```
    break
  end
  if sign(fc)*sign(fa)<0  %a and c make the new interval
    b=c;fb=fc;
  else                    %c and b make the new interval
    a=c;fa=fc;
  end
end
xc=(a+b)/2;               %new midpoint is best estimate
```

To use `bisect.m`, first define a MATLAB function by:

```
>> f=@(x) x^3+x-1;
```

This command actually defines a "function handle" `f`, which can be used as input for other MATLAB functions. See Appendix B for more details on MATLAB functions and function handles. Then the command

```
» xc=bisect (f,0,1,0.00005)
```

returns a solution correct to a tolerance of 0.00005.

1.1.2 How accurate and how fast?

If $[a, b]$ is the starting interval, then after n bisection steps, the interval $[a_n, b_n]$ has length $(b-a)/2^n$. Choosing the midpoint $x_c = (a_n + b_n)/2$ gives a best estimate of the solution r, which is within half the interval length of the true solution. Summarizing, after n steps of the Bisection Method, we find that

$$\text{Solution error} = |x_c - r| < \frac{b-a}{2^{n+1}} \tag{1.1}$$

and

$$\text{Function evaluations} = n + 2. \tag{1.2}$$

A good way to assess the efficiency of the Bisection Method is to ask how much accuracy can be bought per function evaluation. Each step, or each function evaluation, cuts the uncertainty in the root by a factor of two.

DEFINITION 1.3 A solution is **correct within p decimal places** if the error is less than 0.5×10^{-p}. ❒

► **EXAMPLE 1.2** Use the Bisection Method to find a root of $f(x) = \cos x - x$ in the interval $[0, 1]$ to within six correct places.

First we decide how many steps of bisection are required. According to (1.1), the error after n steps is $(b-a)/2^{n+1} = 1/2^{n+1}$. From the definition of p decimal places, we require that

$$\frac{1}{2^{n+1}} < 0.5 \times 10^{-6}$$

$$n > \frac{6}{\log_{10} 2} \approx \frac{6}{0.301} = 19.9.$$

Therefore, $n = 20$ steps will be needed. Proceeding with the Bisection Method, the following table is produced:

k	a_k	$f(a_k)$	c_k	$f(c_k)$	b_k	$f(b_k)$
0	0.000000	+	0.500000	+	1.000000	−
1	0.500000	+	0.750000	−	1.000000	−
2	0.500000	+	0.625000	+	0.750000	−
3	0.625000	+	0.687500	+	0.750000	−
4	0.687500	+	0.718750	+	0.750000	−
5	0.718750	+	0.734375	+	0.750000	−
6	0.734375	+	0.742188	−	0.750000	−
7	0.734375	+	0.738281	+	0.742188	−
8	0.738281	+	0.740234	−	0.742188	−
9	0.738281	+	0.739258	−	0.740234	−
10	0.738281	+	0.738770	+	0.739258	−
11	0.738769	+	0.739014	+	0.739258	−
12	0.739013	+	0.739136	−	0.739258	−
13	0.739013	+	0.739075	+	0.739136	−
14	0.739074	+	0.739105	−	0.739136	−
15	0.739074	+	0.739090	−	0.739105	−
16	0.739074	+	0.739082	+	0.739090	−
17	0.739082	+	0.739086	−	0.739090	−
18	0.739082	+	0.739084	+	0.739086	−
19	0.739084	+	0.739085	−	0.739086	−
20	0.739084	+	0.739085	−	0.739085	−

The approximate root to six correct places is 0.739085. ◄

For the Bisection Method, the question of how many steps to run is a simple one—just choose the desired precision and find the number of necessary steps, as in (1.1). We will see that more high-powered algorithms are often less predictable and have no analogue to (1.1). In those cases, we will need to establish definite "stopping criteria" that govern the circumstances under which the algorithm terminates. Even for the Bisection Method, the finite precision of computer arithmetic will put a limit on the number of possible correct digits. We will look into this issue further in Section 1.3.

1.1 Exercises

1. Use the Intermediate Value Theorem to find an interval of length one that contains a root of the equation. (a) $x^3 = 9$ (b) $3x^3 + x^2 = x + 5$ (c) $\cos^2 x + 6 = x$
2. Use the Intermediate Value Theorem to find an interval of length one that contains a root of the equation. (a) $x^5 + x = 1$ (b) $\sin x = 6x + 5$ (c) $\ln x + x^2 = 3$
3. Consider the equations in Exercise 1. Apply two steps of the Bisection Method to find an approximate root within $1/8$ of the true root.
4. Consider the equations in Exercise 2. Apply two steps of the Bisection Method to find an approximate root within $1/8$ of the true root.
5. Consider the equation $x^4 = x^3 + 10$.
   (a) Find an interval $[a, b]$ of length one inside which the equation has a solution.
   (b) Starting with $[a, b]$, how many steps of the Bisection Method are required to calculate the solution within 10^{-10}? Answer with an integer.
6. Suppose that the Bisection Method with starting interval $[-2, 1]$ is used to find a root of the function $f(x) = 1/x$. Does the method converge to a real number? Is it the root?

