Lecture-1
Algorithmic Mathematics(CSC545)

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Numerical Error in Computation

- Rounding Off Error
- Truncation Error
- Discretization Error

Rounding Off Error:

The round-off error is used because representing every number as a real number isn't possible. So rounding is introduced to adjust for this situation. A round-off error represents the numerical amount between what a figure actually is versus its closest real number value, depending on how the round is applied. For instance, rounding to the nearest whole number means you round up or down to what is the closest whole figure. So if your result is 3.31 then you would round to 3. Rounding the highest amount would be a bit different. In this approach, if your figure is 3.31, your rounding would be to 4. In terms of numerical analysis the round-off error is an attempt to identify what the rounding distance is when it comes up in algorithms. It's also known as a quantization error.

Truncation Error

- A truncation error occurs when approximation is involved in numerical analysis. The error factor is related to how much the approximate value is at variance from the actual value in a formula or math result. For example, take the formula of 3 x 3 + 4. The calculation equals 28. Now, break it down and the root is close to 1.99. The truncation error value is therefore equal to 0.01

Discretization Error

- Discretization involves converting or partitioning variables or continuous attributes to nominal attributes, intervals and variables. As a type of truncation error, the discretization error focuses on how much a discrete math problem is not consistent with a continuous math problem.

Measurement of error in numerical computation

True and Relative True Errors: A true error (E_t) is defined as the difference between the true (exact) value and an approximate value. This type of error is only measurable when the true value is available

true error (E_t) = true value - approximate value

The approximate error (E_a) is defined as the difference between the present approximate value and the previous approximation (i.e. the change between the iterations).

approximate error (E_a) = present approximation – previous approximation

Similarly we can calculate the **relative approximate Error (E_r)** dividing the approximate error by the present approximate value.

relative approximate error (E_r)=approximate error / present approximation

Numerical methods to solve nonlinear equations

- An equation is said to be nonlinear when it involves terms of degree higher than 1 in the unknown quantity. These terms may be polynomial or capable of being broken down into Taylor series of degrees higher than 1.
- Nonlinear equations cannot in general be solved analytically. In this case, therefore, the solutions of the equations must be approached using iterative methods. The principle of these methods of solving consists in starting from an arbitrary point – the closest possible point to the solution sought – and involves arriving at the solution gradually through successive tests.
- The two criteria to take into account when choosing a method for solving nonlinear equations are:

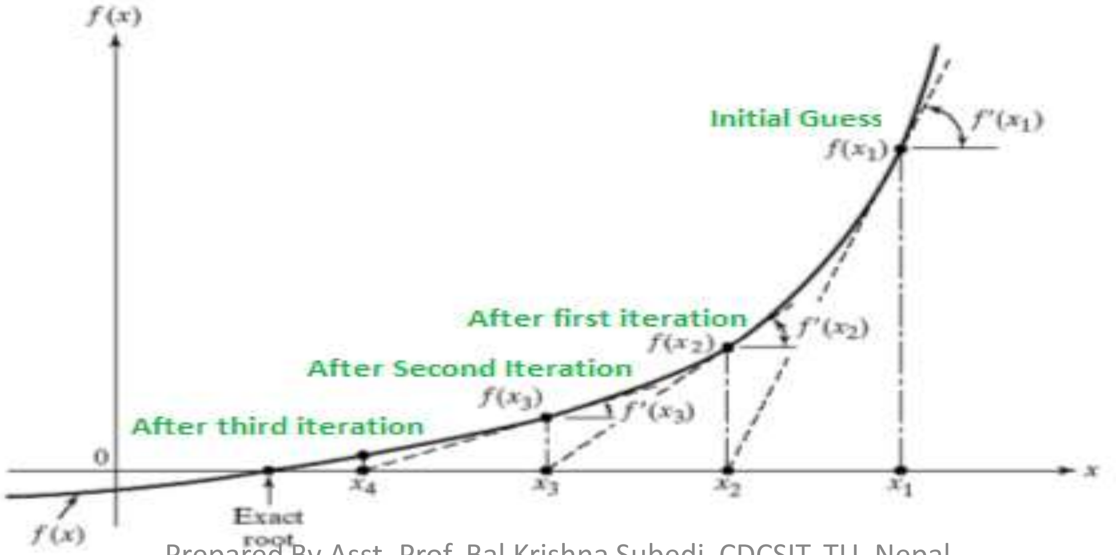
1. Method convergence (conditions of convergence, speed of convergence etc.).
2. The cost of calculating of the method

Some popular methods to solve nonlinear equations

- Bisection method
- Newton's method Or Newton Raphson Method
- Secant method
- Fixed-point iteration method and so on

Newton-Raphson method

- The **Newton-Raphson method** (also known as **Newton's method**) is a way to quickly find a good approximation for the root of a real-valued function f (x) = 0 f(x) = 0 f(x)=0. It uses the idea that a continuous and differentiable function can be approximated by a straight line tangent to it.



