

Algorithm 2.7 computes $P(x_0)$ and $P'(x_0)$ using Horner's method.

ALGORITHM 2.7

Horner's

To evaluate the polynomial

$$P(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0 = (x - x_0)Q(x) + b_0$$

and its derivative at x_0:

INPUT degree n; coefficients $a_0, a_1, \ldots, a_n$; x_0.

OUTPUT $y = P(x_0)$; $z = P'(x_0)$.

Step 1 Set $y = a_n$; (*Compute b_n for P.*)
$z = a_n$. (*Compute b_{n-1} for Q.*)

Step 2 For $j = n-1, n-2, \ldots, 1$
set $y = x_0 y + a_j$; (*Compute b_j for P.*)
$z = x_0 z + y$. (*Compute b_{j-1} for Q.*)

Step 3 Set $y = x_0 y + a_0$. (*Compute b_0 for P.*)

Step 4 OUTPUT (y, z);
STOP. ■

If the Nth iterate, x_N, in Newton's method is an approximate zero for P, then

$$P(x) = (x - x_N)Q(x) + b_0 = (x - x_N)Q(x) + P(x_N) \approx (x - x_N)Q(x),$$

so $x - x_N$ is an approximate factor of $P(x)$. Letting $\hat{x}_1 = x_N$ be the approximate zero of P and $Q_1(x) \equiv Q(x)$ be the approximate factor gives

$$P(x) \approx (x - \hat{x}_1)Q_1(x).$$

We can find a second approximate zero of P by applying Newton's method to $Q_1(x)$.

If $P(x)$ is an nth-degree polynomial with n real zeros, this procedure applied repeatedly will eventually result in $(n-2)$ approximate zeros of P and an approximate quadratic factor $Q_{n-2}(x)$. At this stage, $Q_{n-2}(x) = 0$ can be solved by the quadratic formula to find the last two approximate zeros of P. Although this method can be used to find all the approximate zeros, it depends on repeated use of approximations and can lead to inaccurate results.

The procedure just described is called **deflation**. The accuracy difficulty with deflation is due to the fact that, when we obtain the approximate zeros of $P(x)$, Newton's method is used on the reduced polynomial $Q_k(x)$, that is, the polynomial having the property that

$$P(x) \approx (x - \hat{x}_1)(x - \hat{x}_2) \cdots (x - \hat{x}_k)Q_k(x).$$

An approximate zero $\hat{x}_{k+1}$ of Q_k will generally not approximate a root of $P(x) = 0$ as well as it does a root of the reduced equation $Q_k(x) = 0$, and inaccuracy increases as k increases. One way to eliminate this difficulty is to use the reduced equations to find approximations $\hat{x}_2$, $\hat{x}_3, \ldots, \hat{x}_k$ to the zeros of P, and then improve these approximations by applying Newton's method to the original polynomial $P(x)$.

Complex Zeros: Müller's Method

One problem with applying the Secant, False Position, or Newton's method to polynomials is the possibility of the polynomial having complex roots even when all the coefficients are real numbers. If the initial approximation is a real number, all subsequent approximations will also be real numbers. One way to overcome this difficulty is to begin with a complex initial approximation and do all the computations using complex arithmetic. An alternative approach has its basis in the following theorem.

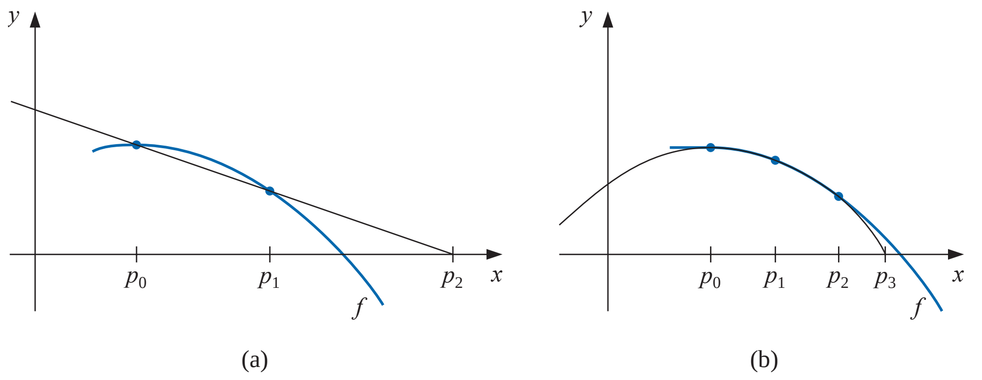
Theorem 2.20 If $z = a+bi$ is a complex zero of multiplicity m of the polynomial $P(x)$ with real coefficients, then $\bar{z} = a - bi$ is also a zero of multiplicity m of the polynomial $P(x)$, and $(x^2 - 2ax + a^2 + b^2)^m$ is a factor of $P(x)$. ■

A synthetic division involving quadratic polynomials can be devised to approximately factor the polynomial so that one term will be a quadratic polynomial whose complex roots are approximations to the roots of the original polynomial. This technique was described in some detail in our second edition [BFR]. Instead of proceeding along these lines, we will now consider a method first presented by D. E. Müller [Mu]. This technique can be used for any root-finding problem, but it is particularly useful for approximating the roots of polynomials.