1.1 Computer Problems

1. Use the Bisection Method to find the root to six correct decimal places. (a) $x^3 = 9$ (b) $3x^3 + x^2 = x + 5$ (c) $\cos^2 x + 6 = x$

2. Use the Bisection Method to find the root to eight correct decimal places. (a) $x^5 + x = 1$ (b) $\sin x = 6x + 5$ (c) $\ln x + x^2 = 3$

3. Use the Bisection Method to locate all solutions of the following equations. Sketch the function by using MATLAB's `plot` command and identify three intervals of length one that contain a root. Then find the roots to six correct decimal places. (a) $2x^3 - 6x - 1 = 0$ (b) $e^{x-2} + x^3 - x = 0$ (c) $1 + 5x - 6x^3 - e^{2x} = 0$

4. Calculate the square roots of the following numbers to eight correct decimal places by using the Bisection Method to solve $x^2 - A = 0$, where A is (a) 2 (b) 3 (c) 5. State your starting interval and the number of steps needed.

5. Calculate the cube roots of the following numbers to eight correct decimal places by using the Bisection Method to solve $x^3 - A = 0$, where A is (a) 2 (b) 3 (c) 5. State your starting interval and the number of steps needed.

6. Use the Bisection Method to calculate the solution of $\cos x = \sin x$ in the interval [0, 1] within six correct decimal places.

7. Use the Bisection Method to find the two real numbers x, within six correct decimal places, that make the determinant of the matrix

$$A = \begin{bmatrix} 1 & 2 & 3 & x \\ 4 & 5 & x & 6 \\ 7 & x & 8 & 9 \\ x & 10 & 11 & 12 \end{bmatrix}$$

equal to 1000. For each solution you find, test it by computing the corresponding determinant and reporting how many correct decimal places (after the decimal point) the determinant has when your solution x is used. (In Section 1.2, we will call this the "backward error" associated with the approximate solution.) You may use the MATLAB command `det` to compute the determinants.

8. The **Hilbert matrix** is the $n \times n$ matrix whose ijth entry is $1/(i + j - 1)$. Let A denote the 5×5 Hilbert matrix. Its largest eigenvalue is about 1.567. Use the Bisection Method to decide how to change the upper left entry A_{11} to make the largest eigenvalue of A equal to π. Determine A_{11} within six correct decimal places. You may use the MATLAB commands `hilb`, `pi`, `eig`, and `max` to simplify your task.

9. Find the height reached by 1 cubic meter of water stored in a spherical tank of radius 1 meter. Give your answer ± 1 mm. (Hint: First note that the sphere will be less than half full. The volume of the bottom H meters of a hemisphere of radius R is $\pi H^2(R - 1/3H)$.)

1.2 FIXED-POINT ITERATION

Use a calculator or computer to apply the `cos` function repeatedly to an arbitrary starting number. That is, apply the `cos` function to the starting number, then apply `cos` to the result, then to the new result, and so forth. (If you use a calculator, be sure it is in radian

mode.) Continue until the digits no longer change. The resulting sequence of numbers converges to 0.7390851332, at least to the first 10 decimal places. In this section, our goal is to explain why this calculation, an instance of Fixed-Point Iteration (FPI), converges. While we do this, most of the major issues of algorithm convergence will come under discussion.

1.2.1 Fixed points of a function

The sequence of numbers produced by iterating the cosine function appears to converge to a number r. Subsequent applications of cosine do not change the number. For this input, the output of the cosine function is equal to the input, or $\cos r = r$.

DEFINITION 1.4 The real number r is a **fixed point** of the function g if $g(r) = r$. ☐

The number $r = 0.7390851332$ is an approximate fixed point for the function $g(x) = \cos x$. The function $g(x) = x^3$ has three fixed points, $r = -1, 0$, and 1.

We used the Bisection Method in Example 1.2 to solve the equation $\cos x - x = 0$. The fixed-point equation $\cos x = x$ is the same problem from a different point of view. When the output equals the input, that number is a fixed point of $\cos x$, and simultaneously a solution of the equation $\cos x - x = 0$.

Once the equation is written as $g(x) = x$, Fixed-Point Iteration proceeds by starting with an initial guess x_0 and iterating the function g.

Fixed-Point Iteration

$$x_0 = \text{initial guess}$$
$$x_{i+1} = g(x_i) \textbf{ for } i = 0, 1, 2, \ldots$$

Therefore,

$$x_1 = g(x_0)$$
$$x_2 = g(x_1)$$
$$x_3 = g(x_2)$$
$$\vdots$$

and so forth. The sequence x_i may or may not converge as the number of steps goes to infinity. However, if g is continuous and the x_i converge, say, to a number r, then r is a fixed point. In fact, Theorem 0.5 implies that

$$g(r) = g\left(\lim_{i\to\infty} x_i\right) = \lim_{i\to\infty} g(x_i) = \lim_{i\to\infty} x_{i+1} = r. \tag{1.3}$$

The Fixed-Point Iteration algorithm applied to a function g is easily written in MATLAB code:

```
%Program 1.2 Fixed-Point Iteration
%Computes approximate solution of g(x)=x
%Input: function handle g, starting guess x0,
%       number of iteration steps k
%Output: Approximate solution xc
function xc=fpi(g, x0, k)
x(1)=x0;
```

Before finishing the calculation, let's decide whether it will converge. According to Theorem 1.6, we need $S < 1$. For this iteration, $g(x) = 1/2(x + 2/x)$ and $g'(x) = 1/2(1 - 2/x^2)$. Evaluating at the fixed point yields

$$g'(\sqrt{2}) = \frac{1}{2}\left(1 - \frac{2}{(\sqrt{2})^2}\right) = 0, \tag{1.15}$$

so $S = 0$. We conclude that the FPI will converge, and very fast.

