Numerical Analysis

Chapter 3 Root Finding

An Ideal Goal: Find the roots of the equation

$$f(x) = 0.$$

Example 1. Solve the following equations.

a) $x^2 - 3x + 2 = 0$ b) $x^3 - 3x + 2 = 0$

c) $x^6 - x - 1 = 0$

Example 2. Given $P_{in},\ P_{out},\ N_{in},\ N_{out}$, find r in the equation

$$f(r) \equiv P_{in}\left[(1+r)^{N_{in}} - 1\right] \ - \ P_{out}\left[1 - (1+r)^{N_{out}}\right] = 0.$$

Read the text on pages 71 and 72 for the application and derivation of this equation.

Practical Goal: Approximate the roots of the equation

$$f(x) = 0.$$

3.1 The Bisection Method

Remark. Assume f is continuous on $[a, b]$ and

$$f(a)f(b) < 0.$$

Then f changes sign on $[a, b]$ and $f(x) = 0$ has at least a root in the interval. (This is the Intermediate Value Theorem of Calculus.)
The simplest numerical procedure for finding a root is repeatedly halving the interval for which $f(x)$ changes sign. This is called the **bisection method**.

Here are the steps. Fix a positive $\epsilon > 0$. This is to decide the accuracy of the approximation.

B1 Define $c = \frac{a+b}{2}$

B2 If $b - c < \epsilon$, then accept c as a root and stop.

B3 If sign$[f(b)]\cdot$ sign$[f(c)] < 0$, then set $c = a$.
Otherwise, set $b = c$ and return to B1

Example 3. Find the largest root of

$$f(x) = x^6 - x - 1 = 0$$

accurate to within $\epsilon = 0.001$.

Solution: First note that $f(1) = -1$ and $f(2) = 61$. Thus $a = 1$ and $b = 2$. The first value of c will be $c = 1.5$. We compute $b - c$ to find that $b - c = .5$. Next we evaluate $f(c) = f(1.5) = 8.8906 > 0$, and hence let $b = c = 1.5$ and go to B1. The new c is $c = 1.25$ and $b - c = .25$ and so we compute $f(c) = f(1.25) = 1.5647 > 0$. We set $b = c = 1.25$ and go to B1 again. Keep repeating this while at the same time keeping track of the difference $b - c$. When this difference becomes less than ϵ we stop. For details, see the table on page 73 of the text.

Error Bounds Given a, b, and ϵ, how many steps do we need to approximate the roo of $f(x) = 0$?

To answer this question, we let a_n, b_n, and c_n denote the nth computed values of a, b, and c respectively. Then

$$b_{n+1} - a_{n+1} = \frac{1}{2}(b_n - a_n)$$

and hence (by induction)

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

Since the root α is in either $[a_n, c_n]$ or $[c_n, b_n]$, we know that

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

and so (again by induction) we have

$$|\alpha - c_n| < \frac{1}{2^n}(b - a).$$

It follows that

$$\lim_{n \to \infty} c_n = \alpha.$$

If we require $|\alpha - c_n| \leq \epsilon$, then it suffices to have

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

or

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

3.2 Newton's Method

Remark. Newton's method use tangent line approximation. More precisely, let x_0 a point near a solution α of $f(x) = 0$. We will discussed a condition on the selection of x_0 later. For the moment assume that $f'(x_0) \neq 0$. The equation of the tangent line at x_0 is given by

$$y - f(x_0) = f'(x_0)(x - x_0).$$

Let x_1 be the $x-$intercept of the tangent line. Then we can solve for x_1 to get

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

We will show later that for suitably chosen x_0, x_1 will be closer to the root α of $f(x) = 0$. Replace x_0 by x_1 and repeat the above to get a better approximation x_2 given by

$$x_2 = x_1 \; - \; \frac{f(x_1)}{f'(x_1)}.$$

Continue this process to obtain

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

This is called the **iteration formula of Newton's Method**. Newton's method is sometimes called **Newton - Raphson Method**

Example 4 Find the iteration formula for Newton's method and use it to approximate the root of $f(x) = x^6 - x - 1$.