Derivation

The Newton-Raphson method is based on the principle that if the initial guess of the root of $f(x)=0$ is at x_i, then if one draws the tangent to the curve at $f(x_i)$, the point x_{i+1} where the tangent crosses the x-axis is an improved estimate of the root (Figure 1).

Using the definition of the slope of a function, at $x = x_i$

$$f'(x_i) = \tan\theta$$

$$= \frac{f(x_i)-0}{x_i - x_{i+1}},$$

which gives

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \qquad (1)$$

Equation (1) is called the Newton-Raphson formula for solving nonlinear equations of the form $f(x)=0$. So starting with an initial guess, x_i, one can find the next guess, x_{i+1}, by using Equation (1). One can repeat this process until one finds the root within a desirable tolerance.

Algorithm

The steps of the Newton-Raphson method to find the root of an equation $f(x)=0$ are

1. Evaluate $f'(x)$ symbolically
2. Use an initial guess of the root, x_i, to estimate the new value of the root, x_{i+1}, as
$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$
3. Find the absolute relative approximate error $|\in_a|$ as
$$|\in_a| = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| \times 100$$
4. Compare the absolute relative approximate error with the pre-specified relative error tolerance, $\in_s$. If $|\in_a| > \in_s$, then go to Step 2, else stop the algorithm. Also, check if the number of iterations has exceeded the maximum number of iterations allowed. If so, one needs to terminate the algorithm and notify the user.

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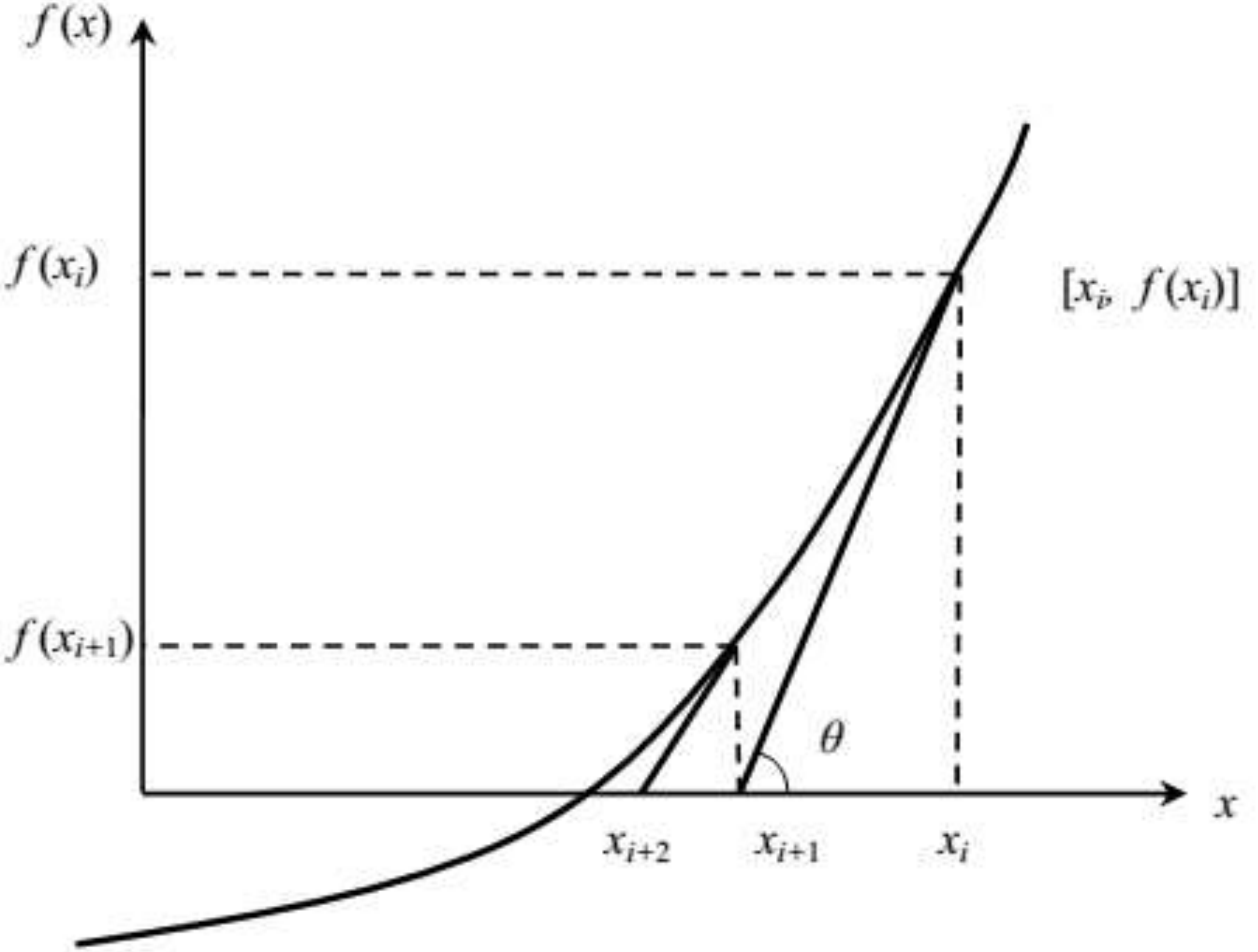