Exercise 18 asks whether this method will be successful in finding the square root of an arbitrary positive number. ◀

1.2.4 Stopping criteria

Unlike the case of bisection, the number of steps required for FPI to converge within a given tolerance is rarely predictable beforehand. In the absence of an error formula like (1.1) for the Bisection Method, a decision must be made about terminating the algorithm, called a **stopping criterion**.

For a set tolerance, TOL, we may ask for an absolute error stopping criterion

$$|x_{i+1} - x_i| < \text{TOL} \tag{1.16}$$

or, in case the solution is not too near zero, the relative error stopping criterion

$$\frac{|x_{i+1} - x_i|}{|x_{i+1}|} < \text{TOL}. \tag{1.17}$$

A hybrid absolute/relative stopping criterion such as

$$\frac{|x_{i+1} - x_i|}{\max(|x_{i+1}|, \theta)} < \text{TOL} \tag{1.18}$$

for some $\theta > 0$ is often useful in cases where the solution is near 0. In addition, good FPI code sets a limit on the maximum number of steps in case convergence fails. The issue of stopping criteria is important, and will be revisited in a more sophisticated way when we study forward and backward error in Section 1.3.

The Bisection Method is guaranteed to converge linearly. Fixed-Point Iteration is only locally convergent, and when it converges it is linearly convergent. Both methods require one function evaluation per step. The bisection cuts uncertainty by 1/2 for each step, compared with approximately $S = |g'(r)|$ for FPI. Therefore, Fixed-Point Iteration may be faster or slower than bisection, depending on whether S is smaller or larger than 1/2. In Section 1.4, we study Newton's Method, a particularly refined version of FPI, where S is designed to be zero.

1.2 Exercises

1. Find all fixed points of the following $g(x)$.
(a) $\dfrac{3}{x}$ (b) $x^2 - 2x + 2$ (c) $x^2 - 4x + 2$

2. Find all fixed points of the following $g(x)$.
(a) $\dfrac{x+6}{3x-2}$ (b) $\dfrac{8+2x}{2+x^2}$ (c) x^5

3. Show that 1, 2, and 3 are fixed points of the following $g(x)$.
(a) $\dfrac{x^3+x-6}{6x-10}$ (b) $\dfrac{6+6x^2-x^3}{11}$

4. Show that $-1, 0$, and 1 are fixed points of the following $g(x)$.
(a) $\dfrac{4x}{x^2+3}$ (b) $\dfrac{x^2-5x}{x^2+x-6}$

5. For which of the following $g(x)$ is $r = \sqrt{3}$ a fixed point?
(a) $g(x) = \dfrac{x}{\sqrt{3}}$ (b) $g(x) = \dfrac{2x}{3} + \dfrac{1}{x}$ (c) $g(x) = x^2 - x$ (d) $g(x) = 1 + \dfrac{2}{x+1}$

6. For which of the following $g(x)$ is $r = \sqrt{5}$ a fixed point?
(a) $g(x) = \dfrac{5+7x}{x+7}$ (b) $g(x) = \dfrac{10}{3x} + \dfrac{x}{3}$ (c) $g(x) = x^2 - 5$ (d) $g(x) = 1 + \dfrac{4}{x+1}$

7. Use Theorem 1.6 to determine whether Fixed-Point Iteration of $g(x)$ is locally convergent to the given fixed point r. (a) $g(x) = (2x-1)^{1/3}, r = 1$ (b) $g(x) = (x^3+1)/2, r = 1$
(c) $g(x) = \sin x + x, r = 0$

8. Use Theorem 1.6 to determine whether Fixed-Point Iteration of $g(x)$ is locally convergent to the given fixed point r. (a) $g(x) = (2x-1)/x^2, r = 1$ (b) $g(x) = \cos x + \pi + 1, r = \pi$
(c) $g(x) = e^{2x} - 1, r = 0$

9. Find each fixed point and decide whether Fixed-Point Iteration is locally convergent to it.
(a) $g(x) = \frac{1}{2}x^2 + \frac{1}{2}x$ (b) $g(x) = x^2 - \frac{1}{4}x + \frac{3}{8}$

10. Find each fixed point and decide whether Fixed-Point Iteration is locally convergent to it.
(a) $g(x) = x^2 - \frac{3}{2}x + \frac{3}{2}$ (b) $g(x) = x^2 + \frac{1}{2}x - \frac{1}{2}$

11. Express each equation as a fixed-point problem $x = g(x)$ in three different ways.
(a) $x^3 - x + e^x = 0$ (b) $3x^{-2} + 9x^3 = x^2$

12. Consider the Fixed-Point Iteration $x \rightarrow g(x) = x^2 - 0.24$. (a) Do you expect Fixed-Point Iteration to calculate the root -0.2, say, to 10 or to correct decimal places, faster or slower than the Bisection Method? (b) Find the other fixed point. Will FPI converge to it?

13. (a) Find all fixed points of $g(x) = 0.39 - x^2$. (b) To which of the fixed-points is Fixed-Point Iteration locally convergent? (c) Does FPI converge to this fixed point faster or slower than the Bisection Method?

