Chapter 3 Rootfinding

Numerical Analysis 1. Winter Semester 2018-19

1 Bisection Method

1.1 Matlab code

The procedure to be constructed will operate on an arbitrary function f . An interval $[a, b]$ is also specified, and the number of steps to be taken, nmax, is given. Pseudocode to perform nmax steps in the bisection algorithm follows:

```
function [c,err,n]=bisection(f,a,b,nmax,ep)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Function bisect aims to find the root of the function f using ...
    Bisection method
% f: function
% a,b: begin & end points
% nmax: maximal number of steps to be taken
% ep: maximal allowable error
% c: the approximated root
% err: absolute error of the root
% n: the number iterated steps
% Copyright: Phi Ha, September 2018
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Use nargin only for advanced students
if nargin ==3
  nmax = 100; ep = 1e-6;
elseif nargin<5
  error('Wrong number of input arguments')
end

% Main program starts here

fa = f(a); fb = f(b);

if sign(fa) == sign(fb)
  error('Function has the same sign at a, b')
end

err = b-a;

for n=0:nmax
  err = err/2;
  c = a+err;
  fc = f(c);

  if err<ep
    disp('Bisection method converges.')
```

```
    break
  end

  if sign(fa) ≠ sign(fc)
    b=c;
    fb = fc;
  else
    a=c;
    fa=fc;
  end
end
```

1.2 Error bound

Let a_n, b_n, and c_n denote the nth computed values of a, b, and c, respectively. Then easily we get

$$b_{n+1} - a_{n+1} = \frac{1}{2}(b_n - a_n), \qquad n \geq 1 \tag{3.5}$$

and it is straightforward to deduce that

$$b_n - a_n = \frac{1}{2^{n-1}}(b - a), \qquad n \geq 1 \tag{3.6}$$

where $b - a$ denotes the length of the original interval with which we started. Since the root α is in either the interval $[a_n, c_n]$ or $[c_n, b_n]$, we know that

$$|\alpha - c_n| \leq c_n - a_n = b_n - c_n = \frac{1}{2}(b_n - a_n) \tag{3.7}$$

This is the error bound for c_n that is used in step B2 of the earlier algorithm. Combining it with (3.6), we obtain the further bound

$$|\alpha - c_n| \leq \frac{1}{2^n}(b - a) \tag{3.8}$$

This shows that the iterates c_n converge to α as $n \to \infty$.

Figure 1: Atkinson-Han, page 74

To see how many iterations will be necessary, suppose we want to have

$$|\alpha - c_n| \leq \epsilon$$

This will be satisfied if

$$\frac{1}{2^n}(b-a) \leq \epsilon$$

Thus we have the following estimation

$$n \geq \frac{\log\left(\dfrac{b-a}{\epsilon}\right)}{\log 2} \quad . \tag{1}$$

There are several advantages to the bisection method. The principal one is that the method is guaranteed to converge. In addition, the error bound, given in (3.7), is guaranteed to decrease by one-half with each iteration. Many other numerical methods have variable rates of decrease for the error, and these may be worse than the bisection method for some equations. The principal disadvantage of the bisection method is that it generally converges more slowly than most other methods. For functions $f(x)$ that have a continuous derivative, other methods are usually faster. These methods may not always converge; when they do converge, however, they are almost always much faster than the bisection method.

Remark 1. *As a final remark, to determine which subinterval of [an, bn] contains a root of f, it is better to make use of the signum function, since the test*

$$\operatorname{sign}(f(a_n)) \cdot \operatorname{sign}(f(c_n)) > 0 \textit{ instead of } f(a_n) \cdot f(c_n) > 0$$

gives the same result but avoids the possibility of overflow or underflow in the multiplication of $f(a_n)$ *and* $f(c_n)$.

2 Fix point iteration

In this section, we give a more general introduction to iteration methods, presenting a general theory for one-point iteration formulas.

2.1 Classical fixed point iteration

As a motivational example, consider solving the equation

$$x^2 - 5 = 0 \tag{3.35}$$

for the root $\alpha = \sqrt{5} \doteq 2.2361$. We give four iteration methods to solve this equation.

