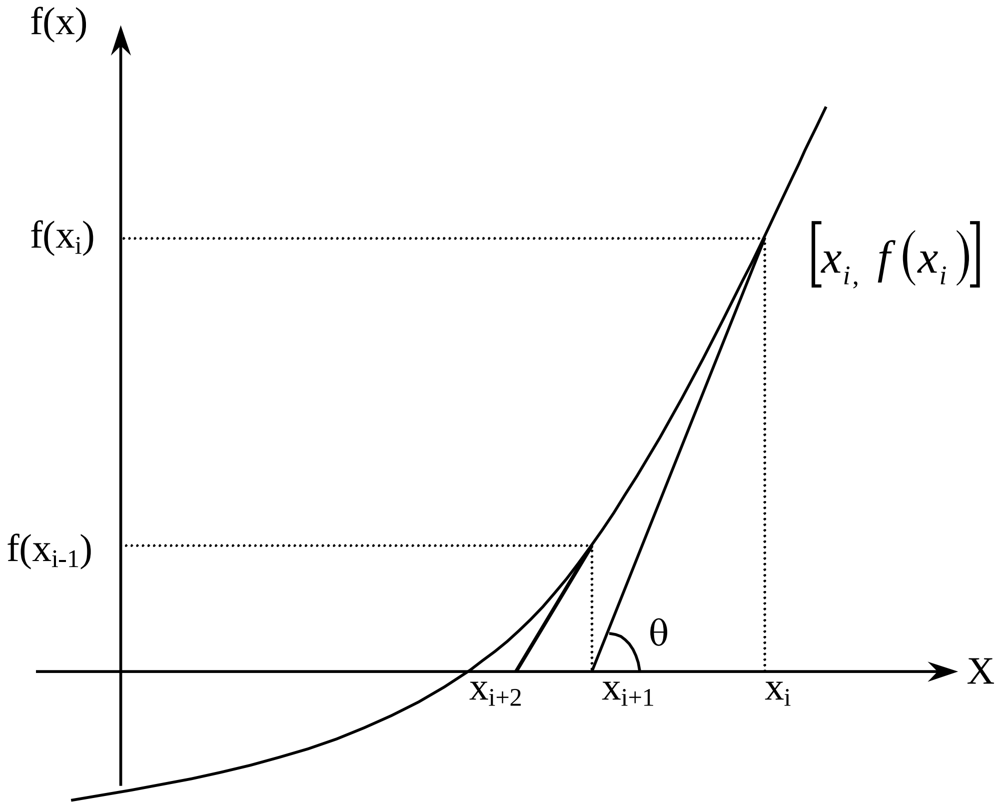
Newton-Raphson Method

Computational Physics

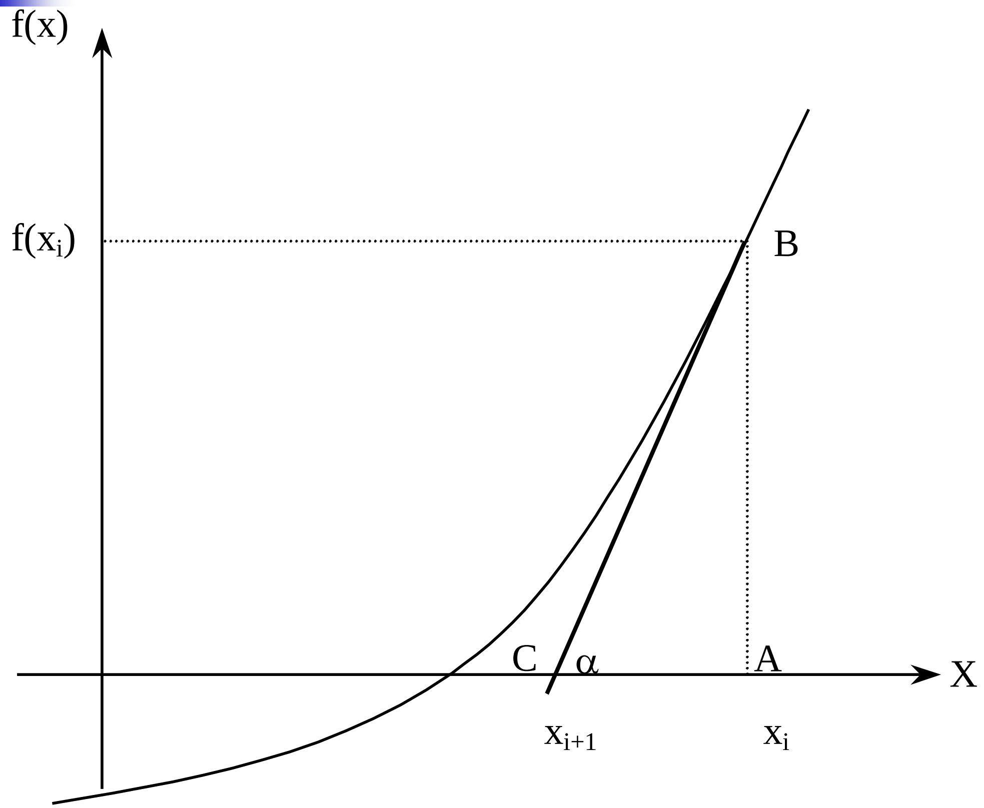
Newton-Raphson Method



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

Figure 1 Geometrical illustration of the Newton-Raphson method.

Derivation



$$\tan(\alpha) = \frac{AB}{AC}$$

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

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

Figure 2 Derivation of the Newton-Raphson method.

Algorithm for Newton-Raphson Method

Step 1

Evaluate $f'(x)$ symbolically.

Step 2

Use an initial guess of the root, x_i , to estimate the new value of the root, x_{i+1} , as