14. Which of the following three Fixed-Point Iterations converge to $\sqrt{2}$? Rank the ones that converge from fastest to slowest.
(A) $x \longrightarrow \dfrac{1}{2}x + \dfrac{1}{x}$ (B) $x \longrightarrow \dfrac{2}{3}x + \dfrac{2}{3x}$ (C) $x \longrightarrow \dfrac{3}{4}x + \dfrac{1}{2x}$

15. Which of the following three Fixed-Point Iterations converge to $\sqrt{5}$? Rank the ones that converge from fastest to slowest.
(A) $x \longrightarrow \dfrac{4}{5}x + \dfrac{1}{x}$ (B) $x \longrightarrow \dfrac{x}{2} + \dfrac{5}{2x}$ (C) $x \longrightarrow \dfrac{x+5}{x+1}$

16. Which of the following three Fixed-Point Iterations converge to the cube root of 4? Rank the ones that converge from fastest to slowest.
(A) $g(x) = \dfrac{2}{\sqrt{x}}$ (B) $g(x) = \dfrac{3x}{4} + \dfrac{1}{x^2}$ (C) $g(x) = \dfrac{2}{3}x + \dfrac{4}{3x^2}$

17. Check that 1/2 and -1 are roots of $f(x) = 2x^2 + x - 1 = 0$. Isolate the x^2 term and solve for x to find two candidates for $g(x)$. Which of the roots will be found by the two Fixed-Point Iterations?

18. Prove that the method of Example 1.6 will calculate the square root of any positive number.

19. Explore the idea of Example 1.6 for cube roots. If x is a guess that is smaller than $A^{1/3}$, then A/x^2 will be larger than $A^{1/3}$, so that the average of the two will be a better approximation than x. Suggest a Fixed-Point Iteration on the basis of this fact, and use Theorem 1.6 to decide whether it will converge to the cube root of A.

20. Improve the cube root algorithm of Exercise 19 by reweighting the average. Setting $g(x) = wx + (1 - w)A/x^2$ for some fixed number $0 < w < 1$, what is the best choice for w?

21. Consider Fixed-Point Iteration applied to $g(x) = 1 - 5x + \frac{15}{2}x^2 - \frac{5}{2}x^3$. (a) Show that $1 - \sqrt{3/5}$, 1, and $1 + \sqrt{3/5}$ are fixed points. (b) Show that none of the three fixed points is locally convergent. (Computer Problem 7 investigates this example further.)

22. Show that the initial guesses 0, 1, and 2 lead to a fixed point in Exercise 21. What happens to other initial guesses close to those numbers?

23. Assume that $g(x)$ is continuously differentiable and that the Fixed-Point Iteration $g(x)$ has exactly three fixed points, $r_1 < r_2 < r_3$. Assume also that $|g'(r_1)| = 0.5$ and $|g'(r_3)| = 0.5$. List all values of $|g'(r_2)|$ that are possible under these conditions.

24. Assume that g is a continuously differentiable function and that the Fixed-Point Iteration $g(x)$ has exactly three fixed points, -3, 1, and 2. Assume that $g'(-3) = 2.4$ and that FPI started sufficiently near the fixed point 2 converges to 2. Find $g'(1)$.

25. Prove the variant of Theorem 1.6: If g is continuously differentiable and $|g'(x)| \le B < 1$ on an interval $[a, b]$ containing the fixed point r, then FPI converges to r from any initial guess in $[a, b]$.

26. Prove that a continuously differentiable function $g(x)$ satisfying $|g'(x)| < 1$ on a closed interval cannot have two fixed points on that interval.

27. Consider Fixed-Point Iteration with $g(x) = x - x^3$. (a) Show that $x = 0$ is the only fixed point. (b) Show that if $0 < x_0 < 1$, then $x_0 > x_1 > x_2 \ldots > 0$. (c) Show that FPI converges to $r = 0$, while $g'(0) = 1$. (Hint: Use the fact that every bounded monotonic sequence converges to a limit.)

28. Consider Fixed-Point Iteration with $g(x) = x + x^3$. (a) Show that $x = 0$ is the only fixed point. (b) Show that if $0 < x_0 < 1$, then $x_0 < x_1 < x_2 < \ldots$. (c) Show that FPI fails to converge to a fixed point, while $g'(0) = 1$. Together with Exercise 27, this shows that FPI may converge to a fixed point r or diverge from r when $|g'(r)| = 1$.

29. Consider the equation $x^3 + x - 2 = 0$, with root $r = 1$. Add the term cx to both sides and divide by c to obtain $g(x)$. (a) For what c is FPI locally convergent to $r = 1$?(b) For what c will FPI converge fastest?

30. Assume that Fixed-Point Iteration is applied to a twice continuously differentiable function $g(x)$ and that $g'(r) = 0$ for a fixed point r. Show that if FPI converges to r, then the error obeys $\lim_{i\to\infty}(e_{i+1})/e_i^2 = M$, where $M = |g''(r)|/2$.

31. Define Fixed-Point Iteration on the equation $x^2 + x = 5/16$ by isolating the x term. Find both fixed points, and determine which initial guesses lead to each fixed point under iteration. (Hint: Plot $g(x)$, and draw cobweb diagrams.)

32. Find the set of all initial guesses for which the Fixed-Point Iteration $x \to 4/9 - x^2$ converges to a fixed point.