Figure 1 Geometrical illustration of the Newton-Raphson method.

Example 1

You are working for 'DOWN THE TOILET COMPANY' that makes floats for ABC commodes. The floating ball has a specific gravity of 0.6 and has a radius of 5.5 cm. You are asked to find the depth to which the ball is submerged when floating in water.

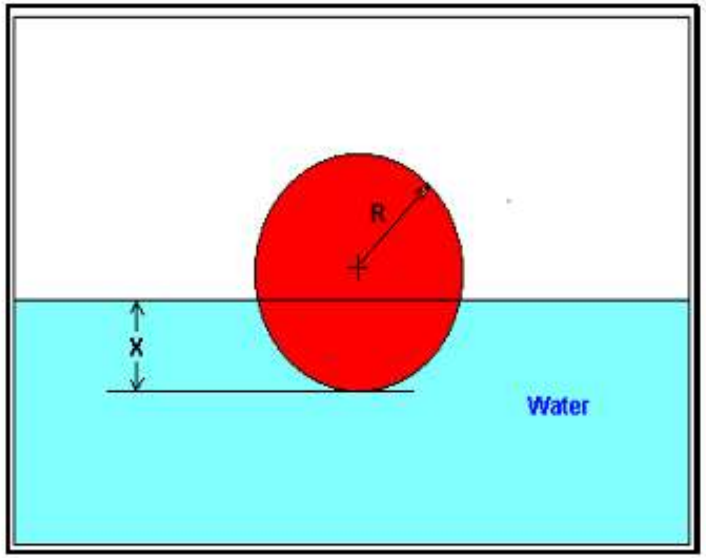

Figure 2 Floating ball problem.

The equation that gives the depth x in meters to which the ball is submerged under water is given by

$$x^3 - 0.165x^2 + 3.993\times10^{-4} = 0$$

Use the Newton-Raphson method of finding roots of equations to find

a) the depth x to which the ball is submerged under water. Conduct three iterations to estimate the root of the above equation.
b) the absolute relative approximate error at the end of each iteration, and
c) the number of significant digits at least correct at the end of each iteration.

Solution

$$f(x) = x^3 - 0.165x^2 + 3.993 \times 10^{-4}$$
$$f'(x) = 3x^2 - 0.33x$$

Let us assume the initial guess of the root of $f(x) = 0$ is $x_0 = 0.05\,\text{m}$. This is a reasonable guess (discuss why $x = 0$ and $x = 0.11\,\text{m}$ are not good choices) as the extreme values of the depth x would be 0 and the diameter (0.11 m) of the ball.

<u>Iteration 1</u>

The estimate of the root is

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$
$$= 0.05 - \frac{(0.05)^3 - 0.165(0.05)^2 + 3.993 \times 10^{-4}}{3(0.05)^2 - 0.33(0.05)}$$
$$= 0.05 - \frac{1.118 \times 10^{-4}}{-9 \times 10^{-3}}$$
$$= 0.05 - (-0.01242)$$
$$= 0.06242$$

The absolute relative approximate error $|\in_a|$ at the end of Iteration 1 is

$$|\in_a| = \left|\frac{x_1 - x_0}{x_1}\right| \times 100$$
$$= \left|\frac{0.06242 - 0.05}{0.06242}\right| \times 100$$
$$= 19.90\%$$

The number of significant digits at least correct is 0, as you need an absolute relative approximate error of 5% or less for at least one significant digit to be correct in your result.