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

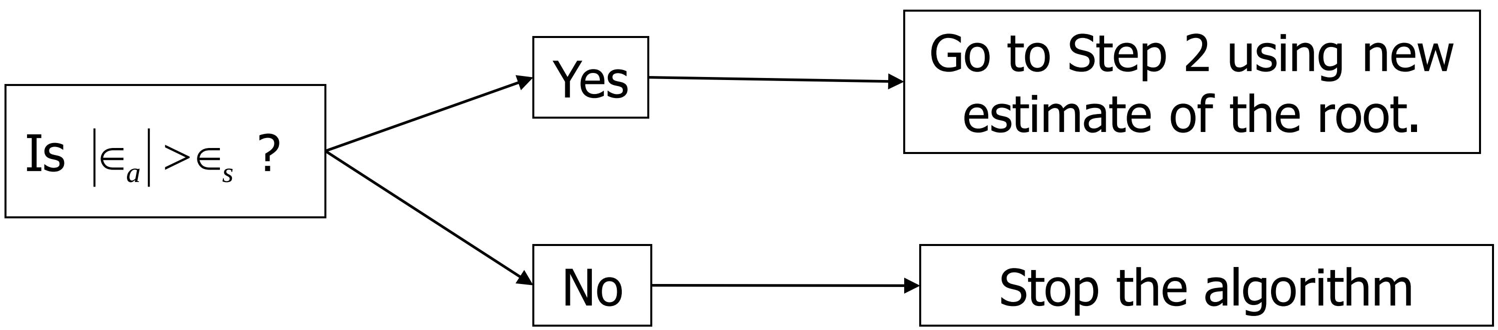
Step 3

Find the absolute relative approximate error $\left|\in_a\right|$ as

$$\left|\in_a\right| = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| \times 100$$

Step 4

Compare the absolute relative approximate error with the pre-specified relative error tolerance $\in_s$.



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.

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.

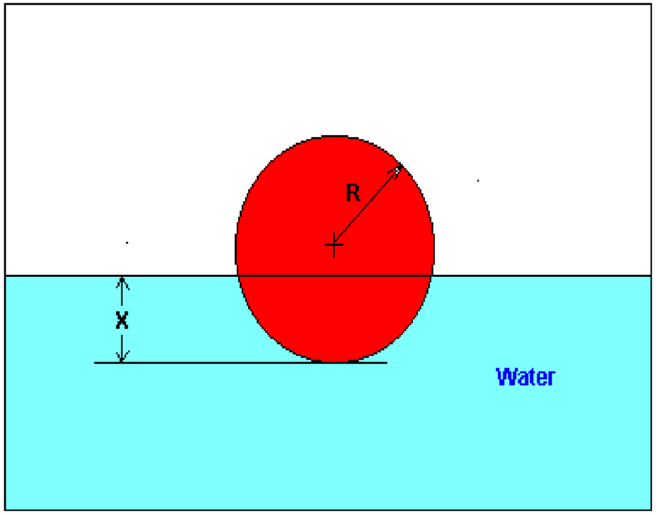


Figure 3 Floating ball problem.