33. Let $g(x) = a + bx + cx^2$ for constants a, b, and c. (a) Specify one set of constants a, b, and c for which $x = 0$ is a fixed-point of $x = g(x)$ and Fixed-Point Iteration is locally convergent to 0. (b) Specify one set of constants a, b, and c for which $x = 0$ is a fixed-point of $x = g(x)$ but Fixed-Point Iteration is not locally convergent to 0.

1.2 Computer Problems

1. Apply Fixed-Point Iteration to find the solution of each equation to eight correct decimal places. (a) $x^3 = 2x + 2$ (b) $e^x + x = 7$ (c) $e^x + \sin x = 4$.

2. Apply Fixed-Point Iteration to find the solution of each equation to eight correct decimal places. (a) $x^5 + x = 1$ (b) $\sin x = 6x + 5$ (c) $\ln x + x^2 = 3$

3. Calculate the square roots of the following numbers to eight correct decimal places by using Fixed-Point Iteration as in Example 1.6: (a) 3 (b) 5. State your initial guess and the number of steps needed.

4. Calculate the cube roots of the following numbers to eight correct decimal places, by using Fixed-Point Iteration with $g(x) = (2x + A/x^2)/3$, where A is (a) 2 (b) 3 (c) 5. State your initial guess and the number of steps needed.

5. Example 1.3 showed that $g(x) = \cos x$ is a convergent FPI. Is the same true for $g(x) = \cos^2 x$? Find the fixed point to six correct decimal places, and report the number of FPI steps needed. Discuss local convergence, using Theorem 1.6.

6. Derive three different $g(x)$ for finding roots to six correct decimal places of the following $f(x) = 0$ by Fixed-Point Iteration. Run FPI for each $g(x)$ and report results, convergence or divergence. Each equation $f(x) = 0$ has three roots. Derive more $g(x)$ if necessary until all roots are found by FPI. For each convergent run, determine the value of S from the errors e_{i+1}/e_i, and compare with S determined from calculus as in (1.11). (a) $f(x) = 2x^3 - 6x - 1$ (b) $f(x) = e^{x-2} + x^3 - x$ (c) $f(x) = 1 + 5x - 6x^3 - e^{2x}$

7. Exercise 21 considered Fixed-Point Iteration applied to $g(x) = 1 - 5x + \frac{15}{2}x^2 - \frac{5}{2}x^3 = x$. Find initial guesses for which FPI (a) cycles endlessly through numbers in the interval $(0, 1)$ (b) the same as (a), but the interval is $(1, 2)$ (c) diverges to infinity. Cases (a) and (b) are examples of chaotic dynamics. In all three cases, FPI is unsuccessful.

1.3 LIMITS OF ACCURACY

One of the goals of numerical analysis is to compute answers within a specified level of accuracy. Working in double precision means that we store and operate on numbers that are kept to 52-bit accuracy, about 16 decimal digits.

Can answers always be computed to 16 correct significant digits? In Chapter 0, it was shown that, with a naive algorithm for computing roots of a quadratic equation, it was possible to lose some or all significant digits. An improved algorithm eliminated the problem. In this section, we will see something new—a calculation that a double-precision computer cannot make to anywhere near 16 correct digits, even with the best algorithm.

SPOTLIGHT ON

Conditioning This is the first appearance of the concept of condition number, a measure of error magnification. Numerical analysis is the study of algorithms, which take data defining the problem as input and deliver an answer as output. Condition number refers to the part of this magnification that is inherent in the theoretical problem itself, irrespective of the particular algorithm used to solve it.

It is important to note that the error magnification factor measures only magnification due to the problem. Along with conditioning, there is a parallel concept, stability, that refers to the magnification of small input errors due to the algorithm, not the problem itself. An algorithm is called stable if it always provides an approximate solution with small backward error. If the problem is well-conditioned and the algorithm is stable, we can expect both small backward and forward error.

The preceding error magnification examples show the sensitivity of root-finding to a particular input change. The problem may be more or less sensitive, depending on how the input change is designed. The **condition number** of a problem is defined to be the maximum error magnification over all input changes, or at least all changes of a prescribed type. A problem with high condition number is called **ill-conditioned**, and a problem with a condition number near 1 is called **well-conditioned**. We will return to this concept when we discuss matrix problems in Chapter 2.

1.3 Exercises

1. Find the forward and backward error for the following functions, where the root is $3/4$ and the approximate root is $x_a = 0.74$: (a) $f(x) = 4x - 3$ (b) $f(x) = (4x - 3)^2$ (c) $f(x) = (4x - 3)^3$ (d) $f(x) = (4x - 3)^{1/3}$
2. Find the forward and backward error for the following functions, where the root is $1/3$ and the approximate root is $x_a = 0.3333$: (a) $f(x) = 3x - 1$ (b) $f(x) = (3x - 1)^2$ (c) $f(x) = (3x - 1)^3$ (d) $f(x) = (3x - 1)^{1/3}$
3. (a) Find the multiplicity of the root $r = 0$ of $f(x) = 1 - \cos x$. (b) Find the forward and backward errors of the approximate root $x_a = 0.0001$.
4. (a) Find the multiplicity of the root $r = 0$ of $f(x) = x^2 \sin x^2$. (b) Find the forward and backward errors of the approximate root $x_a = 0.01$.
5. Find the relation between forward and backward error for finding the root of the linear function $f(x) = ax - b$.
6. Let n be a positive integer. The equation defining the nth root of a positive number A is $x^n - A = 0$. (a) Find the multiplicity of the root. (b) Show that, for an approximate nth root with small forward error, the backward error is approximately $nA^{(n-1)/n}$ times the forward error.
7. Let $W(x)$ be the Wilkinson polynomial. (a) Prove that $W'(16) = 15!4!$ (b) Find an analogous formula for $W'(j)$, where j is an integer between 1 and 20.
8. Let $f(x) = x^n - ax^{n-1}$, and set $g(x) = x^n$. (a) Use the Sensitivity Formula to give a prediction for the nonzero root of $f_\epsilon(x) = x^n - ax^{n-1} + \epsilon x^n$ for small ϵ. (b) Find the nonzero root and compare with the prediction.

