Summary of last session

-Chapter 7. Numerical Differentiation and integration

■ 7.3. Gaussian Quadrature

■ 7.4. Romberg Integration

Chapter Three Solution of Nonlinear Equations

- 3.0 Introduction
- 3.1 Bisection Method
- 3.2 Newton's Method
- 3.3 Secant Method
- 3.4 Fixed Points and Functional Iteration
- 3.5 Computing Roots of Polynomials
- 3.6 Homotopy and Continuation Methods

One of the basic problems in science and engineering is the root-finding problem. This process involves finding a root or solution, of an equation of the form

$$f(x)=0$$

The equation f(x) = 0 is called an algebraic equation if it is purely a polynomial in x. For example

$$x^3 - 5x^2 - 6x + 3 = 0$$

is an algebraic equation.

It is called transcendental(超越) equation if f(x) contains trigonometric(三角的), exponential or logarithmic functions. For example

 $M = E - e \sin E$ and $ax^2 + \log (x - 3) + e^x \sin x = 0$ are transcendental equations.

To find the solution of an equation f(x) = 0, we find those values of x for which f(x) = 0 is satisfied. Such values of x are called the roots of f(x) = 0.

Examples of non-linear equations can be found in many applications. Generally, the root is obtained in a numerical way, using iterative method.

For example: to find the value of root square of 3 is alternatively to find the solution or root of equation:

$$x^2 - 3 = 0$$

(Continued)

Given a initial value x_0 (>0), from the formula: $x_k = (x_{k-1} + 3/x_{k-1})/2$

we can generate a sequence:

$$x_0 = 1$$

 $x_1 = (1+3)/2 = 2$
 $x_2 = (2+3/2)/2 = 1+3/4 = 1.75$
 $x_3 = \dots$

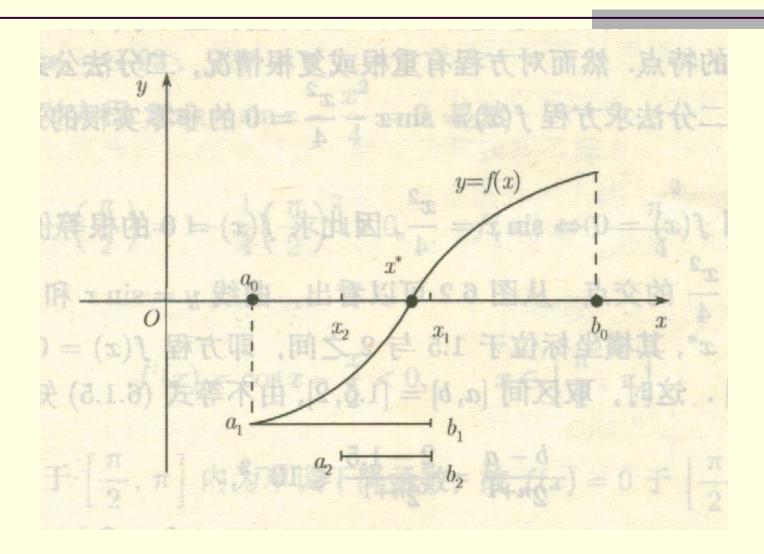
And this sequence converges to the solution.

Concerns of the iterative method: construction of the method, convergence of iterative sequence, the rate of the convergence, the error analysis.

<u>Iterative methods</u> also require first approximation to initiate iteration.

How to get the first approximation? We can find the approximate value of the root of f(x) = 0 either by a graphical method or by an analytical method.

Intermediate value property: if f(x) is a real valued continuous function in the closed interval $a \le x \le b$, and if f(a) and f(b) have opposite signs, then the graph of the function y = f(x) crosses the x-axis at least once; that is f(x) = 0 has at least one root x^* such that $a < x^* < b$.



This method is based on "intermediate value property". We shall illustrate it through an example. Let,

$$f(x) = 3x - \sqrt{1 + \sin x} = 0$$

We can easily verify

$$f(0) = -1$$

$$f(1) = 3 - \sqrt{1 + \sin(1)} = 3 - \sqrt{1 + 0.84147} = 1.64299$$

We observe that f(0) and f(1) are of opposite signs. Therefore, using intermediate value property we infer that there is at least one root between x=0 and x=1. This method is often used to find the first approximation to a root of either transcendental equation or algebraic equation. Hence, in analytical method, we must always start with an initial interval (a,b), so that f(a) and f(b) have opposite signs.