Example 1 Cont.

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

$$f(x) = x^3 - 0.165x^2 + 3.993\times10^{-4}$$

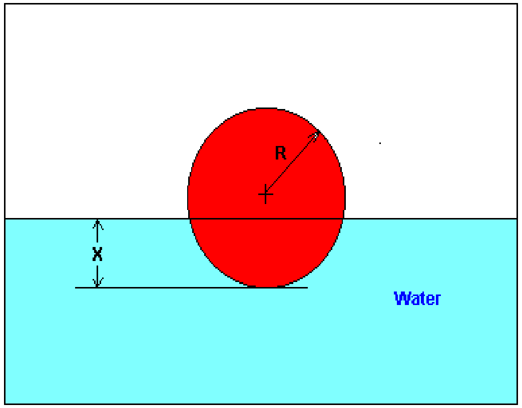


Figure 3 Floating ball problem.

Use the Newton's 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.

Example 1 Cont.

Solution

To aid in the understanding of how this method works to find the root of an equation, the graph of f(x) is shown to the right,

where

$$f(x) = x^3 - 0.165x^2 + 3.993\times10^{-4}$$

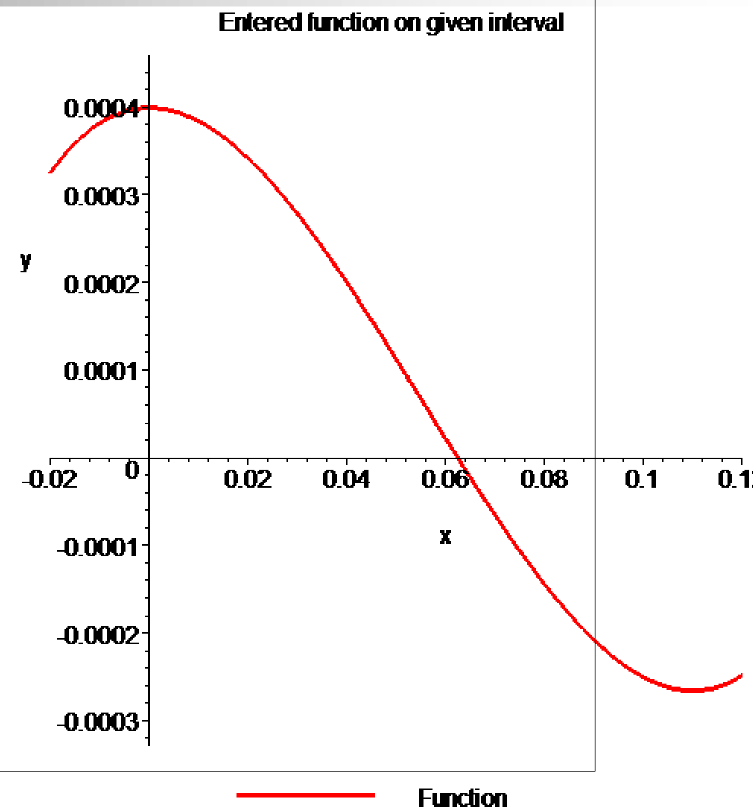


Figure 4 Graph of the function f(x)

Example 1 Cont.

Solve for $f'(x)$

$$f(x)=x^3\text{-}0.165x^2+3.993\times10^{-4}$$

$$f'(x)=3x^2\text{-}0.33x$$

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.

Example 1 Cont.

<u>Iteration 1</u>

The estimate of the root is

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

$$= 0.05 - \frac{(0.05)^3 - 0.165(0.05)^2 + 3.993\times10^{-4}}{3(0.05)^2 - 0.33(0.05)}$$

$$= 0.05 - \frac{1.118\times10^{-4}}{-9\times10^{-3}}$$

$$= 0.05 - (-0.01242)$$

$$= 0.06242$$

Example 1 Cont.