Solution: Since $f'(x) = 6x^5 - 1$, we have

$$x_{n+1} = x_n \; - \; \frac{x_n^6 - x_n - 1}{6x_n^5 - 1}$$

We can use $x_0 = 1.5$ and obtain $x_1 = 1.300490088$. and so on. (See Table 3.2 on page 81)

Example 5 Do Example 3.2.2 of the text on page 81.

<u>**Error Analysis**</u> How do we choose x_0 to ensure convergence of x_n to α?

Assume f has a continuous derivative, $f(\alpha) = 0$, and $f'(\alpha) \neq 0$. Using Taylor's Thereom, we have

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

where c_n is a number between α and x_n.

Since $f(\alpha) = 0$ and $f'(\alpha) \neq 0$ diving the above by $f'(\alpha)$, we get

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

From Newton's method iteration formula, we note that

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

Using this in the above equation, we get

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

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

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

If we now assume that

$$\lim_{n\to\infty} x_n = \alpha,$$

then

$$c_n \approx \alpha \qquad \text{and} \qquad c_n \approx \alpha$$

and hence

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

Thus,

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

and multiply both sides by M, we get

$$M(\alpha - x_{n+1}) \approx (M(\alpha - x_0))^2$$

By induction, we conclude that

$$\alpha - x_n \approx (M(\alpha - x_0))^{2^n}, \qquad (n \geq 1).$$

Consequently for $\lim_{n\to\infty} x_n = \alpha$ to hold we must have

$$|\alpha - x_0| < \frac{1}{M}.$$

Remark. While the above condition ensures the convergence of the iteration formula for Newton, the difficulty is that M uses the value of the unknown α. How would you overcome this difficulty?

Error Estimation How many iterations do we need to approximate α by x_n accurate to within a given $\epsilon > 0$?

To answer this question, we use the Mean Value Theorem on the interval $[\alpha, x_n]$ or $[x_n, \alpha]$ to write

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

for some c_n between x_n and α. But $f(\alpha) = 0$ and so we have

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

or

$$\alpha - x_n = \frac{-f(x_n)}{f'(c_n)}.$$

Now assume $f'(c_n) \approx f'(x_n)$ and use Newton's iteration formula to get

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

Therefore,

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

In other words,

$$|x_{n+1} - x_n| < \epsilon$$

can ensure that the error $|\alpha - x_n|$ is less than ϵ. This is the standard error estimate for Newton's Method.

3.3 Secant Method

Newton's Method uses tangent line. However, we can also use other straight line approximations to $y = f(x)$. One such method is called the **secant method**.

Assume that two initial guesses x_0 and x_1 to α are known. Find the equation of the line passing through $(x_0,\ f(x_0))$ and $(x_1,\ f(x_1))$ to obtain

$$y = P(x) = f(x_1) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_1).$$

Solve $P(x) = 0$ to get the solution x_2:

$$x_2 = x_1 - f(x_1)\frac{x_1 - x_0}{f(x_1) - f(x_0)}.$$

It can be shown that x_2 is a better approximation to α than the previous two guesses. Repeat the above arguement with x_1 and x_2 to get a new approximation x_3 given by

$$x_3 = x_2 - f(x_2)\frac{x_2 - x_1}{f(x_2) - f(x_1)}.$$

We proceed inductively to obtain the **iteration formula for the secant method:**

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

Example Find the iteration formula for to approximate the root of $f(x) = x^6 - x - 1$. (See table 3.3 on page 92)

Error Analysis From

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

we can show that

$$\alpha - x_{n+1} = (\alpha - x_n)(\alpha - x_{n-1})\left[-\frac{f''(d_n)}{2f'(c_d)}\right]$$

where c_n is between x_n and x_{n+1} and d_n is between the smallest and largest of α, x_n and x_{n-1}.

It can be shown that if x_0 and x_1 are chosen to be sufficiently close to α, then

$$\lim_{n\to\infty} \frac{|\alpha - x_{n+1}|}{|\alpha - x_n|^r} = \left|\frac{f''(\alpha)}{2f'(\alpha)}\right|^{r-2} = c$$

where $r = (\sqrt{5} + 1)/2 \approx 1.62$. Thus

$$|\alpha - x_{n+1}| \approx c|\alpha - x_n|^{1.62}.$$

From this we also deduce that

$$\alpha - x_n \approx x_n - x_{n-1}$$

which is the **error estimate** for the iterates of the scant method. Clearly the Newton method is faster than the secant method.

