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

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

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

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

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

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

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

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.

Solution (a) We have

$$f(x) = e^x - x - 1,$$
 $f'(x) = e^x - 1$ and $f''(x) = e^x,$

so

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

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

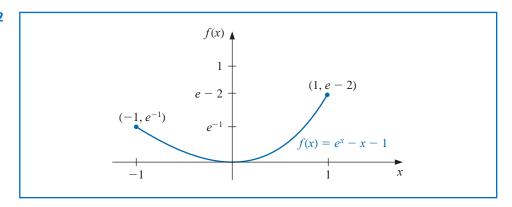
$$p_2 = p_1 - \frac{f(p_1)}{f'(p_1)} \approx 0.58198 - \frac{0.20760}{0.78957} \approx 0.31906.$$

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

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

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

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	$-2.8085217 \times 10^{-7}$

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

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

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

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

With $p_0 = 1.5$, we have

Newton's method

$$p_1 = 1.37333333$$
, $p_2 = 1.36526201$, and $p_3 = 1.36523001$.

Modified Newton's method

$$p_1 = 1.35689898$$
, $p_2 = 1.36519585$, and $p_3 = 1.36523001$.

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 *Numerical-Analysis* 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])

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

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

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 < x < -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 < x < 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 < x < -2
 - c. $\sin 3x + 3e^{-2x} \sin x 3e^{-x} \sin 2x e^{-3x} = 0$, for 3 < x < 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?