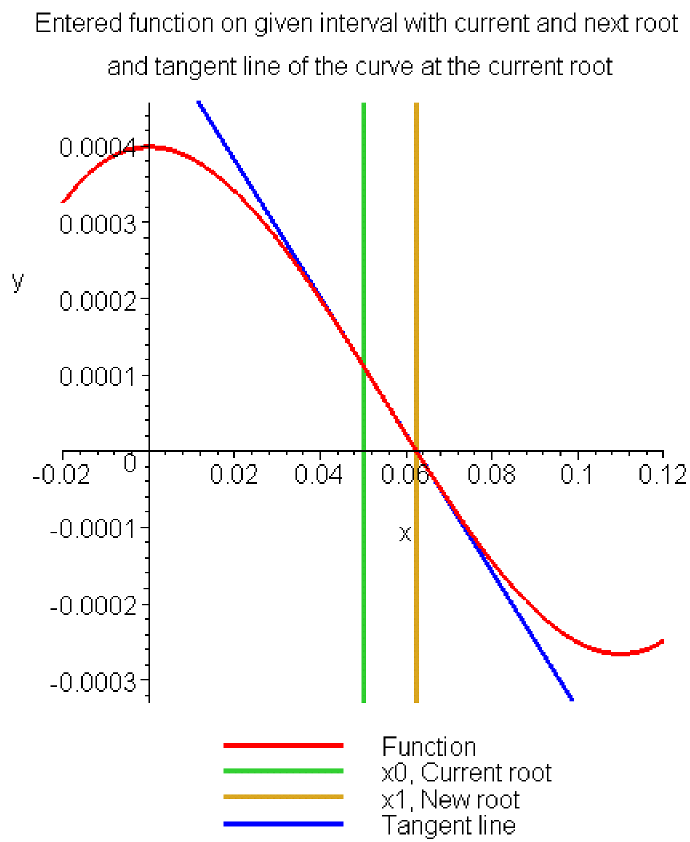


Figure 5 Estimate of the root for the first iteration.

Example 1 Cont.

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

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

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 digits to be correct in your result.

Example 1 Cont.

Iteration 2

The estimate of the root is

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

$$= 0.06242 - \frac{(0.06242)^3 - 0.165(0.06242)^2 + 3.993\times10^{-4}}{3(0.06242)^2 - 0.33(0.06242)}$$

$$= 0.06242 - \frac{-3.97781\times10^{-7}}{-8.90973\times10^{-3}}$$

$$= 0.06242 - \left(4.4646\times10^{-5}\right)$$

$$= 0.06238$$

Example 1 Cont.

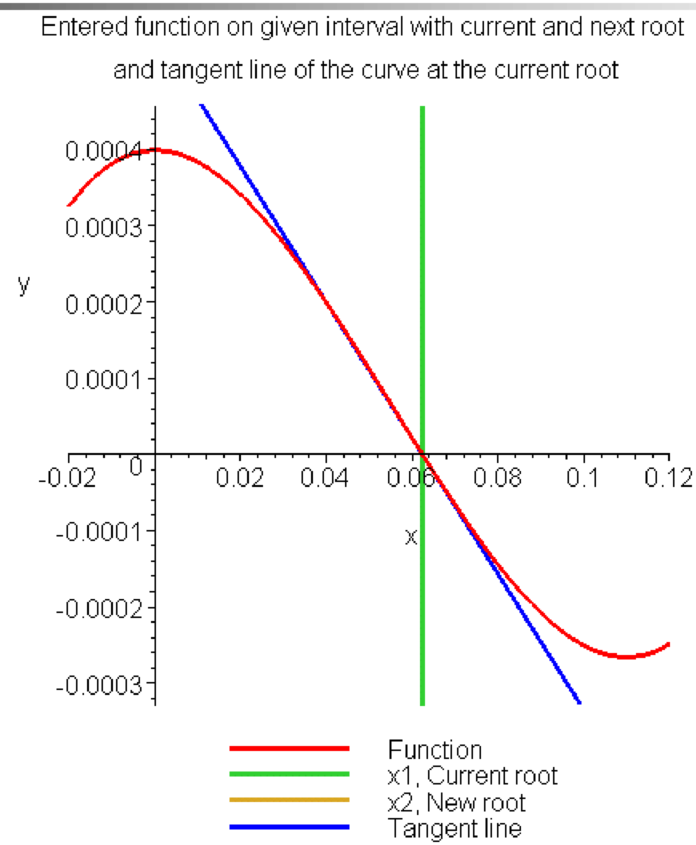


Figure 6 Estimate of the root for the Iteration 2.