Müller's method is similar to the Secant method. But whereas the Secant method uses a line through two points on the curve to approximate the root, Müller's method uses a parabola through three points on the curve for the approximation.

The Secant method begins with two initial approximations p_0 and p_1 and determines the next approximation p_2 as the intersection of the x-axis with the line through $(p_0, f(p_0))$ and $(p_1, f(p_1))$. (See Figure 2.13(a).) Müller's method uses three initial approximations, p_0, p_1, and p_2, and determines the next approximation p_3 by considering the intersection of the x-axis with the parabola through $(p_0, f(p_0))$, $(p_1, f(p_1))$, and $(p_2, f(p_2))$. (See Figure 2.13(b).)

Figure 2.13



The derivation of Müller's method begins by considering the quadratic polynomial

$$P(x) = a(x - p_2)^2 + b(x - p_2) + c$$

that passes through $(p_0, f(p_0))$, $(p_1, f(p_1))$, and $(p_2, f(p_2))$. The constants a, b, and c can be determined from the conditions

$$f(p_0) = a(p_0 - p_2)^2 + b(p_0 - p_2) + c, \tag{2.17}$$

$$f(p_1) = a(p_1 - p_2)^2 + b(p_1 - p_2) + c, \tag{2.18}$$

and

$$f(p_2) = a \cdot 0^2 + b \cdot 0 + c = c \tag{2.19}$$

to be

$$c = f(p_2), \tag{2.20}$$

$$b = \frac{(p_0 - p_2)^2[f(p_1) - f(p_2)] - (p_1 - p_2)^2[f(p_0) - f(p_2)]}{(p_0 - p_2)(p_1 - p_2)(p_0 - p_1)}, \tag{2.21}$$

and

$$a = \frac{(p_1 - p_2)[f(p_0) - f(p_2)] - (p_0 - p_2)[f(p_1) - f(p_2)]}{(p_0 - p_2)(p_1 - p_2)(p_0 - p_1)}. \tag{2.22}$$

To determine p_3, a zero of P, we apply the quadratic formula to $P(x) = 0$. However, because of round-off error problems caused by the subtraction of nearly equal numbers, we apply the formula in the manner prescribed in Eq (1.2) and (1.3) of Section 1.2:

$$p_3 - p_2 = \frac{-2c}{b \pm \sqrt{b^2 - 4ac}}.$$

This formula gives two possibilities for p_3, depending on the sign preceding the radical term. In Müller's method, the sign is chosen to agree with the sign of b. Chosen in this manner, the denominator will be the largest in magnitude and will result in p_3 being selected as the closest zero of P to p_2. Thus

$$p_3 = p_2 - \frac{2c}{b + \operatorname{sgn}(b)\sqrt{b^2 - 4ac}},$$

where a, b, and c are given in Eqs. (2.20) through (2.22).

Once p_3 is determined, the procedure is reinitialized using p_1, p_2, and p_3 in place of p_0, p_1, and p_2 to determine the next approximation, p_4. The method continues until a satisfactory conclusion is obtained. At each step, the method involves the radical $\sqrt{b^2 - 4ac}$, so the method gives approximate complex roots when $b^2 - 4ac < 0$. Algorithm 2.8 implements this procedure.

ALGORITHM 2.8

Müller's

To find a solution to $f(x) = 0$ given three approximations, p_0, p_1, and p_2:

INPUT p_0, p_1, p_2; tolerance TOL; maximum number of iterations N_0.

OUTPUT approximate solution p or message of failure.

Step 1 Set $h_1 = p_1 - p_0$;
$h_2 = p_2 - p_1$;
$\delta_1 = (f(p_1) - f(p_0))/h_1$;
$\delta_2 = (f(p_2) - f(p_1))/h_2$;
$d = (\delta_2 - \delta_1)/(h_2 + h_1)$;
$i = 3$.

Step 2 While $i \le N_0$ do Steps 3–7.