<u>Iteration 2</u>

The estimate of the root is

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$
$$= 0.06242 - \frac{(0.06242)^3 - 0.165(0.06242)^2 + 3.993 \times 10^{-4}}{3(0.06242)^2 - 0.33(0.06242)}$$
$$= 0.06242 - \frac{-3.97781 \times 10^{-7}}{-8.90973 \times 10^{-3}}$$
$$= 0.06242 - \left(4.4646 \times 10^{-5}\right)$$
$$= 0.06238$$

The absolute relative approximate error $|\in_a|$ at the end of Iteration 2 is

$$|\in_a| = \left|\frac{x_2 - x_1}{x_2}\right| \times 100$$
$$= \left|\frac{0.06238 - 0.06242}{0.06238}\right| \times 100$$
$$= 0.0716\%$$

The maximum value of m for which $|\in_a| \le 0.5\times10^{2-m}$ is 2.844. Hence, the number of significant digits at least correct in the answer is 2.

Iteration 3

The estimate of the root is

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

$$= 0.06238 - \frac{(0.06238)^3 - 0.165(0.06238)^2 + 3.993\times10^{-4}}{3(0.06238)^2 - 0.33(0.06238)}$$

$$= 0.06238 - \frac{4.44\times10^{-11}}{-8.91171\times10^{-3}}$$

$$= 0.06238 - \left(-4.9822\times10^{-9}\right)$$

$$= 0.06238$$

The absolute relative approximate error $|\in_a|$ at the end of Iteration 3 is

$$|\in_a| = \left|\frac{0.06238 - 0.06238}{0.06238}\right|\times100$$

$$= 0$$

The number of significant digits at least correct is 4, as only 4 significant digits are carried through in all the calculations.

Drawbacks of the Newton-Raphson Method

1. Divergence at inflection points

If the selection of the initial guess or an iterated value of the root turns out to be close to the inflection point (see the definition in the appendix of this chapter) of the function $f(x)$ in the equation $f(x)=0$, Newton-Raphson method may start diverging away from the root. It may then start converging back to the root. For example, to find the root of the equation

$$f(x)=(x-1)^3+0.512=0$$

the Newton-Raphson method reduces to

$$x_{i+1}=x_i-\frac{(x_i^3-1)^3+0.512}{3(x_i-1)^2}$$

Starting with an initial guess of $x_0=5.0$, Table 1 shows the iterated values of the root of the equation. As you can observe, the root starts to diverge at Iteration 6 because the previous estimate of 0.92589 is close to the inflection point of $x=1$ (the value of $f'(x)$ is zero at the inflection point). Eventually, after 12 more iterations the root converges to the exact value of $x=0.2$.

Table 1 Divergence near inflection point.

Iteration Number	x_i
0	5.0000
1	3.6560
2	2.7465
3	2.1084
4	1.6000
5	0.92589
6	–30.119
7	–19.746
8	–12.831
9	–8.2217
10	–5.1498
11	–3.1044
12	–1.7464
13	–0.85356
14	–0.28538
15	0.039784
16	0.17475
17	0.19924
18	0.2