1.3 Computer Problems

1. Let $f(x) = \sin x - x$. (a) Find the multiplicity of the root $r = 0$. (b) Use MATLAB's `fzero` command with initial guess $x = 0.1$ to locate a root. What are the forward and backward errors of `fzero`'s response?
2. Carry out Computer Problem 1 for $f(x) = \sin x^3 - x^3$.
3. (a) Use `fzero` to find the root of $f(x) = 2x\cos x - 2x + \sin x^3$ on $[-0.1, 0.2]$. Report the forward and backward errors. (b) Run the Bisection Method with initial interval $[-0.1, 0.2]$ to find as many correct digits as possible, and report your conclusion.
4. (a) Use (1.21) to approximate the root near 3 of $f_\epsilon(x) = (1+\epsilon)x^3 - 3x^2 + x - 3$ for a constant ϵ. (b) Setting $\epsilon = 10^{-3}$, find the actual root and compare with part (a).
5. Use (1.21) to approximate the root of $f(x) = (x-1)(x-2)(x-3)(x-4) - 10^{-6}x^6$ near $r = 4$. Find the error magnification factor. Use `fzero` to check your approximation.
6. Use the MATLAB command `fzero` to find the root of the Wilkinson polynomial near $x = 15$ with a relative change of $\epsilon = 2 \times 10^{-15}$ in the x^{15} coefficient, making the coefficient slightly more negative. Compare with the prediction made by (1.21).

1.4 NEWTON'S METHOD

Newton's Method, also called the Newton–Raphson Method, usually converges much faster than the linearly convergent methods we have seen previously. The geometric picture of Newton's Method is shown in Figure 1.8. To find a root of $f(x) = 0$, a starting guess x_0 is given, and the tangent line to the function f at x_0 is drawn. The tangent line will approximately follow the function down to the x-axis toward the root. The intersection point of the line with the x-axis is an approximate root, but probably not exact if f curves. Therefore, this step is iterated.

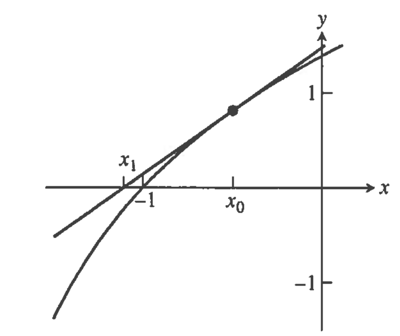

Figure 1.8 One step of Newton's Method. Starting with x_0, the tangent line to the curve $y = f(x)$ is drawn. The intersection point with the x-axis is x_1, the next approximation to the root.

From the geometric picture, we can develop an algebraic formula for Newton's Method. The tangent line at x_0 has slope given by the derivative $f'(x_0)$. One point on the tangent line is $(x_0, f(x_0))$. The point-slope formula for the equation of a line is

We know that 0 is a multiple root. While the backward error is driven near ϵ_{mach} by Newton's Method, the forward error, equal to x_i, is several orders of magnitude larger.

Newton's Method, like FPI, may not converge to a root. The next example shows just one of its possible nonconvergent behaviors.

► **EXAMPLE 1.15** Apply Newton's Method to $f(x) = 4x^4 - 6x^2 - 11/4$ with starting guess $x_0 = 1/2$.

This function has roots, since it is continuous, negative at $x = 0$, and goes to positive infinity for large positive and large negative x. However, no root will be found for the starting guess $x_0 = 1/2$, as shown in Figure 1.10. The Newton formula is

$$x_{i+1} = x_i - \frac{4x_i^4 - 6x_i^2 - \frac{11}{4}}{16x_i^3 - 12x_i}. \tag{1.33}$$

Substitution gives $x_1 = -1/2$, and then $x_2 = 1/2$ again. Newton's Method alternates on this example between the two nonroots $1/2$ and $-1/2$, and fails to find a root.

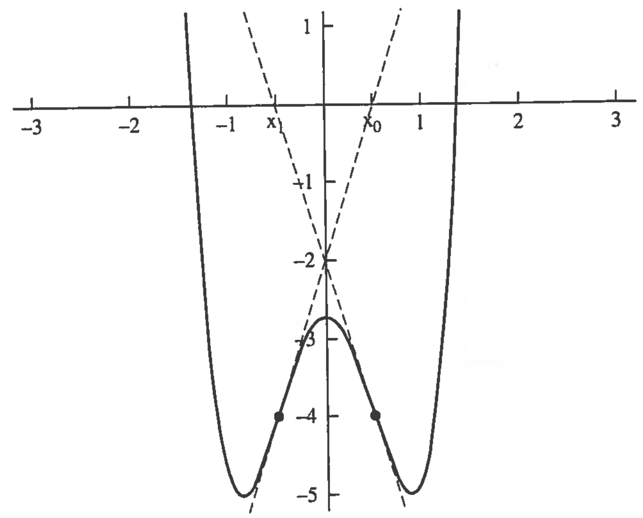

Figure 1.10 Failure of Newton's Method in Example 1.15. The iteration alternates between 1/2 and −1/2, and does not converge to a root. ◄

Newton's Method can fail in other ways. Obviously, if $f'(x_i) = 0$ at any iteration step, the method cannot continue. There are other examples where the iteration diverges to infinity (see Exercise 6) or mimics a random number generator (see Computer Problem 13). Although not every initial guess leads to convergence to a root, Theorems 1.11 and 1.12 guarantee a neighborhood of initial guesses surrounding each root for which convergence to that root is assured.