Step 3 $b = \delta_2 + h_2 d$;
$D = (b^2 - 4f(p_2)d)^{1/2}$. (*Note: May require complex arithmetic.*)

Step 4 If $|b - D| < |b + D|$ then set $E = b + D$
else set $E = b - D$.

Step 5 Set $h = -2f(p_2)/E$;
$p = p_2 + h$.

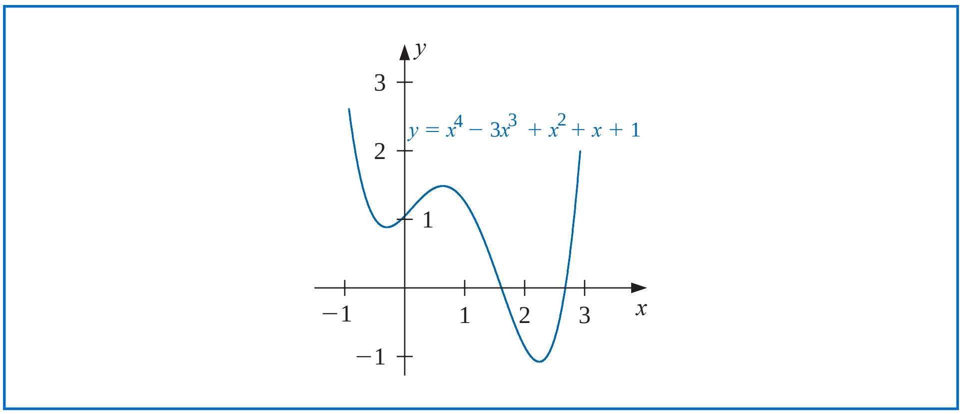
Step 6 If $|h| < TOL$ then
OUTPUT (p); (*The procedure was successful.*)
STOP.

Step 7 Set $p_0 = p_1$; (*Prepare for next iteration.*)
$p_1 = p_2$;
$p_2 = p$;
$h_1 = p_1 - p_0$;
$h_2 = p_2 - p_1$;
$\delta_1 = (f(p_1) - f(p_0))/h_1$;
$\delta_2 = (f(p_2) - f(p_1))/h_2$;
$d = (\delta_2 - \delta_1)/(h_2 + h_1)$;
$i = i + 1$.

Step 8 OUTPUT ('Method failed after N_0 iterations, $N_0 =$', N_0);
(*The procedure was unsuccessful.*)
STOP. ■

Illustration Consider the polynomial $f(x) = x^4 - 3x^3 + x^2 + x + 1$, part of whose graph is shown in Figure 2.14.

Figure 2.14



Three sets of three initial points will be used with Algorithm 2.8 and $TOL = 10^{-5}$ to approximate the zeros of f. The first set will use $p_0 = 0.5$, $p_1 = -0.5$, and $p_2 = 0$. The parabola passing through these points has complex roots because it does not intersect the x-axis. Table 2.12 gives approximations to the corresponding complex zeros of f.

Table 2.12

	$p_0 = 0.5,\ p_1 = -0.5,\ p_2 = 0$	
i	p_i	$f(p_i)$
3	$-0.100000 + 0.888819i$	$-0.01120000 + 3.014875548i$
4	$-0.492146 + 0.447031i$	$-0.1691201 - 0.7367331502i$
5	$-0.352226 + 0.484132i$	$-0.1786004 + 0.0181872213i$
6	$-0.340229 + 0.443036i$	$0.01197670 - 0.0105562185i$
7	$-0.339095 + 0.446656i$	$-0.0010550 + 0.000387261i$
8	$-0.339093 + 0.446630i$	$0.000000 + 0.000000i$
9	$-0.339093 + 0.446630i$	$0.000000 + 0.000000i$

Table 2.13 gives the approximations to the two real zeros of f. The smallest of these uses $p_0 = 0.5$, $p_1 = 1.0$, and $p_2 = 1.5$, and the largest root is approximated when $p_0 = 1.5$, $p_1 = 2.0$, and $p_2 = 2.5$.