Example 1 Cont.

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

$$\left|\in_a\right| = \left|\frac{x_2 - x_1}{x_2}\right| \times 100$$

$$= \left|\frac{0.06238 - 0.06242}{0.06238}\right| \times 100$$

$$= 0.0716\%$$

The maximum value of m for which $\left|\in_a\right| \leq 0.5 \times 10^{2-m}$ is 2.844. Hence, the number of significant digits at least correct in the answer is 2.

Example 1 Cont.

<u>Iteration 3</u>

The estimate of the root is

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

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

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

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

$$= 0.06238$$

Example 1 Cont.

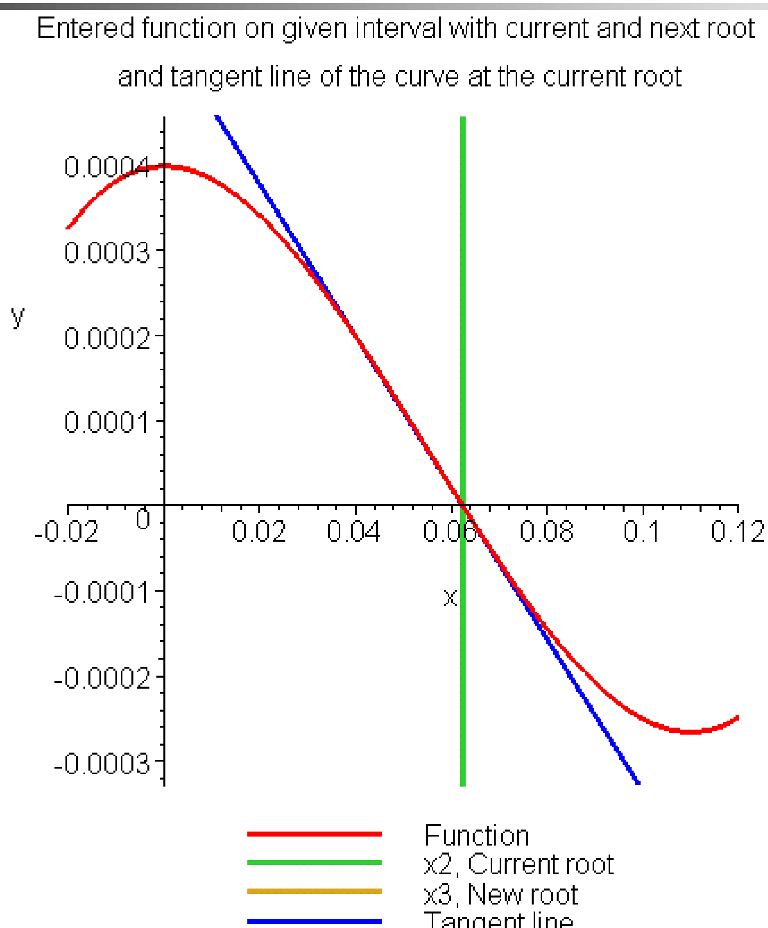


Figure 7 Estimate of the root for the Iteration 3.

Example 1 Cont.

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

$$\left|\in_a\right| = \left|\frac{x_2 - x_1}{x_2}\right| \times 100$$

$$= \left|\frac{0.06238 - 0.06238}{0.06238}\right| \times 100$$

$$= 0\%$$

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

Advantages and Drawbacks of Newton Raphson Method

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Advantages

- Converges fast (quadratic convergence), if it converges.
- Requires only one guess

Drawbacks

1. <u>Divergence at inflection points</u>
   Selection of the initial guess or an iteration value of the root that is close to the inflection point of the function $f(x)$ may start diverging away from the root in ther Newton-Raphson method.