This method is also called Interval halving method.

Suppose we wish to locate the root of an equation f(x) = 0in an interval, say (a, b).

Let f(a) and f(b) be of opposite signs, such that f(a) f(b) < 0.

This shows that the graph of the function crosses the x-axis between a and b, which guarantees the existence of at least one root in the interval (a, b).

The desired root is approximately defined by the midpoint

$$c = \frac{a+b}{2}$$
 (continued)

If f(c)=0, then x=c is the desired root of f(x)=0. However, if $f(c) \neq 0$, then the root may be between a and c or c and b.

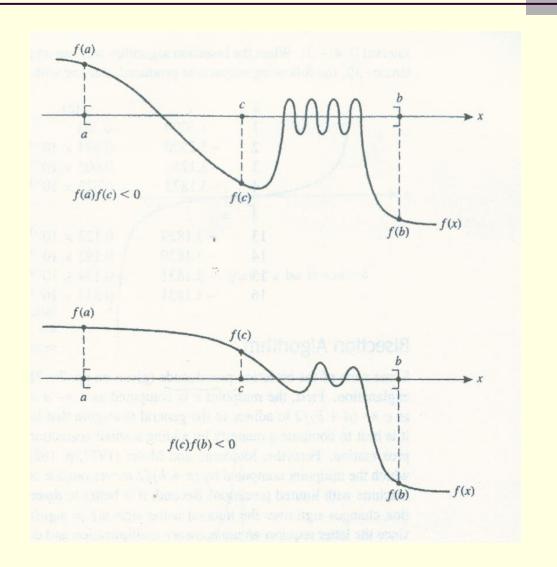
Now, we define the next approximation by

$$d = \frac{a+c}{2}$$

provided f(a)f(c) < 0, then the root may be found between a and c or by

$$e = \frac{c+b}{2}$$

provided f(c)f(b) < 0, then the root lies between c and b etc. (continued)



We repeatedly halve the interval. At each step, we either find the desired root to the required accuracy or narrow the range to half of the previous Interval. This process of halving the interval is continued to determine a smaller and smaller interval within which the desired root lies. Continuation of this process eventually gives us the desired root. This method is illustrated in the following example.

EXAMPLE 1: Solve $x^3 - 9x + 1 = 0$ for the root between x = 2 and x = 4 by the bisection method.

Solution: Given $f(x) = x^3 - 9x + 1$, we can verify that f(2) = -9, f(4) = 29.

Therefore, f(2)f(4) < 0 and hence the root lies between 2 and 4.

Now, let $x_0 = 2$, $x_1 = 4$ and we define

$$x_2 = \frac{x_0 + x_1}{2} = \frac{2+4}{2} = 3$$

as a first approximation to a root of f(x) = 0, and note that

$$f(3) = 1$$
, so that $f(2) f(3) < 0$.

Thus, the root lies between 2 and 3. We then further define,

$$x_3 = \frac{x_0 + x_2}{2} = \frac{2+3}{2} = 2.5$$
 (continued)

and note that $f(x_3) = f(2.5) < 0$, so that f(2.5) f(3) < 0. Therefore,

we define the mid-point
$$x_4 = \frac{x_3 + x_2}{2} = \frac{2.5 + 3}{2} = 2.75$$
.

Similarly, we find that

$$x_5 = 2.875$$
, $x_6 = 2.9375$, and so on....

The same process can be continued until the root is finally obtained to the desired accuracy. These results are presented in the table.

$$\begin{array}{cccc}
n & x_n & f(x_n) \\
2 & 3 & 1.0 \\
3 & 2.5 & -5.875
\end{array}$$

$$4 \quad 2.75 \quad -2.9531$$

$$6 \quad 2.9375 \quad -0.0901$$

— graphical method to find the first approximation

EXAMPLE 2: Find the root of the equation $e^x = \sin x$ closest to 0.