I1. $x_{n+1} = 5 + x_n - x_n^2$

I2. $x_{n+1} = \dfrac{5}{x_n}$

I3. $x_{n+1} = 1 + x_n - \dfrac{1}{5}x_n^2$

I4. $x_{n+1} = \dfrac{1}{2}\left(x_n + \dfrac{5}{x_n}\right)$

Table 3.4. Iterations I1 to I4

n	x_n : I1	x_n : I2	x_n : I3	x_n : I4
0	2.5	2.5	2.5	2.5
1	1.25	2.0	2.25	2.25
2	4.6875	2.5	2.2375	2.2361
3	−12.2852	2.0	2.2362	2.2361

The iterations I1 to I4 all have the form

$$x_{n+1} = g(x_n) \tag{3.36}$$

for appropriate continuous functions $g(x)$. For example, with I1, $g(x) = 5 + x - x^2$. If the iterates x_n converge to a point α, then

$$\lim_{n\to\infty} x_{n+1} = \lim_{n\to\infty} g(x_n)$$
$$\alpha = g(\alpha)$$

Thus, α is a solution of the equation $x = g(x)$, and α is called a *fixed point* of the function g.

Figure 2: Page 97 Atkinson - Han

Theorem 1. *(Contraction mapping theorem)*
Assume $g(x)$ and $g'(x)$ are continuous function and assume g satisfies $g : [a, b] \to [a, b]$. Further

assume that

$$\lambda \equiv \max_{t\in[a,b]} |g'(x)| < 1.$$

Then

S1. *There is a unique solution of $x = g(x)$ in the interval $[a, b]$ and for any initial estimate x_0 in $[a, b]$, the iterates x_n will converge to α.*

S2. ***Priori error estimation***

$$|\alpha - x_n| \leqslant \frac{\lambda^n}{1-\lambda} |x_1 - x_0| \, . \tag{2}$$

S3. ***Posteriori error estimation***

$$|\alpha - x_n| \leqslant \frac{\lambda}{1-\lambda} |x_n - x_{n-1}| \, . \tag{3}$$

S4.

$$\lim_{n\to\infty} \frac{\alpha - x_{n+1}}{\alpha - x_n} = g'(\alpha) \, .$$

Thus,

$$|\alpha - x_{n+1}| \approx g'(\alpha)|\alpha - x_n| \, . \tag{4}$$

Proof. The proof is taken from Atkinson-Han, [2]. □

To show that the iterates converge, subtract $x_{n+1} = g(x_n)$ from $\alpha = g(\alpha)$, obtaining

$$\begin{aligned} \alpha - x_{n+1} &= g(\alpha) - g(x_n) \\ &= g'(c_n)(\alpha - x_n) \end{aligned} \tag{3.43}$$

for some c_n between α and x_n. Using the assumption (3.38), we get

$$|\alpha - x_{n+1}| \leq \lambda \, |\alpha - x_n| \, , \qquad n \geq 0 \tag{3.44}$$

Inductively, we can then show that

$$|\alpha - x_n| \leq \lambda^n \, |\alpha - x_0| \, , \qquad n \geq 0 \tag{3.45}$$

Since $\lambda < 1$, the right side of (3.45) goes to zero as $n \to \infty$, and this then shows that $x_n \to \alpha$ as $n \to \infty$.

S3. Use (3.44) with $n = 1$ to obtain

$$\begin{aligned}
|\alpha - x_0| &\le |\alpha - x_1| + |x_1 - x_0| \\
&\le \lambda\, |\alpha - x_0| + |x_1 - x_0| \\
(1-\lambda)\, |\alpha - x_0| &\le |x_1 - x_0| \\
|\alpha - x_0| &\le \frac{1}{1-\lambda}\, |x_1 - x_0| \qquad (3.46)
\end{aligned}$$

Combine this with (3.45) to conclude the derivation of (3.39).

Figure 3: AtkinsonHan p100

Remark 2. *i) With the priori error estimation, we can compute the number of iteration needed to achieve a desired error* ε *without computing the approximated solution.*
ii) On the other hand, the posteriori error estimation is convenient for computing, since if the absolute error between two consecutive error $|x_{n+1} - x_n| < \dfrac{\varepsilon(1-\lambda)}{\lambda}$ *then* $|x_n - \alpha| < \varepsilon$.
iii) The approx. (4) *is useful for later.*

We need a more precise way to deal with the concept of the speed of convergence of an iteration method. We say that a sequence $\{x_n \mid n \ge 0\}$ converges to α with an *order of convergence* $p \ge 1$ if

$$|\alpha - x_{n+1}| \le c\, |\alpha - x_n|^p\,, \qquad n \ge 0$$

for some constant $c \ge 0$. The cases $p = 1$, $p = 2$, and $p = 3$ are referred to as *linear convergence*, *quadratic convergence*, and *cubic convergence*, respectively. Newton's method usually converges quadratically; and the secant method has order of convergence $p = (1 + \sqrt{5})/2$. For linear convergence, we make the additional requirement that $c < 1$; as otherwise, the error $\alpha - x_n$ need not converge to zero.