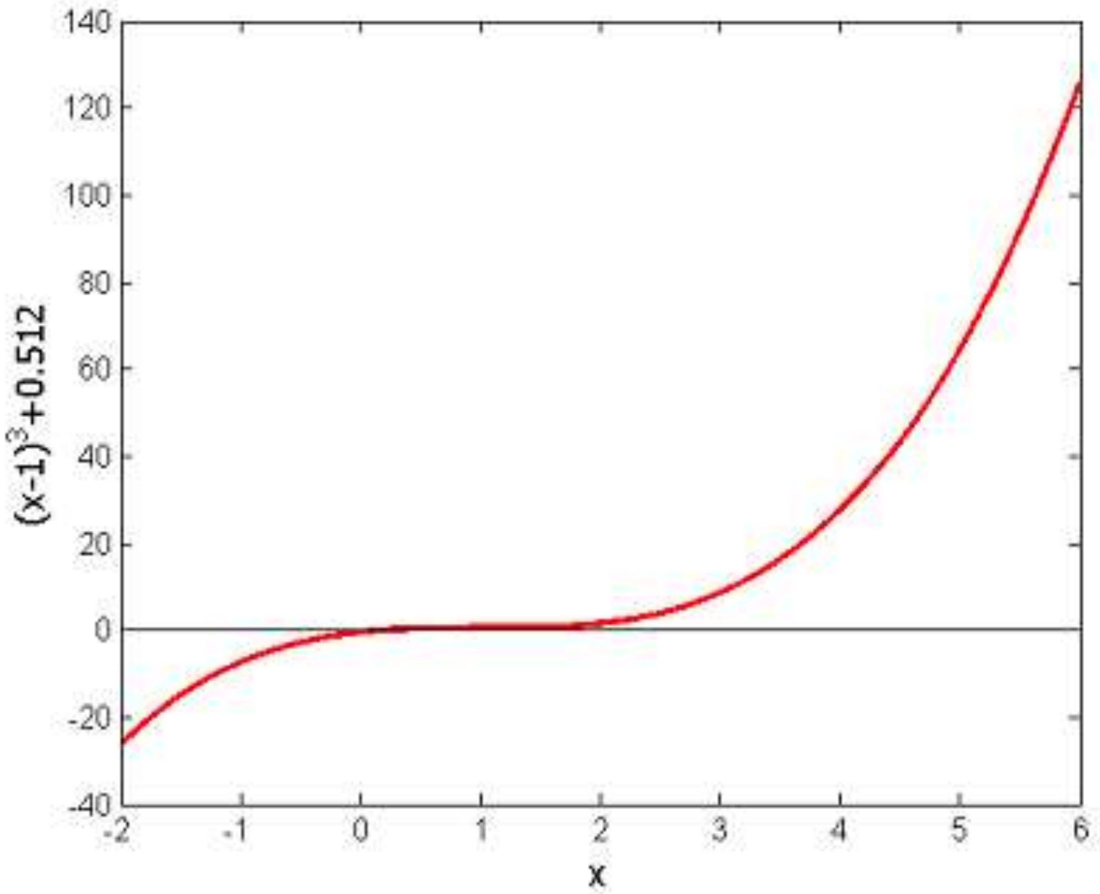

Figure 3 Divergence at inflection point for $f(x) = (x-1)^3 = 0$.

2. Division by zero

For the equation

$$f(x) = x^3 - 0.03x^2 + 2.4\times10^{-6} = 0$$

the Newton-Raphson method reduces to

$$x_{i+1} = x_i - \frac{x_i^3 - 0.03x_i^2 + 2.4\times10^{-6}}{3x_i^2 - 0.06x_i}$$

For $x_0 = 0$ or $x_0 = 0.02$, division by zero occurs (Figure 4). For an initial guess close to 0.02 such as $x_0 = 0.01999$, one may avoid division by zero, but then the denominator in the formula is a small number. For this case, as given in Table 2, even after 9 iterations, the Newton-Raphson method does not converge.

Table 2 Division by near zero in Newton-Raphson method.

Iteration Number	x_i	$f(x_i)$	$\lvert\epsilon_a\rvert\%$
0	0.019990	-1.60000×10^{-6}	——
1	–2.6480	18.778	100.75
2	–1.7620	–5.5638	50.282
3	–1.1714	–1.6485	50.422
4	–0.77765	–0.48842	50.632
5	–0.51518	–0.14470	50.946
6	–0.34025	–0.042862	51.413
7	–0.22369	–0.012692	52.107
8	–0.14608	–0.0037553	53.127
9	–0.094490	–0.0011091	54.602