Solution: If the graphs of e^x and $\sin x$ are roughly plotted, it becomes clear that there are no positive roots of $f(x) = e^x - \sin x$ and that the first root to the left of 0 is in the interval [-4, -3]. Using the bisection algorithm, the following output was obtained with the interval [-4, -3];

n	\mathcal{X}_n	$f(x_n)$	
1	-3.5000	-0.321	
2	-3.2500	-0.694×10^{-1}	
3	-3.1250	0.605×10^{-1}	
4	-3.1875	0.625×10^{-1}	
M	M	M	
M 13	M -3.1829	$M \\ 0.122 \times 10^{-3}$	
	7.7		
13	-3.1829	0.122×10^{-3}	

3.1 Bisection Method - Error Analysis

To analyze the bisection method, let us denote the successive intervals that arise in the process by $[a_0,b_0]$, $[a_1,b_1]$, and so on. Here are some observations about these numbers:

$$a_{0} \leq a_{1} \leq a_{2} \leq \dots \leq b_{0}$$

$$b_{0} \geq b_{1} \geq b_{2} \geq \dots \geq a_{0}$$

$$b_{n+1} - a_{n+1} = \frac{1}{2} (b_{n} - a_{n}) \qquad (n \geq 0)$$
(1)

Since $[a_n]$ is nondecreasing and bounded above, it converges. Likewise $[b_n]$ converges. If we apply equation (1) repeatedly, we find that

$$b_n - a_n = 2^{-n} \left(b_0 - a_0 \right)$$

Thus,
$$\lim_{n\to\infty} b_n - \lim_{n\to\infty} a_n = \lim_{n\to\infty} 2^{-n} \left(b_0 - a_0 \right) = 0$$

If we put
$$r = \lim_{n \to \infty} a_n = \lim_{n \to \infty} b_n$$

By taking a limit in the inequality $0 \ge f(a_n) f(b_n)$, we obtain $0 \ge [f(r)]^2$ Hence f(r) = 0.

3.1 Bisection Method- Error Analysis

Suppose that, at a certain stage in the process, the interval $[a_n, b_n]$ has just been defined. If the process is now stopped, the root is certain to lie in this interval. The best estimate of the root at this stage is not a_n , or b_n but the midpoint of the interval

$$c_n = \frac{\left(a_n + b_n\right)}{2}$$

The error is then bounded as follows:

$$|r-c_n| \le \frac{1}{2} (b_n - a_n) = 2^{-(n+1)} (b_0 - a_0)$$

Therefore, we have the following theorem.

Theorem 1 Theorem on Bisection Method

If $[a_0,b_0]$, $[a_1,b_1]$, ... $[a_n,b_n]$, ... denote the intervals in the bisection method, then the limits $\lim_{n\to\infty}a_n$ and $\lim_{n\to\infty}b_n$ exist, are equal, and represent a zero of

(2)

f. If
$$r = \lim_{n \to \infty} c_n$$
 and $c_n = \frac{1}{2} (a_n + b_n)$, then $|r - c_n| \le 2^{-(n+1)} (b_0 - a_0)$

- Theorem on Bisection Method

EXAMPLE 3: Suppose that the bisection method is started with the interval [50, 63]. How many steps should be taken to compute a root with relative accuracy of 10^{-12} ?

Solution: The stated requirement on relative accuracy means that

$$\frac{\left|r-c_{n}\right|}{\left|r\right|} \leq 10^{-12}$$

We know that $r \ge 50$, and thus it suffices to secure the inequality

$$\frac{|r - c_n|}{50} \le 10^{-12}$$
 $\left(\frac{|r - c_n|}{|r|} \le \frac{|r - c_n|}{50}\right)$

By means of Theorem 1, we infer that the following condition is sufficient:

$$|r - c_n| \le \frac{1}{2} (b_n - a_n) = 2^{-(n+1)} (b_0 - a_0) \implies (\frac{|r - c_n|}{50} \le) 2^{-(n+1)} \times (\frac{13}{50}) \le 10^{-12}$$

Solving this for n, we conclude that $n \ge 37$.