For example, to find the root of the equation $f(x) = (x-1)^3 + 0.512 = 0$.

The Newton-Raphson method reduces to $x_{i+1} = x_i - \dfrac{(x_i^3 - 1)^3 + 0.512}{3(x_i - 1)^2}$.

Table 1 shows the iterated values of the root of the equation.

The root starts to diverge at Iteration 6 because the previous estimate of 0.92589 is close to the inflection point of $x = 1$.

Eventually after 12 more iterations the root converges to the exact value of $x = 0.2$.

Drawbacks – Inflection Points

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
18	0.2000

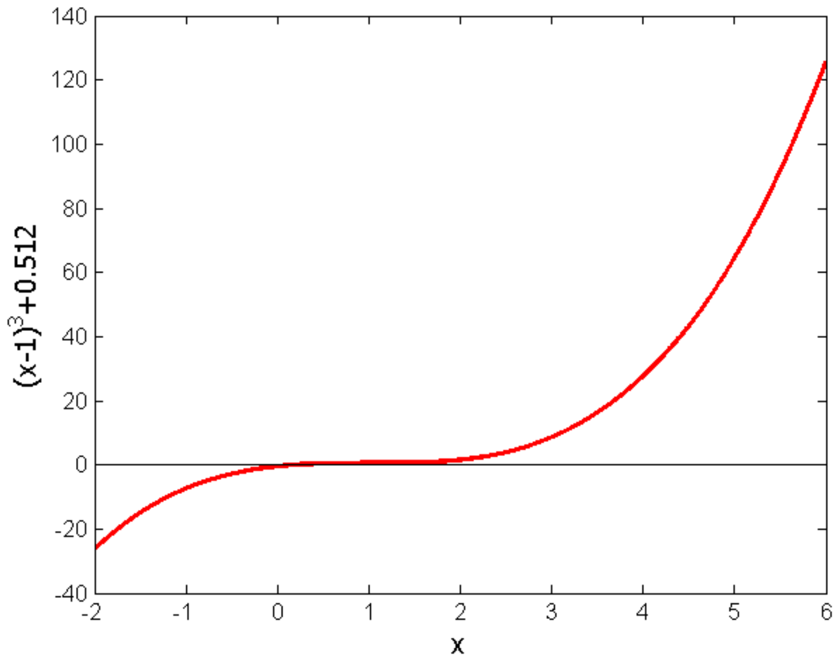

Figure 8 Divergence at inflection point for

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

Drawbacks – Division by Zero

2. <u>Division by zero</u>
   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 $x_0 = 0.02$, the denominator will equal zero.

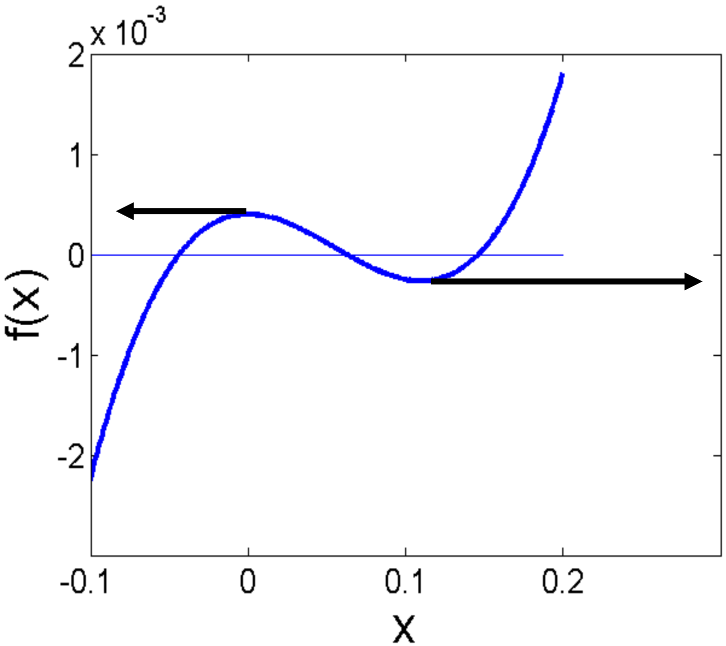

Figure 9 Pitfall of division by zero or near a zero number

Drawbacks – Oscillations near local maximum and minimum

3. <u>Oscillations near local maximum and minimum</u>

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.