If $|g'(\alpha)| < 1$ in the preceding theorem, then formula (3.44) shows that the iterates x_n are linearly convergent. If in addition, $g'(\alpha) \ne 0$, then formula (3.41) proves the convergence is exactly linear, with no higher order of convergence being possible. In this case, we call the value of $|g'(\alpha)|$ the linear rate of convergence.

Figure 4: AtkinsonHan - very important

In practice, Theorem 1 is seldom used directly. The main reason is that it is difficult to find an interval $[a, b]$ for which the condition $g : [a, b] \to [a, b]$ is satisfied. Instead, we look for a way to use the theorem in a practical way. The key idea is the result (4), which shows how the iteration error behaves when the iterates x_n are near α.

Corollary 1. *i) Assume that $g(x)$ and $g'(x)$ are continuous for some interval $c < x < d$, with the fixed point (α contained in this interval. Moreover, assume that $|g'(a)| < 1$. Then, there is an interval $[a, b]$ around α for which the hypotheses, and hence also the conclusions, of Theorem 1 are true.*
ii) If the contrary, $|g'(\alpha)| > 1$, then the iteration method $x_{n+1} = g(x_n)$ will not converge to α.
iii) When $|g'(\alpha)| = 1$, no conclusion can be drawn; and even if convergence were to occur, the method would be far too slow for the iteration method to be practical.

Other remarks can be found in [1], pages 139, 141.

2.2 Aitken Error Estimation and Extrapolation

With the formula (4), it is possible estimate the error in the iterate x_n and to accelerate their convergence. Let $g'(\alpha)$ be denoted by λ. Thus,

$$|\alpha - x_{n+1}| \approx \lambda|\alpha - x_n| \;\Rightarrow\; \alpha \approx x_n + \frac{\lambda}{1-\lambda}(x_n - x_{n-1}). \tag{5}$$

We need an estimate of λ. It cannot be calculated from its definition, since that requires knowing the solution α. To estimate λ, we use the ratios

$$\lambda_n := \frac{x_n - x_{n-1}}{x_{n-1} - x_{n-2}} = g'(c_n) \overset{n\to\infty}{\longrightarrow} g'(\alpha) = \lambda\,. \tag{6}$$

The **Aitken's extrapolation formula**

$$\alpha \approx x_n + \frac{\lambda_n}{1-\lambda_n}(x_n - x_{n-1}) \;=\; \frac{x_{n-2}x_n - x_{n-1}^2}{x_{n-2} - 2x_{n-1} + x_n}.$$

The **Aitken's error estimate**

$$\alpha - x_n \approx \frac{\lambda_n}{1-\lambda_n}(x_n - x_{n-1}) \;=\; \frac{(x_n - x_{n-1})^2}{x_{n-2} - 2x_{n-1} + x_n}.$$

Table 3.5. The Iteration $x_{n+1} = 1 + x_n - \frac{1}{5}x_n^2$

n	x_n	$\alpha - x_n$	r_n
0	2.5	−2.64E − 1	
1	2.25	−1.39E − 2	0.0528
2	2.2375	−1.43E − 3	0.1028
3	2.23621875	−1.51E − 4	0.1053
4	2.23608389	−1.59E − 5	0.1055
5	2.23606966	−1.68E − 6	0.1056
6	2.23606815	−1.77E − 7	0.1056
7	2.23606800	−1.87E − 8	0.1056

Table 3.6. The Iteration $x_{n+1} = 1 + x_n - \frac{1}{5}x_n^2$ and Aitken Error Estimation

n	x_n	$x_n - x_{n-1}$	λ_n	Estimate
0	2.5			
1	2.25	−2.50E − 1		
2	2.2375	−1.25E − 2	0.0500	−6.58E − 4
3	2.23621875	−1.28E − 3	0.1025	−1.46E − 4
4	2.23608389	−1.35E − 4	0.1053	−1.59E − 5
5	2.23606966	−1.42E − 5	0.1055	−1.68E − 6
6	2.23606815	−1.50E − 6	0.1056	−1.77E − 7
7	2.23606800	−1.59E − 7	0.1056	−1.87E − 8