- Theorem on Bisection Method

Therefore, for a given tolerance ε , by this theorem we can find the value of n from

$$2^{-(n+1)}(b_0 - a_0) < \varepsilon$$

which provides an interation stopping criterion

$$n > \frac{\log \frac{\left(b_0 - a_0\right)}{\varepsilon}}{\log 2} - 1$$

Theorem on Bisection Method

Example 4: The equation $f(x) = x^3 + 4x^2 - 10 = 0$ has a root in [1, 2] since f(1) = -5 and f(2) = 14. The bisection method gives the results

n	a_n	b_n	C_n	$f(c_n)$
0	1.0	2.0	1.5	2.375
1	1.0	1.5	1.25	-1.79687
2	1.25	1.5	1.375	0.16211
M	M	M	M	M
8	1.36328125	1.3671875	1.365234375	0.000072
9	1.36328125	1.365234375	1.364257813	-0.01605
10	1.364257813	1.365234375	1.364746094	-0.00799
11	1.364746094	1.365234375	1.364990235	-0.00396
12	1.364990235	1.365234375	1.365112305	-0.00194

- Theorem on Bisection Method

After 12 iterations, $c_{12} = 1.365112305$ approximates the root r with an error

$$|r - c_{12}| < \frac{1}{2} |b_{12} - a_{12}| = \frac{1}{2} |1.365234375 - 1.364990235| = 0.000122070$$
Since $|a_{13}| < |r|, |b_{13} - a_{13}| = \frac{1}{2} |b_{12} - a_{12}|, a_{13} = 1.365112305, b_{13} = 1.365234375$

$$\frac{|r - c_{12}|}{|r|} < \frac{|b_{13} - a_{13}|}{|a_{13}|} = 0.0000894212 < 9.0 \times 10^{-5},$$

The correct value of r to nine decimal places, is r = 1.365230013.

$$n > \frac{\log \frac{(b_0 - a_0)}{\varepsilon}}{\log 2} - 1 = \frac{\log \frac{(2 - 1)}{1 \times 10^{-9}}}{\log 2} - 1 = \frac{\log(2 \times 10^9)}{\log 2} - 1 = \frac{9}{\log 2} = 29.9$$

- Theorem on Bisection Method

To determine the number of iterations necessary to solve the equation with accuracy 10^{-3} using $a_0 = 1$ and $b_0 = 2$ requires finding an integer n that satisfies

$$|r - c_n| \le 2^{-(n+1)} (b_0 - a_0) = 2^{-(n+1)} < 10^{-3}$$

$$n > \frac{\log 10^3}{\log 2} - 1 = \frac{3}{\log 2} - 1 \approx 8.96$$

Hence, nine iterations will ensure an approximation accurate to within 10^{-3} .

It is important to keep in mind that the error analysis gives only a bound for the number of iterations, and in many cases this bound is much larger than the actual number required.

The Bisection method, though conceptually clear, has significant drawbacks. It is slow to converge (that is, n may become quite large before $|r-c_n|$ is sufficiently small) and a good intermediate approximation can be inadvertently discarded. However, the method has the important property that it always converges to a solution, and for that reason it is often used as a starter for the more efficient methods.

Newton's method is a general procedure that can be applied in many diverse situations. In general, Newton's method is faster than the bisection and the secant methods (to be discussed later) since its convergence is quadratic rather than linear. Once the quadratic convergence becomes effective, the convergence is so rapid that only a few more values are needed.

Unfortunately, the method is not garanteed always to converge. So often Newton's method is combined with other slower methods in a hybrid method that is numerically globally convergence.

This method is also called **Newton-Raphson Method**. It is to find the real root of an equation in the form, f(x) = 0. Its formula can be derived by the method based on Taylor polynomial.

Suppose x_0 is an approximate root of f(x) = 0. Let $r = x_0 + h$,

where h is small, and r be the exact root of f(x) = 0, then f(r) = 0.

Now, expanding $f(x_0 + h)$ by Taylor's theorem, we get

$$f(r) = f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \dots = 0$$
 (1)

Since h is small, we neglect terms containing h^2 and its higher powers, then

$$0 = f(r) \approx f(x_0) + hf'(x_0) \qquad \Rightarrow \qquad h \approx \frac{-f(x_0)}{f'(x_0)}$$

Therefore, a better approximation to the root is given by

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

and better and successive approximations x_2 , x_3 ,..., x_n to the root can obviously be obtained from the iteration formula,

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{2}$$

Graphical Interpretation

Before examining the theoretical basis for Newton's method, let's give a graphical interpretation of it.

