Indian Institute of Technology Roorkee

CHN-323

Computer Applications in Chemical Engineering

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Solving nonlinear algebraic equations

- Single equation

$$f(x) = 0$$
$$f(x, p) = 0$$

p = parameter

- Set of equations

$$f_1(x_1, x_2) = 0$$
$$f_2(x_1, x_2) = 0$$

- Generalized

$$\underline{f}(\underline{x}) = 0$$

$$\underline{f}\left(\underline{x}, \underline{p}\right) = 0$$

Single nonlinear equation

$$f(x) = 0$$
$$f(x, p) = 0$$

x = unknown variable, p = parameter

- Example: $ax^2 + bx + c = 0$

$$f(x) = ax^2 + bx + c$$

- Solving this equation means finding the roots
  - Values of x that make $f(x)$ equal to zero
  - Also called the zeros of $f(x)$
- The roots depends on the values of parameters (a, b and c)

Example 1

- Van der Waals equation of state

$$\left(P + \frac{a}{V^2}\right)(V - b) = RT \qquad a = \frac{27}{64}\left(\frac{R^2T_c^2}{P_c}\right) \qquad b = \frac{RT_c}{8P_c}$$

- P (atm), V(L/gmol), R=0.08206 atm.L/(gmol. K)
- T_c=405.5 K, P_c=111.3 atm for ammonia

- Calculate the molar volume and compressibility factor for ammonia gas at a pressure of 56 atm and a temperature of 450 K.

Example 2

- Second law of motion,
  - rate of change of momentum of a body is equal to the resultant force acting on it

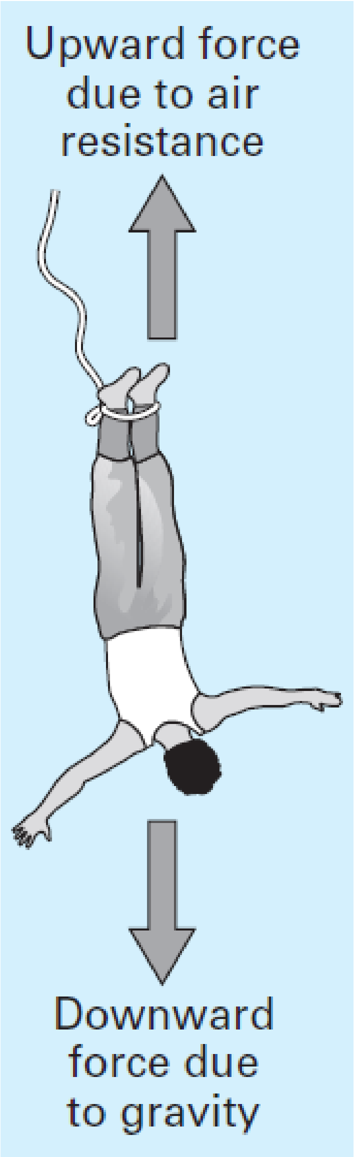
$$\frac{d(mv)}{dt} = F_{net}$$

- The net force on the body is

$$F_{net} = F_g - F_r = mg - c_d v^2$$

- Substituting, we get

$$\frac{dv}{dt} = g - \frac{c_d}{m} v^2$$



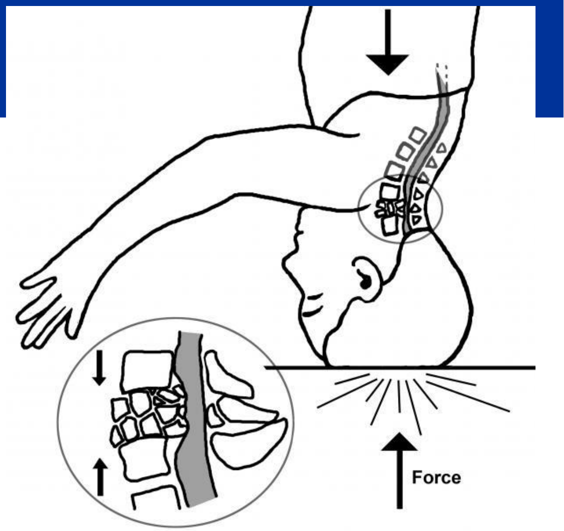
Example 2 continued…

- Analytical solution

$$v(t) = \sqrt{\frac{gm}{c_d}} \tanh\left(\sqrt{\frac{gc_d}{m}}\, t\right)$$

- Model for the bungee jumper's velocity
- You can predict the jumper's velocity
- Such computations can be performed directly because *v* is expressed ***explicitly*** as a function of the model parameters. That is, it is isolated on one side of the equal sign.