3.4 Fixed Point Iteration

An other method of solving $f(x) = 0$ is to rewrite it as

$$x = g(x).$$

We then begin with an initial guess x_0 and define the **fixed point iteration formula**

$$x_{n+1} = g(x_n).$$

Under what condition(s) does the statement 'if $\alpha = g(\alpha)$, then $f(\alpha) = 0$' hold? Note that

$$\lim_{n\to\infty} x_n = \alpha \qquad \text{implies} \qquad \alpha = g(\alpha)$$

and x_n gives an approximation to α. Since $\alpha = g(\alpha)$, we say that α is a fixed point of g and hence the name of the method.

Example Consider the equation

$$f(x) = x^2 - 5 = 0.$$

Each of the following iterations can be considered a fixed point iteration.

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

I2 $x_{n+1} = 5/x_n$

I3 $x_{n+1} = 1 + x_n - \frac{1}{5}x^2$

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

Construct a table to see which of the above iterations gives the desired result of approximate the positive root $\alpha = \sqrt{5}$?

Lemma Let g be continuous on $[a, b]$ and suppose $a \le g(x) \le b$ for all $x \in [a, b]$. The the equation $x = g(x)$ has at least one solution α in $[a, b]$.

Proof: Apply IVT to $f(x) = x - g(x)$.

Theorem (Contraction Mapping Theorem) Assume that g and g' are continuous on $[a, b]$and that $a \le g(x) \le b$ for all $x \in [a, b]$. Suppose

$$\lambda = \max_{a \le x \le b} |g'(x)| < 1.$$

Then

S1 There is a unique solution of $x = g(x)$ in $[a, b]$

S2 For any initial estimate x_0 in $[a, b]$, the iterate x_n converges to α.

S3

$$|\alpha - x_n| = \frac{\lambda^n}{1-\lambda}|x_0 - x_1| \qquad (n \ge 1$$

S4

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

Thus

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

Corollary If g and g' are continuous on $[c, d]$ with a fixed point α and if $|g'(\alpha)| < 1$, then there exists an in interval $[a, b]$ around α for which the hypothesis of the theorem holds.

Example Redo I1 to I4 of the previous example.

Aitken Error Estimation and Extrapolation

Let $\lambda = g'(\alpha)$ and assume that

$$\alpha - x_n \approx g'(\alpha)(\alpha - x_{n-1})$$

as in the above theorem. Solving this equation for α, we get

$$\alpha \approx x_n + \frac{\lambda}{1-\lambda}(x_n - x_{n-1}).$$

Since we do not yet know α, we do not know the exact value of λ. We now make an estimate on λ

Define

$$\lambda_n = \frac{x_n - x_{n-1}}{x_{n-1} - x_{n-2}} = \frac{g(x_{n-1}) - g(x_{n-2})}{x_{n-1} - x_{n-2}}$$

My the Mean Value Theorem, there exists c_n between x_{n-1} and x_{n-2} such that $\lambda_n = g'(c_n)$. Since $x_n \to \alpha$, we have $c_n \to \alpha$. By continuity of g', we conclude that $g(c_n) \to g'(\alpha) = \lambda$. Thus

$$\lambda = \lim_{n\to\infty} \lambda_n$$

and therefore

$$\lambda \approx x_n + \frac{\lambda_n}{1-\lambda_n}(x_n - x_{n-1}).$$

The approximation

$$\alpha - x_n \approx \frac{\lambda_n}{1-\lambda_n}(x_n - x_{n-1}) \qquad \lambda_n = \frac{x_n - x_{n-1}}{x_{n-1} - x_{n-2}}$$

is called **Aitken error estimate**.

Remark If $g'(\alpha) = 0$, then we use Taylor's Theorem and write

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

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

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

or

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

Taking limit and noting that $c_n \to \alpha$, we obtain

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

From this limit we conclude

$$\alpha - x_{n+1} \approx N(\alpha - x_n)^2.$$

For this reason the iterate $x_{n+1} = g(x_n)$ is said be of **order** 2 or **quadratically convergent**.