2.3 Matlab code

```
function [x,n] = fix_iter(f,x0,nmax,eps,varargin)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Function fix_iter is an implementation for the Fixed Point Iteration ...
    (phuong phap lap don)
% Form : [x,n] = fix_iter(f,x0,nmax,eps)
% f: function
% x0 : starting point
% nmax: maximal number of steps to be taken
% ep: maximal allowable error between two consecutive steps
% c: the approximated root
% n: the number iterated steps
% Stopping Criteria: The method stops after nmax iterations
% or the difference between two consecutive iterates is smaller than eps
% Copyright: Phi Ha, September 2018
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Use nargin only for advanced students
if nargin ==2
  nmax = 100; eps = 1e-4;
elseif nargin<4
  error('Wrong number of input arguments')
end

x = x0; n = 0;

tic
for i = 1:nmax
  y = f(x); diff = abs(y-x);
  if diff ⩽ eps
    disp('Fixpoint iteration converges.')
    break
  else
     x = y;
     n = n+1;
  end
```

```
end
toc

% tic
% for i=1:nmax
%     if abs(x-f(x))⩽ eps
%         break
%     else
%         x = f(x);
%         n = n + 1;
%     end
% end
% toc

if (n == nmax && diff > eps)
    disp('Fix point iteration fails to converges.')
end
```

2.4 Higher order iteration formulas

The convergence formula (3.41) gives less information in the case $g'(\alpha) = 0$, although the convergence is clearly quite good. To improve on the results in Theorem 3.4.2, consider the Taylor expansion of $g(x_n)$ about α, assuming that $g(x)$ is twice continuously differentiable:

$$g(x_n) = g(\alpha) + (x_n - \alpha)g'(\alpha) + \frac{1}{2}(x_n - \alpha)^2 g''(c_n) \tag{3.55}$$

with c_n between x_n and α. Using $x_{n+1} = g(x_n)$, $\alpha = g(\alpha)$, and $g'(\alpha) = 0$, we have

$$x_{n+1} = \alpha + \frac{1}{2}(x_n - \alpha)^2 g''(c_n)$$

$$\alpha - x_{n+1} = -\frac{1}{2}(\alpha - x_n)^2 g''(c_n) \tag{3.56}$$

$$\lim_{n\to\infty} \frac{\alpha - x_{n+1}}{(\alpha - x_n)^2} = -\frac{1}{2} g''(\alpha) \tag{3.57}$$

If $g''(\alpha) \neq 0$, then this formula shows that the iteration $x_{n+1} = g(x_n)$ is of *order* 2 or is *quadratically convergent*.

If also $g''(\alpha) = 0$, and perhaps also some higher-order derivatives are zero at α, then expand the Taylor series through higher-order terms in (3.55), until the final error term contains a derivative of g that is nonzero at α. This leads to methods with an order of convergence greater than 2.

3 Newton method

There are two ways to interpret the Newton (also named Newton-Raphson) method.

1. **Geometrical way**

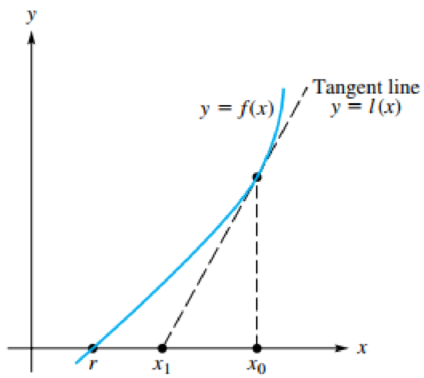

Figure 5: Newton method

The **Newton method** reads

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} .$$

The geometry of Newton's method is shown in Figure 5. The line $y = \ell(x)$ is tangent to the curve $y = f(x)$. It intersects the x-axis at a point x_1. The slope of $\ell(x)$ is $f'(x_0)$.