From the description already given, we can say that **Newton's method involves linearizing the function**. That is, f was replaced by a linear function. The usual way of doing this is to replace f by the first two terms in its Taylor series. Thus, if

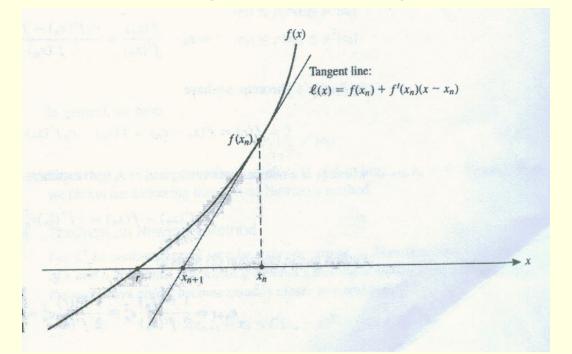
$$f(x) = f(c) + f'(c)(x-c) + \frac{1}{2!}f''(c)(x-c)^2 + L$$

then the linearization (at c) produces the linear function

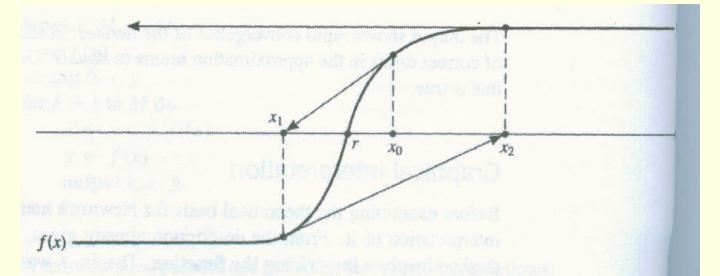
$$l(x) = f(c) + f'(c)(x - c)$$

$$l(x) = f(c) + f'(c)(x - c)$$

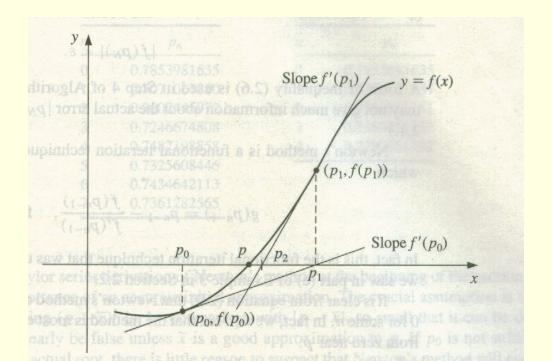
Notice that l is a good approxomation to f in the vicinity of c, and in fact we have l(c) = f(c) and l'(c) = f'(c). Thus, the linear function has the same value and the same slope as f at the point c. So in Newton's method we are constructing the tangent to the f-curve at a point near r, and finding where the tangent line intersects the x-axis.



Keeping in mind this graphical interpretation, we can easily imagine functions and starting points for which the **Newton iteration fails.** Such a function is shown in the figure below. In this example, the shape of the curve is such that for certain starting values, the sequence $[x_n]$ diverges. Thus, any formal statement about Newton's method must involve an assumption that x_0 is sufficiently close to a zero or that the graph of f has a prescribed shape.



The next figure illustrates how the approximations are obtained using successive tangents. Starting with the initial approximation p_0 , the approximation p_1 is the x-intercept of the tangent line to the graph of f at $(p_0, f(p_0))$. The approximation p_2 is the x-intercept of the tangent line to the graph of f at $(p_1, f(p_1))$ and so on.



EXAMPLE: Set up Newton's scheme of iteration for finding the square root of a positive number N.

Solution: The square root of N can be carried out as a root of the equation $x^2 - N = 0$. Let $f(x) = x^2 - N$.

By Newton's method, we have

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

In this problem, $f(x) = x^2 - N$, f'(x) = 2x. Therefore,

$$x_{n+1} = x_n - \frac{x_n^2 - N}{2x_n}$$
$$= \frac{1}{2} \left(x_n + \frac{N}{x_n} \right)$$

If, for example, we wish to compute $\sqrt{17}$ and begin with $x_0 = 4$, the successive approximations are as follows (given in rounded form to exhibit only correct figures):

$$x_1 = 4.12$$

 $x_2 = 4.123106$
 $x_3 = 4.1231056256177$
 $x_4 = 4.123105625617660549821409856$

The value given by x_4 is correct to 28 figures, and we observe the expected doubling of significant digits in the results.