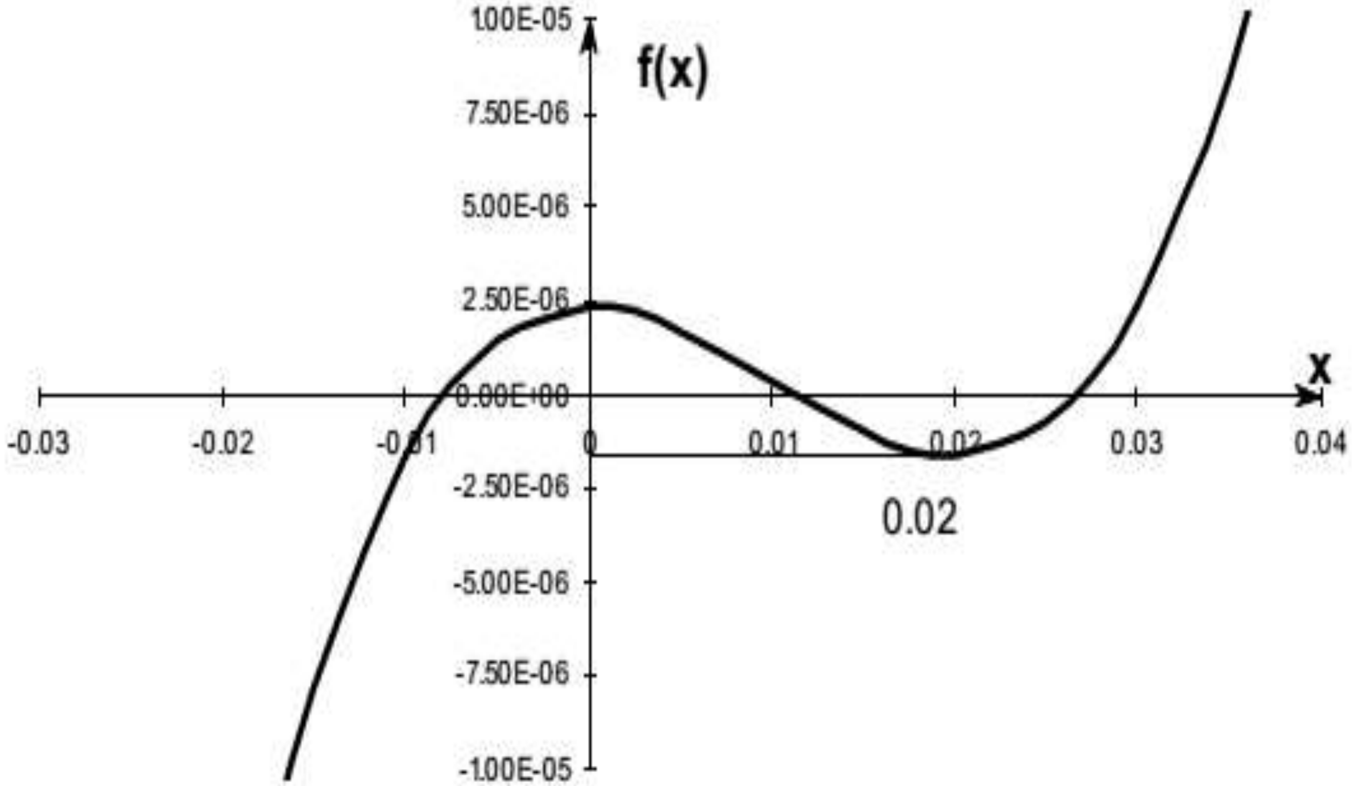

Figure 4 Pitfall of division by zero or a near zero number.

3. Oscillations near local maximum and minimum

Results obtained from the Newton-Raphson method may oscillate about the local maximum or minimum without converging on a root but converging on the local maximum or minimum. Eventually, it may lead to division by a number close to zero and may diverge.

For example, for

$$f(x) = x^2 + 2 = 0$$

the equation has no real roots (Figure 5 and Table 3).