Example 2 continued…



$$v(t) = \sqrt{\frac{gm}{c_d}}\tanh\left(\sqrt{\frac{gc_d}{m}}t\right)$$

- According to medical studies, bungee jumper's chances of sustaining a significant vertebrae injury increase significantly if the free fall velocity exceeds 36 m/s after 4 s of free fall
- Determine the critical mass at which this criterion is exceeded given a drag coefficient of 0.25 kg/m

Example 2 continued…

$$v(t) = \sqrt{\frac{gm}{c_d}}\tanh\left(\sqrt{\frac{gc_d}{m}}t\right)$$

- All unknowns, except m
- We have an equations (to determine m), but it cannot be solved explicitly for m
- m is said to be **implicit**
- To solve for m, we can write

$$f(m) = \sqrt{\frac{gm}{c_d}}\tanh\left(\sqrt{\frac{gc_d}{m}}t\right) - v(t) = 0$$

$$\sqrt{\frac{9.81m}{0.25}}\tanh\left(\sqrt{\frac{9.81(0.25)}{m}}4\right) - 36 = 0$$

Single nonlinear equation

$$ax^2 + bx + c = 0$$

- Direct solution

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

- There are many equations that could not be solved directly → Approximate solution techniques
  1. Graphical method
  2. Trial and error method
  3. Numerical methods: systematic strategies to arrive at the roots

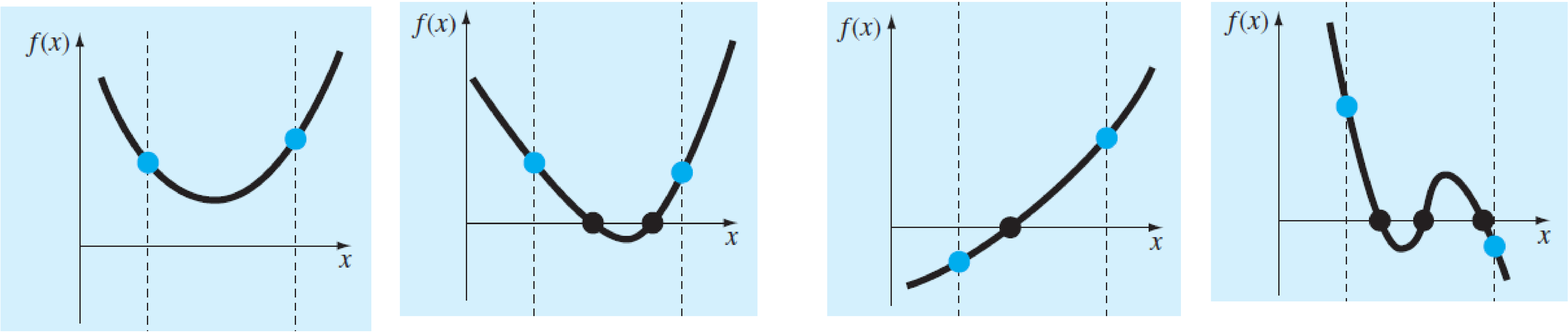
Graphical method

- Make a plot of the function
- Observe where it crosses the x axis
- This point, which represents the x value for which $f(x) = 0$, provides a rough approximation of the root

Solve example 2 by graphical method in MATLAB

Graphical method

- Number of ways in which roots can occur (or be absent) in an interval prescribed by a lower and upper bound



Trial and error method

- Guess a value of x and evaluate whether $f(x)$ is zero
- If not, make another guess for x
- Again evaluate $f(x)$ to check if the new value of x provides a better estimate of the root
- Repeat until a guess results in an $f(x)$ that is close to zero.

Numerical methods

- Bracketing methods: Based on two initial guesses that bracket the root
  - Bisection method
  - False position method
- Open methods: Can involve one or more initial guesses, but there is no need for them to bracket the root.
  - Secant method
  - Newton's method
  - Muller's method
  - Fixed point iteration method

Bisection method

- <u>Key idea</u>: if $f(x)$ is continuous and it changes signs at two x-values, there must be at least one root between these x-values
- To determine a root of $f(x) = 0$ given values x_0 and x_1 such that $f(x_0) * f(x_1) < 0$

Repeat
  Set $x_2 = (x_0 + x_1)/2$
  If $f(x_2) * f(x_0) < 0$ Then
    Set $x_1 = x_2$
    Else Set $x_0 = x_2$
  End if
Until $(|x_0 - x_1|) < 2 * tolerance$