Example Suppose we would like to approximate a fixed point of

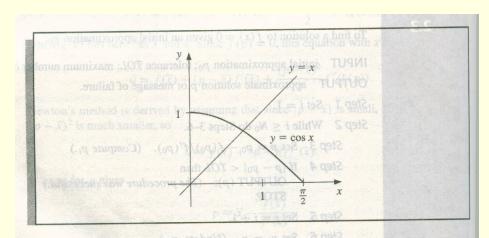
 $x = \cos x$.

The graph in the following figure implies that a single fixed-point p lies in $[0, \pi/2]$.

The following Table 1 shows the results of fixed-point iteration with $p_0 = \pi/4$. The best we could conclude from these results is that $p \approx 0.74$.

To approach this problem differently, define $f(x) = \cos x - x$ and apply Newton's method. Since $f'(x) = -\sin x - 1$, the sequence is generated by

$$p_n = p_{n-1} - \frac{\cos p_{n-1} - p_{n-1}}{-\sin p_{n-1} - 1}$$
, for $n \ge 1$.



7	Γable 1	Table 2
n	p_n	
0 0.	7853981635	n n
1 0.	7071067810	$ \begin{array}{ccc} n & p_n \\ 0 & 0.7853981635 \end{array} $
2 0.	7602445972	1 0.7395361337
3 0.	7246674808	2 0.7390851781
4 0.	7487198858	3 0.7390851781
5 0.	7325608446	4 0.7390851332
6 0.	7434642113	T 0./390031332
7 0.	7361282565	

With $p_0 = \pi/4$, the approximations in Table 2 are generated. An excellent approximation is obtained with n = 3. We would expect this result to be accurate to the places listed because of the agreement of p_3 and p_4 .

The Taylor series derivation of Newton's method at the beginning of the section points out the importance of an accurate initial appraximation. The crucial assumption is that the term involving h^2 is, by comparison with h, so small that it can be deleted. This will clearly be false unless x_0 is a good approximation to the root r. If \mathbf{x}_0 is not sufficiently close to the actual root, there is little reason to suspect that Newton's method will converge to the root. However, in some instances, even poor initial approximations will produce convergence.

The following example using Newton's method illustrates the theoretical importance of the choice of x_0 .

Example Use Newton's method to find the root for the function $f(x) = e^{-x/4}(2-x) - 1 = 0$ with the interval [0, 2].

Solution Obviously f(0)f(2) < 0, i.e. f(x) = 0 has at least a root in the interval [0, 2]. Since $f'(x) = \frac{1}{4}(x-6)e^{-x/4}$,

Newton iteration formula is

$$x_{k+1} = x_k - \frac{e^{-x_k/4}(2 - x_k) - 1}{\frac{1}{4}(x_k - 6)e^{-x_k/4}}, \quad k = 0, 1, 2L.$$

Starting with two initial values $x_0 = 1.0$ and $x_0 = 8.0$ resepectively, and obtain two sequences of $\{x_k\}$. When $x_0 = 1.0$, we got $x^* \approx x_6$ where $f(x_6) = -3.8 \times 10^{-8} (\approx 0)$. When $x_0 = 8.0$, the iteration diverges.

```
kx_kkx_k01.008.01-1.15599134.77810720.1894332869.151930.714143..40.782542..50.783595..60.783596divergence
```

It is seen that the convergency of the Newton method is very much affected by the initial value chosen. The advantage of the Newton method is that it convergences fast and the drawback is that it is sensitive to the initial value and requires the information of f'.

- Convergence of Newton-Raphson method

Theorem Consider a function f(x), $x \in [a,b]$ and f''(x) is continuous, and f(x) satisfies: (i) f(a)f(b) < 0; (ii) $f'(x) \ne 0$, $x \in [a,b]$; (iii) f''(x) does not change the sign in [a,b], then for any x_0 , if $f(x_0)f''(x) > 0$, then $\{x_k\}$ converges to the only root of f(x) = 0.