2. **Analytical way** We ask: What correction h should be added to x_0 to obtain the root precisely? Obviously, we want $f(x_0 + h) = 0$. If f is a sufficiently well-behaved function, it will have a Taylor series at x_0. Thus, we could write

$$f(x_0) + hf'(x_0) + h^2 \frac{f''(x_0)}{2!} + \cdots = 0 .$$

Determining h from this equation is, of course, not easy. Therefore, we give up the expectation of arriving at the true root in one step and seek only an approximation to h. This can be obtained by ignoring all but the first two terms in the series: $f(x_0) + hf'(x_0) = 0$. The h that solves this is not the h that solves $f(x_0 + h) = 0$, but it is the easily computed number & our new approximation is then

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} .$$

and the process can be repeated.
This analytical way makes sense also in the case of systems of nonlinear equations, and we then have the Newton iterations

$$\mathbf{X_{n+1}} = \mathbf{X_n} - \mathbf{J_f}(\mathbf{X_n})^{-1}\mathbf{F}(\mathbf{X_n}) \overset{\text{MATLAB}}{=} \mathbf{X_n} - \mathbf{J_f}(\mathbf{X_n}) \setminus \mathbf{F}(\mathbf{X_n}).)$$

3.1 Matlab code

```
function [x,n] = newton(f,df,x0,nmax,eps,Δ,varargin)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Function newton is an implementation of Newton method for solving f(x)=0
% Form: [x,n] = newton(f,df,x0,nmax,eps,Δ,varargin)
% f: function
% df: the derivatice function
% x0 : starting point
% nmax: maximal number of steps to be taken
% eps: maximal allowable error between two consecutive iterations
% Δ: maximal allowable of f'(x0)
% x: the approximated root
% n: the number iterated steps
% Stopping Criteria: The method stops after nmax iterations or the ...
    difference
% between two consecutive iterates is smaller than eps
% Copyright: Phi Ha, September 2018
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% Use nargin only for advanced students

disp("Please input both f(x) and f'(x)-could be in finite difference")

if nargin ==3
  nmax = 1000; eps = 1e-6; Δ = 1e-12;
elseif (nargin ≠ 3 | nargin ≠ 6)
  error('Wrong number of input arguments')
end

if abs(df(x0)) < Δ
  error("Derivative of function is nearly zero. Stops.")
end

x = x0; n = 0; diff = 1;

for i=1:nmax
  %if abs(y)⩽ eps       % Do not use this, since the number of ...
      significant ...
                         % ... figures in x is not guarantee
  if abs(diff) ⩽ eps
    disp('Newton method converges since |x_{n+1} - x_n| < eps.')
    break
  else
    xnew = x - df(x)\f(x); % The division df(x)\f(x) is also applicable ...
        for matrix ...
                           % ... so it is better than f(x)/df(x)
                           % eventhough they have the same meaning
    diff = x - xnew;
    x = xnew;
    n = n + 1;
  end
end
```

```

if (abs(diff) > eps  && n == nmax)
  disp("Newton method may diverges.")
end
```

3.2 Experiments and Error analysis

Example 1. *Example 3.2.1 in [2] is nice.*

Example 2. *Example 3.2.2 in [2] to demonstrate that* $Rel(x_{n+1}) = Rel(x_n)^2$. *But it should be left for students to read at home.*

Assume $f(x)$ has at least two continuous derivatives for all x in some interval about the root α. Further assume that

$$f'(\alpha) \neq 0 \tag{3.18}$$

This says that the graph of $y = f(x)$ is not tangent to the x-axis when the graph intersects it at $x = \alpha$. The case in which $f'(\alpha) = 0$ is treated in Section 3.5. Also, note that combining (3.18) with the continuity of $f'(x)$ implies that $f'(x) \neq 0$ for all x near α.

Use Taylor's theorem to write

$$f(\alpha) = f(x_n) + (\alpha - x_n) f'(x_n) + \tfrac{1}{2}(\alpha - x_n)^2 f''(c_n)$$

with c_n an unknown point between α and x_n. Note that $f(\alpha) = 0$ by assumption, and then divide $f'(x_n)$ to obtain

$$0 = \frac{f(x_n)}{f'(x_n)} + \alpha - x_n + (\alpha - x_n)^2 \frac{f''(c_n)}{2f'(x_n)}$$

From (3.11), the first term on the right side is $x_n - x_{n+1}$, and we have

$$0 = x_n - x_{n+1} + \alpha - x_n + (\alpha - x_n)^2 \frac{f''(c_n)}{2f'(x_n)}$$