1.4 Exercises

1. Apply two steps of Newton's Method with initial guess $x_0 = 0$. (a) $x^3 + x - 2 = 0$ (b) $x^4 - x^2 + x - 1 = 0$ (c) $x^2 - x - 1 = 0$

2. Apply two steps of Newton's Method with initial guess $x_0 = 1$. (a) $x^3 + x^2 - 1 = 0$ (b) $x^2 + 1/(x + 1) - 3x = 0$ (c) $5x - 10 = 0$

3. Use Theorem 1.11 or 1.12 to estimate the error e_{i+1} in terms of the previous error e_i as Newton's Method converges to the given roots. Is the convergence linear or quadratic?

(a) $x^5 - 2x^4 + 2x^2 - x = 0$; $r = -1, r = 0, r = 1$ (b) $2x^4 - 5x^3 + 3x^2 + x - 1 = 0$; $r = -1/2, r = 1$

4. Estimate e_{i+1} as in Exercise 3. (a) $32x^3 - 32x^2 - 6x + 9 = 0$; $r = -1/2, r = 3/4$ (b) $x^3 - x^2 - 5x - 3 = 0$; $r = -1, r = 3$

5. Consider the equation $8x^4 - 12x^3 + 6x^2 - x = 0$. For each of the two solutions $x = 0$ and $x = 1/2$, decide which will converge faster (say, to eight-place accuracy), the Bisection Method or Newton's Method, without running the calculation.

6. Sketch a function f and initial guess for which Newton's Method diverges.

7. Let $f(x) = x^4 - 7x^3 + 18x^2 - 20x + 8$. Does Newton's Method converge quadratically to the root $r = 2$? Find $\lim_{i \to \infty} e_{i+1}/e_i$, where e_i denotes the error at step i.

8. Prove that Newton's Method applied to $f(x) = ax + b$ converges in one step.

9. Show that applying Newton's Method to $f(x) = x^2 - A$ produces the iteration of Example 1.6.

10. Find the Fixed-Point Iteration produced by applying Newton's Method to $f(x) = x^3 - A$. See Exercise 1.2.10.

11. Use Newton's Method to produce a quadratically convergent method for calculating the nth root of a positive number A, where n is a positive integer. Prove quadratic convergence.

12. Suppose Newton's Method is applied to the function $f(x) = 1/x$. If the initial guess is $x_0 = 1$, find x_{50}.

13. (a) The function $f(x) = x^3 - 4x$ has a root at $r = 2$. If the error $e_i = x_i - r$ after four steps of Newton's Method is $e_4 = 10^{-6}$, estimate e_5. (b) Apply the same question as (a) to the root $r = 0$. (Caution: The usual formula is not useful.)

14. Let $g(x) = x - f(x)/f'(x)$ denote the Newton's Method iteration for the function f. Define $h(x) = g(g(x))$ to be the result of two successive steps of Newton's Method. Then $h'(x) = g'(g(x))g'(x)$ according to the Chain Rule of calculus. (a) Assume that c is a fixed point of h, but not of g, as in Example 1.15. Show that if c is an inflection point of $f(x)$, that is, $f''(x) = 0$, then the fixed point iteration h is locally convergent to c. It follows that for initial guesses near c, Newton's Method itself does not converge to a root of f, but tends toward the oscillating sequence $\{c, g(c)\}$ (b) Verify that the stable oscillation described in (a) actually occurs in Example 1.15. Computer Problem 14 elaborates on this example.

1.4 Computer Problems

1. Each equation has one root. Use Newton's Method to approximate the root to eight correct decimal places. (a) $x^3 = 2x + 2$ (b) $e^x + x = 7$ (c) $e^x + \sin x = 4$

2. Each equation has one real root. Use Newton's Method to approximate the root to eight correct decimal places. (a) $x^5 + x = 1$ (b) $\sin x = 6x + 5$ (c) $\ln x + x^2 = 3$

3. Apply Newton's Method to find the only root to as much accuracy as possible, and find the root's multiplicity. Then use Modified Newton's Method to converge to the root quadratically. Report the forward and backward errors of the best approximation obtained from each method. (a) $f(x) = 27x^3 + 54x^2 + 36x + 8$ (b) $f(x) = 36x^4 - 12x^3 + 37x^2 - 12x + 1$

4. Carry out the steps of Computer Problem 3 for (a) $f(x) = 2e^{x-1} - x^2 - 1$ (b) $f(x) = \ln(3-x) + x - 2$.

5. A silo composed of a right circular cylinder of height 10 m surmounted by a hemispherical dome contains 400 m^3 of volume. Find the base radius of the silo to four correct decimal places.