Drawbacks – Oscillations near local maximum and minimum

Table 3 Oscillations near local maxima and mimima 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

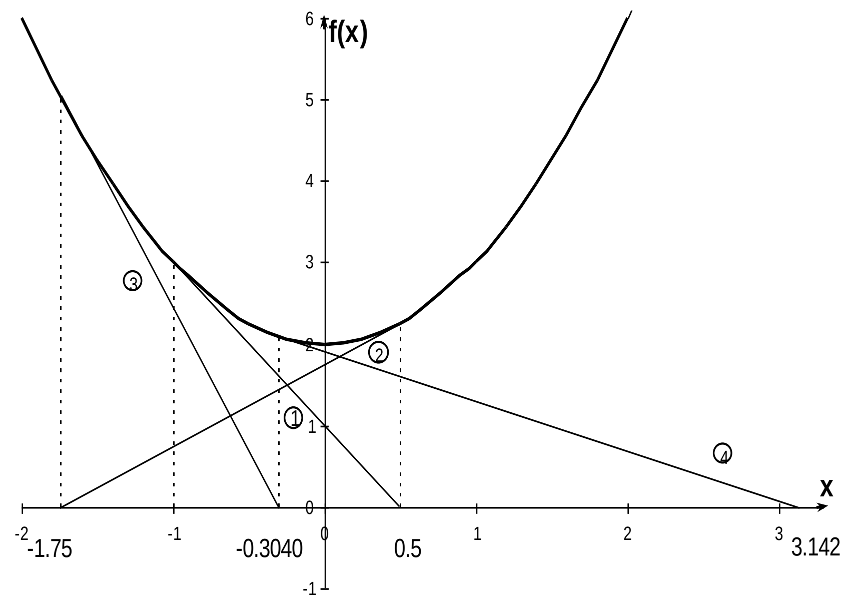

Figure 10 Oscillations around local minima for $f(x) = x^2 + 2$.

Drawbacks – Root Jumping

4. Root Jumping

In some cases 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

$$f(x) = \sin x = 0$$

Choose

$$x_0 = 2.4\pi = 7.539822$$

It will converge to $x = 0$

instead of $x = 2\pi = 6.2831853$

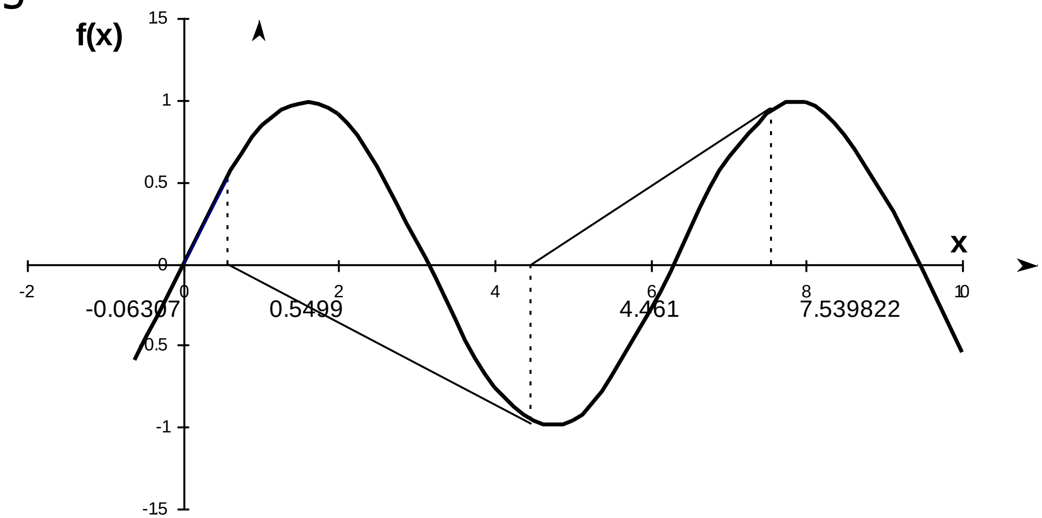

Figure 11 Root jumping from intended location of root for $f(x) = \sin x = 0$

THE END

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