Solving for $\alpha - x_{n+1}$, we have

$$\alpha - x_{n+1} = (\alpha - x_n)^2 \left[\frac{-f''(c_n)}{2f'(x_n)}\right] \tag{3.19}$$

Example 3. *We consider again the first example above.*

For the earlier iteration (3.12), $f''(x) = 30x^4$. If we are near the root α, then

$$\frac{-f''(c_n)}{2f'(x_n)} \approx \frac{-f''(\alpha)}{2f'(\alpha)} = \frac{-30\alpha^4}{2(6\alpha^5 - 1)} \doteq -2.42$$

Thus for the error in (3.12),

$$\alpha - x_{n+1} \approx -2.42(\alpha - x_n)^2 \tag{3.20}$$

This explains the rapid convergence of the final iterates in Table 3.2. For example, consider the case of $n = 3$, with $\alpha - x_3 \doteq -4.73\text{E} - 3$. Then (3.20) predicts

$$\alpha - x_4 \doteq -2.42(4.73\text{E} - 3)^2 \doteq -5.42\text{E} - 5$$

which compares well to the actual error of $\alpha - x_4 \doteq -5.35\text{E} - 5$. ■

If we assume that the iterate x_n is near the root α, the multiplier on the right of (3.19) can be written as

$$\frac{-f''(c_n)}{2f'(x_n)} \approx \frac{-f''(\alpha)}{2f'(\alpha)} \equiv M \tag{3.21}$$

Thus,

$$\alpha - x_{n+1} \approx M(\alpha - x_n)^2, \qquad n \geq 0 \tag{3.22}$$

Multiply both sides by M to get

$$M(\alpha - x_{n+1}) \approx [M(\alpha - x_n)]^2 \tag{3.23}$$

Assuming that all of the iterates are near α, then inductively we can show that

$$M(\alpha - x_n) \approx [M(\alpha - x_0)]^{2^n}, \qquad n \geq 0$$

Since we want $\alpha - x_n$ to converge to zero, this says that we must have

$$|M(\alpha - x_0)| < 1$$

$$|\alpha - x_0| < \frac{1}{|M|} = \left|\frac{2f'(\alpha)}{f''(\alpha)}\right| \tag{3.24}$$

If the quantity $|M|$ is very large, then x_0 will have to be chosen very close to α to obtain convergence. In such situations, the bisection method is probably an easier method to use. An example of this situation is given in Problem 5.

The choice of x_0 can be very important in determining whether Newton's method will converge. Unfortunately, there is no single strategy that is always effective in choosing x_0. In most instances, a choice of xo arises from the physical situation that led to the rootfinding problem. In other instances, graphing $y = f(x)$ will probably be needed, possibly combined with the bisection method for a few iterates.

3.2.2 Error Estimation

We are computing a sequence of iterates x_n, and we would like to estimate their accuracy to know when to stop the iteration. To estimate $\alpha - x_n$, note that, since $f(\alpha) = 0$, we have

$$f(x_n) = f(x_n) - f(\alpha) = f'(\xi_n)(x_n - \alpha)$$

for some ξ_n between x_n and α, by the mean-value theorem. Solving for the error, we obtain

$$\alpha - x_n = \frac{-f(x_n)}{f'(\xi_n)} \approx \frac{-f(x_n)}{f'(x_n)}$$

provided that x_n is so close to α that $f'(x_n) \doteq f'(\xi_n)$. From (3.11), this becomes

$$\alpha - x_n \approx x_{n+1} - x_n \tag{3.25}$$

This is the standard error estimation formula for Newton's method, and it is usually fairly accurate. However, this formula is not valid if $f'(\alpha) = 0$, a case that is discussed in Section 3.5 of this chapter.

3.3 Extra reading

In the use of Newton's method, consideration must be given to the proper choice of a starting point. Usually, onemust have some insight into the shape of the graph of thefunction.Sometimes a coarse graph is adequate, but in other cases, a step-by-step evaluation of the function at various points may be necessary to find a point near the root. Often several steps of the bisection method is used initially to obtain a suitable starting point, and Newton's method is used to improve the precision. Although Newton's method is truly a marvelous invention, its convergence depends upon hypotheses that are difficult to verify a priori. Some graphical examples will show what can happen.