In order to illustrate this method, we consider the following examples.

EXAMPLE 1: Find the real root of the equation $xe^x - 2 = 0$ correct to two decimal places, using N-R method.

Solution: Given $f(x) = xe^x - 2$, we have

$$f'(x) = xe^{x} + e^{x}$$
 and $f''(x) = xe^{x} + 2e^{x}$

Clearly, we have

$$f(0) = -2$$
 and $f(1) = e - 2 = 0.711828$

Hence, the required root lies in the interval (0,1) and is nearer to 1. Also, f'(x) and f''(x) do not vanish in (0,1), and f(x) and f''(x) will have the same sign at x = 1.

Therefore, we take the first approximation $x_0 = 1$, and using N-R

method, we get

$$x_{1} = x_{0} - \frac{f(x_{0})}{f'(x_{0})}$$
$$= \frac{e+2}{2e} = 0.867879$$

and

$$f(x_1) = 6.71607 \times 10^{-2}$$

The second approximation is

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

$$= 0.867879 - \frac{0.06716}{4.44902} = 0.85278$$

and

$$f(x_2) = 7.655 \times 10^{-4}$$

Thus, the required root is 0.853.

EXAMPLE 2: Use Newton's method, with double-precision computation, to find the negative zero of the function $f(x) = e^x - 1.5 - \tan^{-1} x$.

<u>Solution</u>: Double-precision machine numbers have 96 bits, corresponding to about 28 decimal places.

The function $f'(x) = e^x - (1+x^2)^{-1}$, as well as f, had to be programmed for this. A starting point of $x_0 = -7$ is chosen. The output from the computer program is shown here.

k	\boldsymbol{x}	f(x)
0	-7.000000000000000000000000000000000000	-0.702×10^{-1}
1	-10.67709617664001399296984386	-0.226×10^{-1}
2	-13.27916737563271290859786319	-0.437×10^{-2}
3	-14.05365585426923873474831753	-0.239×10^{-3}
4	-14.10110995686641347616312706	-0.800×10^{-6}
5	-14.10126977093941594621579506	-0.901×10^{-11}
6	-14.10126977273996842508300314	-0.114×10^{-20}
7	-14.10126977273996842531155122	0.000
8	-14.10126977273996842531155122	0.000

The output shows very rapid convergence of the iteration.

- Error Analysis

Now we shall analyze the errors in Newton's method. By errors we mean the quantities

$$e_n = x_n - r$$

(We are not considering roundoff errors) Let us assume that f'' is continuous and r is a **simple zero** of f, so that f(r) = 0 and $f'(r) \neq 0$. From the definition of the Newton iteration, we have

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

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

$$= \frac{e_n f'(x_n) - f(x_n)}{f'(x_n)}$$
(1)

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

Error Analysis

By Taylor's Theorem, we have

$$0 = f(r) = f(x_n - e_n) = f(x_n) - e_n f'(x_n) + \frac{1}{2}e_n^2 f''(\xi_n)$$

where ξ_n is a number between x_n and r. A rearrangement of this equation

yields
$$e_n f'(x_n) - f(x_n) = \frac{1}{2} f''(\xi_n) e_n^2$$

Putting this in Equation (1) leads to

$$e_{n+1} = \frac{1}{2} \frac{f''(\xi_n)}{f'(x_n)} e_n^2 \approx \frac{1}{2} \frac{f''(r)}{f'(r)} e_n^2 = Ce_n^2$$
 (2)

Supposing that $C \approx 1$ and $e_n \approx 10^{-4}$, then by Equation (2), we have $e_{n+1} \approx 10^{-8}$ and $e_{n+2} \approx 10^{-16}$. We see that only a few additional iterations are needed to obtain more than machine precision! This tells us that e_{n+1} is roughly a constant times e_n^2 . This is called **quadratic convergence**.

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习题

Ex1. Use the Bisection method to find the root of $f(x) = x^3 - 2 = 0$ on [1, 2] accurate to within 10^{-3} .

Ex2. Use Newton method to find the solution for $f(x) = x^2 - N = 0$, for N = 2, $x_0 = 1$, and accuracy of 10^{-3} .