6. A 10-cm-high cone contains 60 cm^3 of ice cream, including a hemispherical scoop on top. Find the radius of the scoop to four correct decimal places.

7. Consider the function $f(x) = e^{\sin^3 x} + x^6 - 2x^4 - x^3 - 1$ on the interval $[-2, 2]$. Plot the function on the interval, and find all three roots to six correct decimal places. Determine which roots converge quadratically, and find the multiplicity of the roots that converge linearly.

8. Carry out the steps of Computer Problem 7 for the function $f(x) = 94\cos^3 x - 24\cos x + 177\sin^2 x - 108\sin^4 x - 72\cos^3 x \sin^2 x - 65$ on the interval $[0, 3]$.

9. Apply Newton's Method to find both roots of the function $f(x) = 14xe^{x-2} - 12e^{x-2} - 7x^3 + 20x^2 - 26x + 12$ on the interval $[0, 3]$. For each root, print out the sequence of iterates, the errors e_i, and the relevant error ratio e_{i+1}/e_i^2 or e_{i+1}/e_i that converges to a nonzero limit. Match the limit with the expected value M from Theorem 1.11 or S from Theorem 1.12.

10. Set $f(x) = 54x^6 + 45x^5 - 102x^4 - 69x^3 + 35x^2 + 16x - 4$. Plot the function on the interval $[-2, 2]$, and use Newton's Method to find all five roots in the interval. Determine for which roots Newton converges linearly and for which the convergence is quadratic.

11. The ideal gas law for a gas at low temperature and pressure is $PV = nRT$, where P is pressure (in atm), V is volume (in L), T is temperature (in K), n is the number of moles of the gas, and $R = 0.0820578$ is the molar gas constant. The van der Waals equation

$$\left(P + \frac{n^2 a}{V^2}\right)(V - nb) = nRT$$

covers the nonideal case where these assumptions do not hold. Use the ideal gas law to compute an initial guess, followed by Newton's Method applied to the van der Waals equation to find the volume of one mole of oxygen at 320 K and a pressure of 15 atm. For oxygen, $a = 1.36$ L^2-atm/mole^2 and $b = 0.003183$ L/mole. State your initial guess and solution with three significant digits.

12. Use the data from Computer Problem 11 to find the volume of 1 mole of benzene vapor at 700 K under a pressure of 20 atm. For benzene, $a = 18.0$ L^2-atm/mole^2 and $b = 0.1154$ L/mole.

13. (a) Find the root of the function $f(x) = (1 - 3/(4x))^{1/3}$. (b) Apply Newton's Method using an initial guess near the root, and plot the first 50 iterates. This is another way Newton's Method can fail, by producing a chaotic trajectory. (c) Why are Theorems 1.11 and 1.12 not applicable?

14. (a) Fix real numbers $a, b > 0$ and plot the graph of $f(x) = a^2x^4 - 6abx^2 - 11b^2$ for your chosen values. Do not use $a = 2, b = 1/2$, since that case already appears in Example 1.15. (b) Apply Newton's method to find both the negative root and the positive root of $f(x)$. Then find intervals of positive initial guesses $[d_1, d_2]$, where $d_2 > d_1$, for which Newton's Method: (c) converges to the positive root, (d) converges to the negative root, (e) is defined, but does not converge to any root. Your intervals should not contain any initial guess where $f'(x) = 0$, at which Newton's Method is not defined.

1.5 ROOT-FINDING WITHOUT DERIVATIVES

Apart from multiple roots, Newton's Method converges at a faster rate than the bisection and FPI methods. It achieves this faster rate because it uses more information—in particular, information about the tangent line of the function, which comes from the function's derivative. In some circumstances, the derivative may not be available.

The Secant Method is a good substitute for Newton's Method in this case. It replaces the tangent line with an approximation called the secant line, and converges almost as quickly. Variants of the Secant Method replace the line with an approximating parabola, whose axis is either vertical (Muller's Method) or horizontal (inverse quadratic interpolation). The section ends with the description of Brent's Method, a hybrid method which combines the best features of iterative and bracketing methods.

1.5.1 Secant Method and variants

The Secant Method is similar to the Newton's Method, but replaces the derivative by a difference quotient. Geometrically, the tangent line is replaced with a line through the two last known guesses. The intersection point of the "secant line" is the new guess.

An approximation for the derivative at the current guess x_i is the difference quotient

$$\frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}.$$

A straight replacement of this approximation for $f'(x_i)$ in Newton's Method yields the Secant Method.

Secant Method

$$x_0, x_1 = \text{initial guesses}$$
$$x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})} \quad \textbf{for } i = 1, 2, 3, \ldots.$$

Unlike Fixed-Point Iteration and Newton's Method, two starting guesses are needed to begin the Secant Method.

It can be shown that under the assumption that the Secant Method converges to r and $f'(r) \neq 0$, the approximate error relationship

$$e_{i+1} \approx \left|\frac{f''(r)}{2f'(r)}\right| e_i e_{i-1}$$

holds and that this implies that

$$e_{i+1} \approx \left|\frac{f''(r)}{2f'(r)}\right|^{\alpha - 1} e_i^{\alpha},$$

where $\alpha = (1 + \sqrt{5})/2 \approx 1.62$. (See Exercise 6.) The convergence of the Secant Method to simple roots is called **superlinear**, meaning that it lies between linearly and quadratically convergent methods.