In Figure 6(a), the tangent to the graph of the function f at x_0 intersects the x-axis at a point remote from the root r, and successive points in Newton's iteration recede from r instead of converging to r. The difficulty can be ascribed to a poor choice of the initial point x_0; it is not sufficiently close to r. In Figure 6(b), the tangent to the curve is parallel to the x-axis and $x_1 = \infty$, or it is assigned the value of machine infinity in a computer. In Figure 6(c), the iteration values cycle because $x_2 = x_0$. In a computer, roundoff errors or limited precision may eventually cause this situation to become

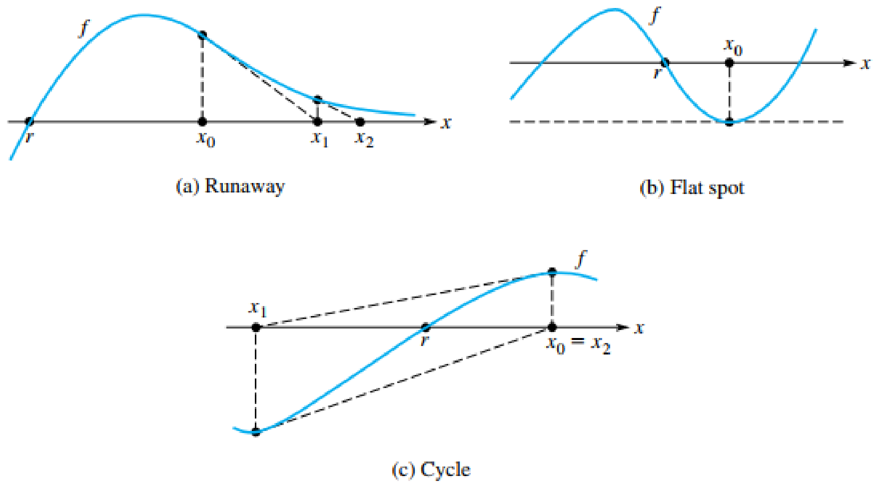

Figure 6: Failure of Newton's method due to bad starting points

unbalanced such that the iterates either spiral inward and converge or spiral outward and diverge. The analysis that establishes the quadratic convergence discloses another troublesome hypothesis; namely, $f'(r) \neq 0$.

If $f'(r) = 0$, then r is a zero of f and f'. Such a zero is termed a multiple zero of f. In this case, at least a double zero. Newton's iteration for a multiple zero converges only linearly! Ordinarily, one would not know in advance that the zero sought was a multiple zero. If one knew that the multiplicity was m, however, Newton's method could be accelerated by modifying the equation to read

$$x_{n+1} = x_n - m\frac{f(x_n)}{f'(x_n)}$$

in which m is the multiplicity of the zero in question.

Summary

(1) For finding a zero of a continuous and differentiable function f, **Newton's method** is given by

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \qquad (n \geqq 0)$$

It requires a given initial value x_0 and two function evaluations (for f and f') per step.

(2) The errors are related by

$$e_{n+1} = -\frac{1}{2}\left(\frac{f''(\xi_n)}{f'(x_n)}\right)e_n^2$$

which leads to the inequality

$$|e_{n+1}| \leqq c|e_n|^2$$

This means that Newton's method has **quadratic convergence** behavior for x_0 sufficiently close to the root r.

(3) For an $N \times N$ system of nonlinear equations $\mathbf{F}(\mathbf{X}) = \mathbf{0}$, **Newton's method** is written as

$$\mathbf{X}^{(k+1)} = \mathbf{X}^{(k)} - \left[\mathbf{F}'\left(\mathbf{X}^{(k)}\right)\right]^{-1}\mathbf{F}\left(\mathbf{X}^{(k)}\right) \qquad (k \geqq 0)$$

which involves the Jacobian matrix $\mathbf{F}'\left(\mathbf{X}^{(k)}\right) = \mathbf{J} = \left[\left(\partial f_i\left(\mathbf{X}^{(k)}\right)/\partial x_j\right)\right]_{N\times N}$. In practice, one solves the **Jacobian linear system**

$$\left[\mathbf{F}'(\mathbf{X}^{(k)})\right]\mathbf{H}^{(k)} = -\mathbf{F}\left(\mathbf{X}^{(k)}\right)$$

using Gaussian elimination and then finds the next iterate from the equation

$$\mathbf{X}^{(k+1)} = \mathbf{X}^{(k)} + \mathbf{H}^{(k)}$$

4 Secant method

In analog to Newton method, the secant method can be viewed from two different perspectives, geometrical and analytical.