Example

- Solve in MATLAB by bisection method

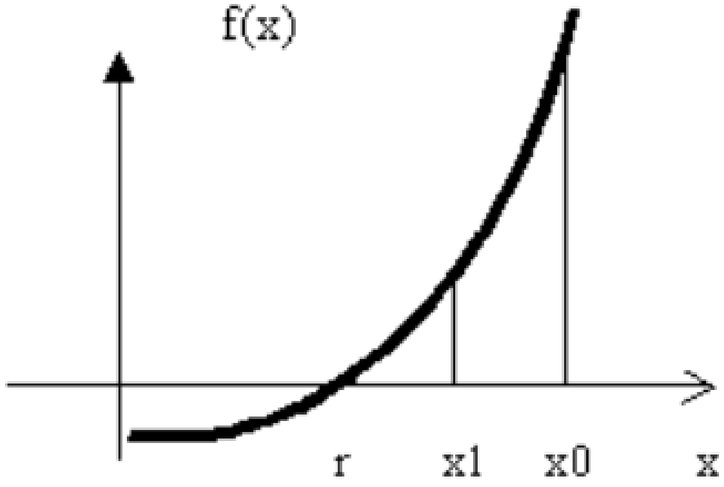
$$f(x) = 3x + \sin x - e^x = 0$$

$x0 = 0$ and $x1 = 1$

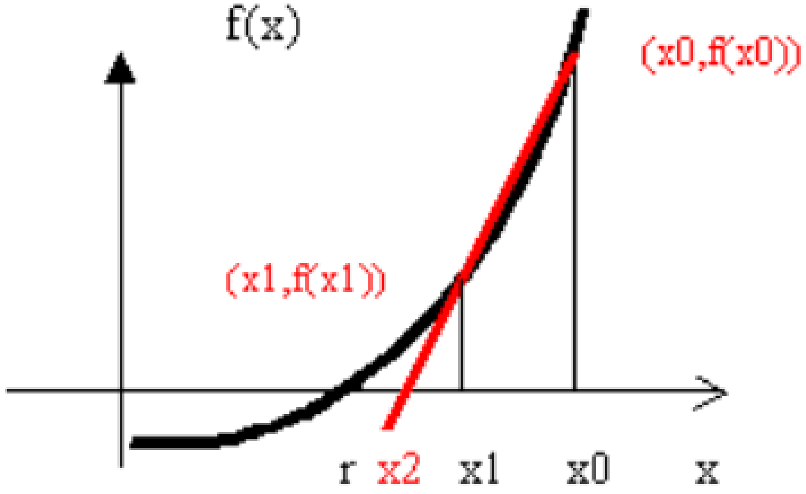
$$tolerance = 1 \times 10^{-4}$$

Secant method

- <u>Key idea</u>: approximate the curve with a straight line for x between the values of x_0 and r.



The straight line is assumed to be the secant which connects the two points (x_0, $f(x_0)$) and (x_1, $f(x_1)$)



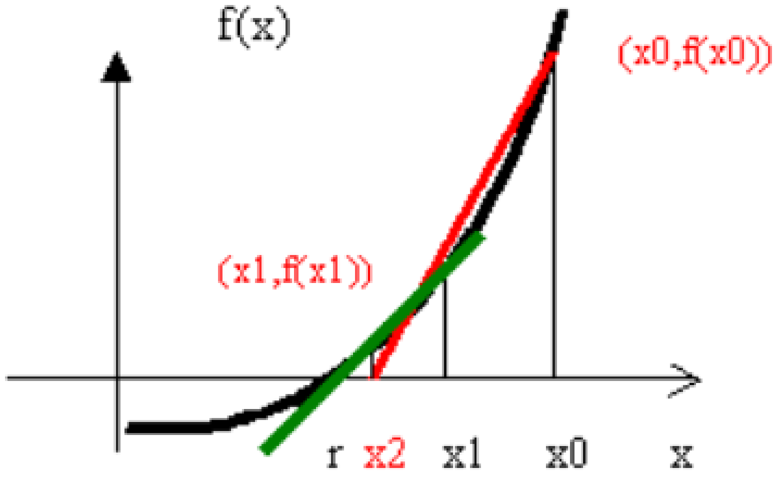
Both the secant line and the new root estimate $\mathbf{x_2}$ are shown in red

$\mathbf{x_2}$ is closer to the root **r** than either $\mathbf{x_1}$ or $\mathbf{x_0}$

https://www.lehigh.edu/~ineng2/clipper/notes/secant.htm

Secant method

- Repeat this process (green line)
- Getting closer to r



Secant method

- Slope of red line $m = \frac{f(x_1)-f(x_0)}{x_1-x_0}$
- Equation of red line considering one point as $(x_1, f(x_1))$