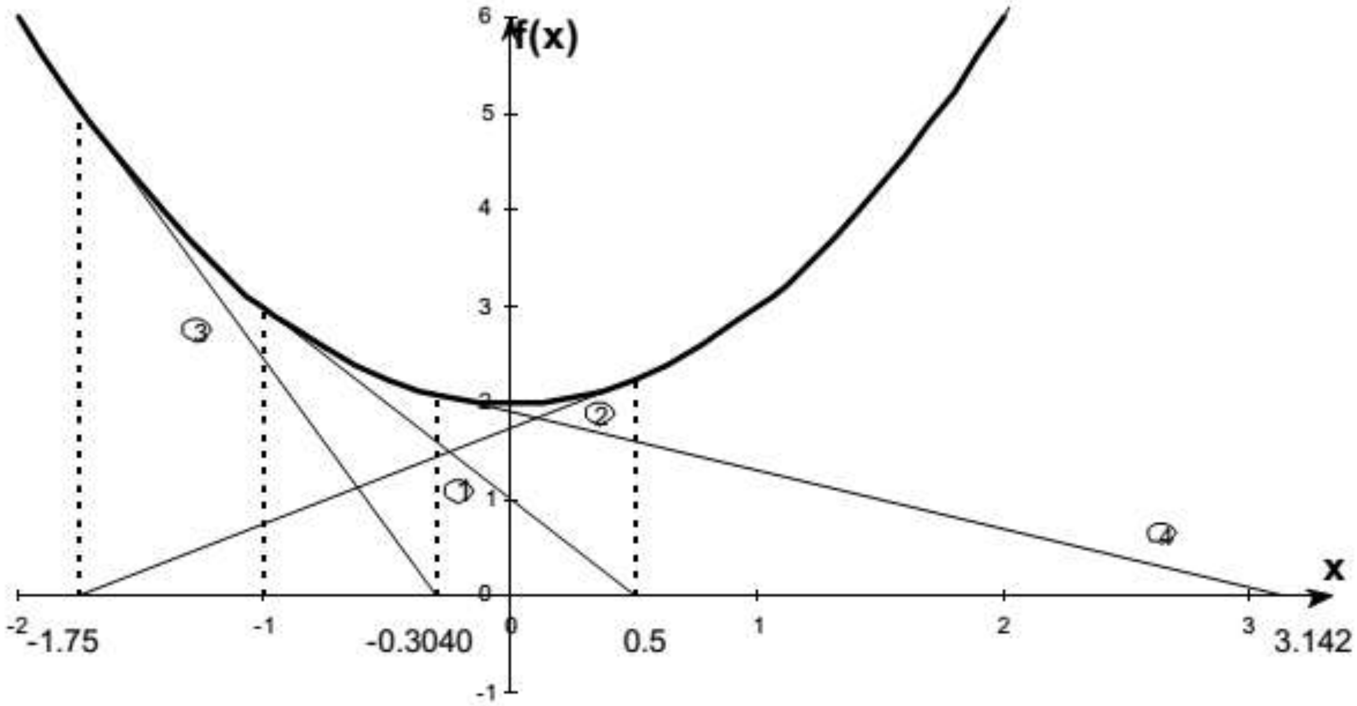

Figure 5 Oscillations around local minima for $f(x) = x^2 + 2$.

Table 3 Oscillations near local maxima and minima in Newton-Raphson method.

Iteration Number	x_i	$f(x_i)$	$\lvert\in_a\rvert\%$
0	–1.0000	3.00	——
1	0.5	2.25	300.00
2	–1.75	5.063	128.571
3	–0.30357	2.092	476.47
4	3.1423	11.874	109.66
5	1.2529	3.570	150.80
6	–0.17166	2.029	829.88
7	5.7395	34.942	102.99
8	2.6955	9.266	112.93
9	0.97678	2.954	175.96

4. Root jumping

In some case where the function $f(x)$ is oscillating and has a number of roots, one may choose an initial guess close to a root. However, the guesses may jump and converge to some other root. For example for solving the equation $\sin x = 0$ if you choose $x_0 = 2.4\pi = (7.539822)$ as an initial guess, it converges to the root of $x = 0$ as shown in Table 4 and Figure 6. However, one may have chosen this as an initial guess to converge to $x = 2\pi = 6.2831853$.

Table 4 Root jumping in Newton-Raphson method.

Iteration Number	x_i	$f(x_i)$	$\lvert\in_a\rvert\%$
0	7.539822	0.951	—
1	4.462	–0.969	68.973
2	0.5499	0.5226	711.44
3	–0.06307	–0.06303	971.91
4	8.376×10^{-4}	8.375×10^{-5}	7.54×10^{4}
5	-1.95861×10^{-13}	-1.95861×10^{-13}	4.28×10^{10}