Geometrical

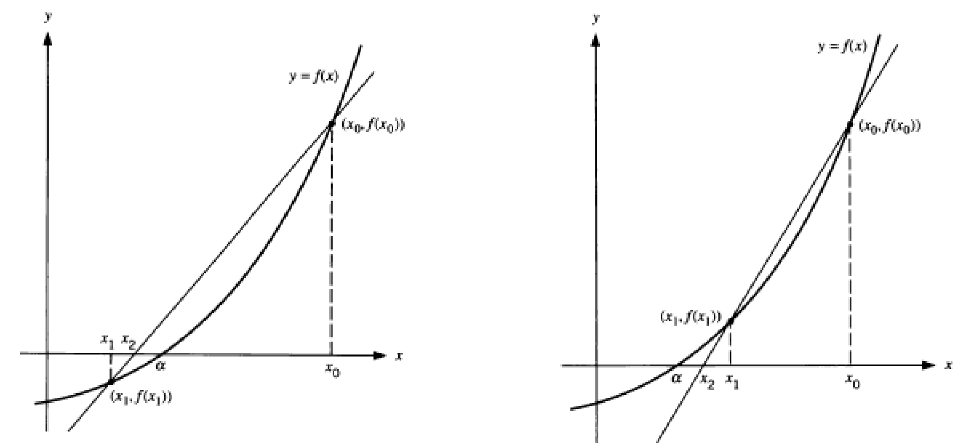

Figure 7: A geometrical schematic of the secant method: left $x_1 < \alpha < x_0$ and right $\alpha < x_1 < x_0$.

Analytical From Newton's method

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \approx \mathbf{x_n} - \mathbf{f}(\mathbf{x_n})\, \frac{\mathbf{x_n} - \mathbf{x_{n-1}}}{\mathbf{f}(\mathbf{x_n}) - \mathbf{f}(\mathbf{x_{n-1}})}\,.$$

Notice that, first secant method requires two initial values x_0 and x_1. After the first step, only one new function evaluation per step is needed.

4.1 Error analysis

After $n+1$ steps of the secant method, the error iterates $e_i = \alpha - x_i$ obey the equation

$$e_{n+1} = -\frac{1}{2}\frac{f''(\xi_n)}{f'(\zeta_n)}\, e_n\, e_{n-1}.$$

which leads to the approximation

$$|e_{n+1}| \approx C|e_n|^{1/2(1+\sqrt{5})} \approx C|e_n|^{1.62}\,.$$

Therefore, the secant method has **superlinear convergence** behavior.

5 Comparison of Methods

In this chapter, three primary methods for solving an equation $f(x) = 0$ have been presented. The bisection method is reliable but slow. Newton's method is fast but often only near the root and requires f'. The secant method is nearly as fast as Newton's method and does not require knowledge of the derivative f', which may not be available or may be too expensive to compute. The user of the bisection method must provide two points at which the signs of $f(x)$ differ, and the function f need only be continuous. In using Newton's method, one must specify a starting point near the root, and f must be differentiable. The secant method requires two good starting points. Newton's procedure can be interpreted as the repetition of a two-step procedure summarized by the prescription linearize and solve. This strategy is applicable in many other numerical problems, and its importance cannot be overemphasized. Both Newton's method and the secant method fail to bracket a root. The modified false position method can retain the advantages of both methods. The secant method is often faster at approximating roots of nonlinear functions in comparison to bisection and false position. Unlike these two methods, the intervals $[a_k, b_k]$ do not have to be on opposite sides of the root and have a change of sign. Moreover, the slope of the secant line can become quite small, and a step can move far from the current point. The secant method can fail to find a root of a nonlinear function that has a small slope near the root because the secant line can jump a large amount. For nice functions and guesses relatively close to the root, most of these methods require relatively few iterations before coming close to the root. However, there are pathological functions that can cause troubles for any of those methods. When selecting a method for solving a given nonlinear problem, one must consider many issues such as what you know about the behavior of the function, an interval $[a, b]$ satisfying $f(a)f(b) < 0$, the first derivative of the function, a good initial guess to the desired root, and so on.

6 Ill behavior

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