Table 2.13

$p_0 = 0.5$,	$p_1 = 1.0$,	$p_2 = 1.5$	$p_0 = 1.5$,	$p_1 = 2.0$,	$p_2 = 2.5$
i	p_i	$f(p_i)$	i	p_i	$f(p_i)$
3	1.40637	−0.04851	3	2.24733	−0.24507
4	1.38878	0.00174	4	2.28652	−0.01446
5	1.38939	0.00000	5	2.28878	−0.00012
6	1.38939	0.00000	6	2.28880	0.00000
			7	2.28879	0.00000

The values in the tables are accurate approximations to the places listed. □

We used Maple to generate the results in Table 2.12. To find the first result in the table, define $f(x)$ with

$$f := x \to x^4 - 3x^3 + x^2 + x + 1$$

Then enter the initial approximations with

$$p0 := 0.5; p1 := -0.5; p2 := 0.0$$

and evaluate the function at these points with

$$f0 := f(p0); f1 := f(p1); f2 := f(p2)$$

To determine the coefficients a, b, c, and the approximate solution, enter

$$c := f2;$$

$$b := \frac{\left((p0 - p2)^2 \cdot (f1 - f2) - (p1 - p2)^2 \cdot (f0 - f2)\right)}{(p0 - p2) \cdot (p1 - p2) \cdot (p0 - p1)}$$

$$a := \frac{((p1 - p2) \cdot (f0 - f2) - (p0 - p2) \cdot (f1 - f2))}{(p0 - p2) \cdot (p1 - p2) \cdot (p0 - p1)}$$

$$p3 := p2 - \frac{2c}{b + \left(\frac{b}{abs(b)}\right)\sqrt{b^2 - 4a \cdot c}}$$

This produces the final Maple output

$$-0.1000000000 + 0.8888194418I$$

and evaluating at this approximation gives $f(p3)$ as

$$-0.0112000001 + 3.014875548I$$

This is our first approximation, as seen in Table 2.12.

The illustration shows that Müller's method can approximate the roots of polynomials with a variety of starting values. In fact, Müller's method generally converges to the root of a polynomial for any initial approximation choice, although problems can be constructed for which convergence will not occur. For example, suppose that for some i we have $f(p_i) = f(p_{i+1}) = f(p_{i+2}) \neq 0$. The quadratic equation then reduces to a nonzero constant function and never intersects the x-axis. This is not usually the case, however, and general-purpose software packages using Müller's method request only one initial approximation per root and will even supply this approximation as an option.

EXERCISE SET 2.6

1. Find the approximations to within 10^{-4} to all the real zeros of the following polynomials using Newton's method.
   - **a.** $f(x) = x^3 - 2x^2 - 5$
   - **b.** $f(x) = x^3 + 3x^2 - 1$
   - **c.** $f(x) = x^3 - x - 1$
   - **d.** $f(x) = x^4 + 2x^2 - x - 3$
   - **e.** $f(x) = x^3 + 4.001x^2 + 4.002x + 1.101$
   - **f.** $f(x) = x^5 - x^4 + 2x^3 - 3x^2 + x - 4$
2. Find approximations to within 10^{-5} to all the zeros of each of the following polynomials by first finding the real zeros using Newton's method and then reducing to polynomials of lower degree to determine any complex zeros.
   - **a.** $f(x) = x^4 + 5x^3 - 9x^2 - 85x - 136$
   - **b.** $f(x) = x^4 - 2x^3 - 12x^2 + 16x - 40$
   - **c.** $f(x) = x^4 + x^3 + 3x^2 + 2x + 2$
   - **d.** $f(x) = x^5 + 11x^4 - 21x^3 - 10x^2 - 21x - 5$
   - **e.** $f(x) = 16x^4 + 88x^3 + 159x^2 + 76x - 240$
   - **f.** $f(x) = x^4 - 4x^2 - 3x + 5$
   - **g.** $f(x) = x^4 - 2x^3 - 4x^2 + 4x + 4$
   - **h.** $f(x) = x^3 - 7x^2 + 14x - 6$
3. Repeat Exercise 1 using Müller's method.
4. Repeat Exercise 2 using Müller's method.
5. Use Newton's method to find, within 10^{-3}, the zeros and critical points of the following functions. Use this information to sketch the graph of f.
   - **a.** $f(x) = x^3 - 9x^2 + 12$
   - **b.** $f(x) = x^4 - 2x^3 - 5x^2 + 12x - 5$
6. $f(x) = 10x^3 - 8.3x^2 + 2.295x - 0.21141 = 0$ has a root at $x = 0.29$. Use Newton's method with an initial approximation $x_0 = 0.28$ to attempt to find this root. Explain what happens.
7. Use Maple to find a real zero of the polynomial $f(x) = x^3 + 4x - 4$.
8. Use Maple to find a real zero of the polynomial $f(x) = x^3 - 2x - 5$.
9. Use each of the following methods to find a solution in $[0.1, 1]$ accurate to within 10^{-4} for

$$600x^4 - 550x^3 + 200x^2 - 20x - 1 = 0.$$

   - **a.** Bisection method
   - **b.** Newton's method
   - **c.** Secant method
   - **d.** method of False Position
   - **e.** Müller's method