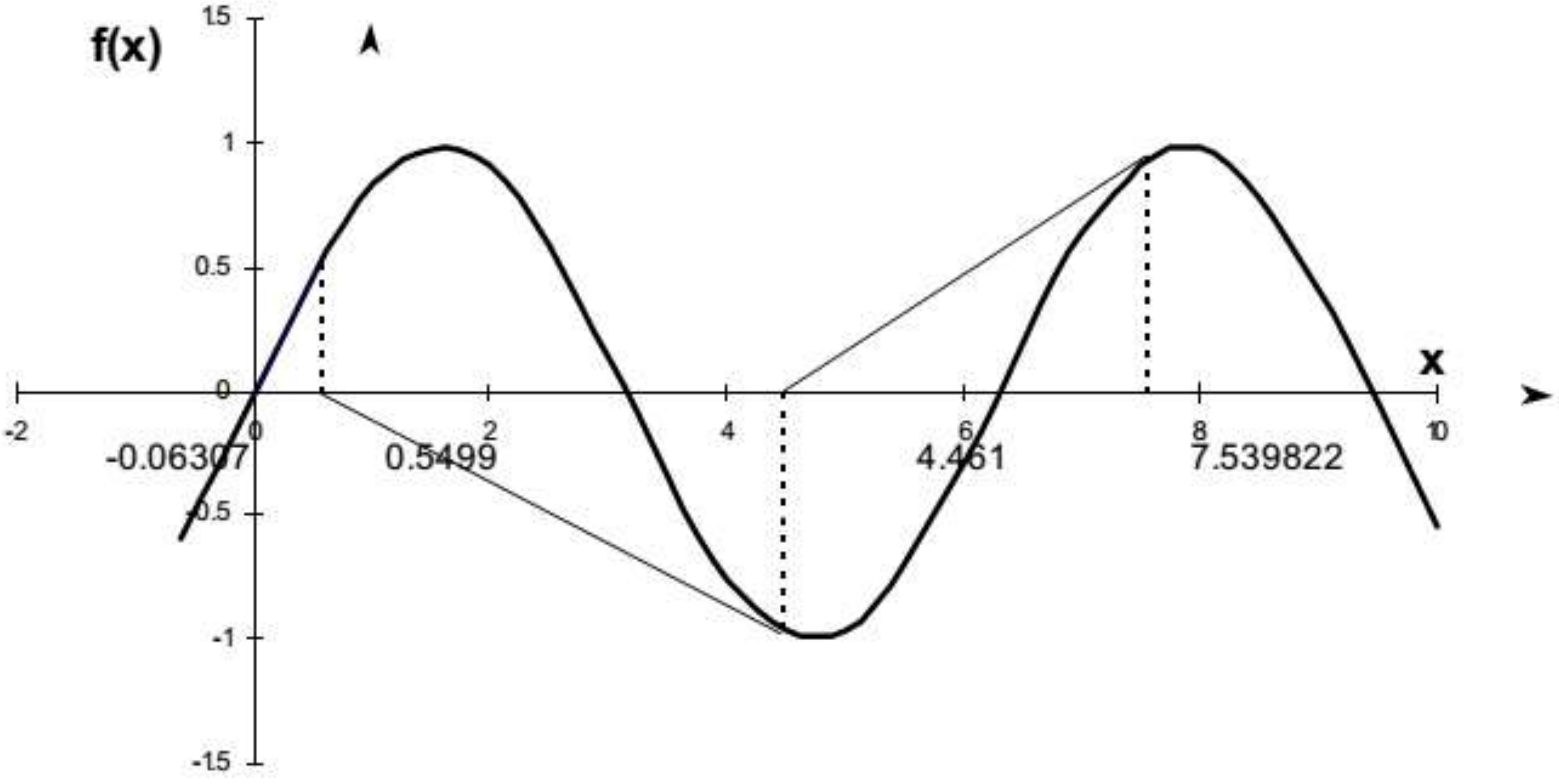

Figure 6 Root jumping from intended location of root for $f(x) = \sin x = 0$.

Appendix A. What is an inflection point?

For a function $f(x)$, the point where the concavity changes from up-to-down or down-to-up is called its inflection point. For example, for the function $f(x)=(x-1)^3$, the concavity changes at $x=1$ (see Figure 3), and hence (1,0) is an inflection point.

An inflection points MAY exist at a point where $f''(x)=0$ and where $f''(x)$ does not exist. The reason we say that it MAY exist is because if $f''(x)=0$, it only makes it a possible inflection point. For example, for $f(x)=x^4-16$, $f''(0)=0$, but the concavity does not change at $x=0$. Hence the point (0, –16) is not an inflection point of $f(x)=x^4-16$.

For $f(x)=(x-1)^3$, $f''(x)$ changes sign at $x=1$ ($f''(x)<0$ for $x<1$, and $f''(x)>0$ for $x>1$), and thus brings up the *Inflection Point Theorem* for a function $f(x)$ that states the following.

"If $f'(c)$ exists and $f''(c)$ changes sign at $x=c$, then the point $(c, f(c))$ is an inflection point of the graph of f."

Appendix B. Derivation of Newton-Raphson method from Taylor series

Newton-Raphson method can also be derived from Taylor series. For a general function $f(x)$, the Taylor series is

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \cdots$$

As an approximation, taking only the first two terms of the right hand side,

$$f(x_{i+1}) \approx f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

and we are seeking a point where $f(x) = 0$, that is, if we assume

$$f(x_{i+1}) = 0,$$

$$0 \approx f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

which gives

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

This is the same Newton-Raphson method formula series as derived previously using the geometric method.

Thanks You

Any Query??