$$y - f(x_1) = m(x - x_1)$$

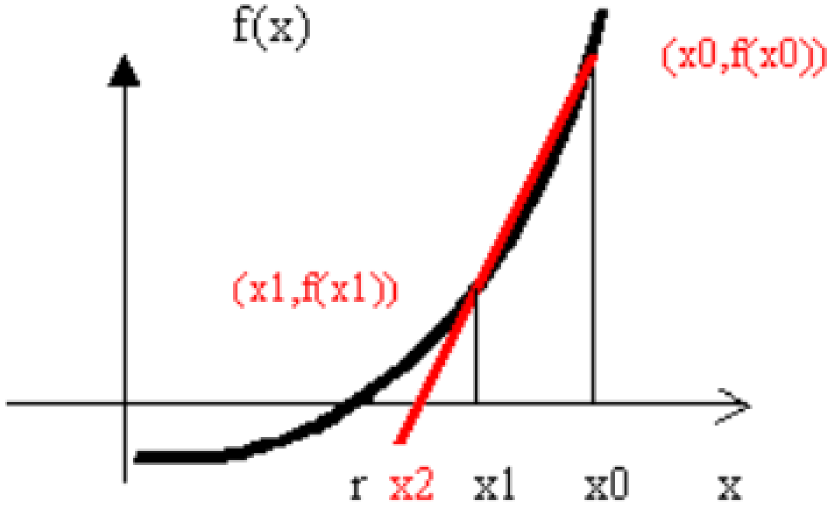
- The point $x = x_2$ corresponds to the point of the straight line where $y = 0$

$$-f(x_1) = m(x_2 - x_1)$$

- Thus

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

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



Secant method

- Generalizing, we get

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

- To determine a root of $f(x) = 0$, given two values, x_0 and x_1, that are near the root,

If $|f(x_0)| < |f(x_1)|$ Then
  Swap x_0 with x_1
Repeat
  Set $x_2 = x_1 - f(x_1)\frac{x_1 - x_0}{f(x_1) - f(x_0)}$
  Set $x_0 = x_1$
  Set $x_1 = x_2$
Until $|f(x_2)| < tolerance$

Example

- Solve in MATLAB by secant method

$$f(x) = 3x + \sin x - e^x = 0$$

$$x_0 = 0 \text{ and } x_1 = 1$$

$$tolerance = 1 \times 10^{-4}$$

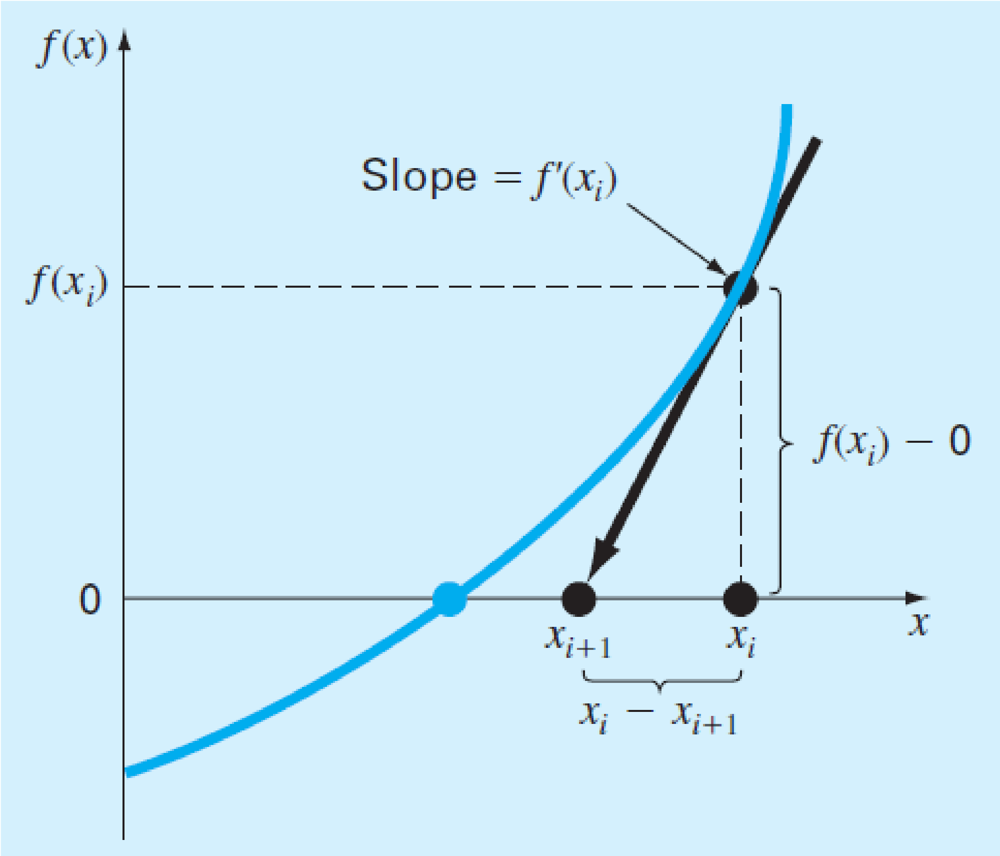
False position (linear interpolation method)

- <u>Key idea</u>: mix of bisection and secant method.

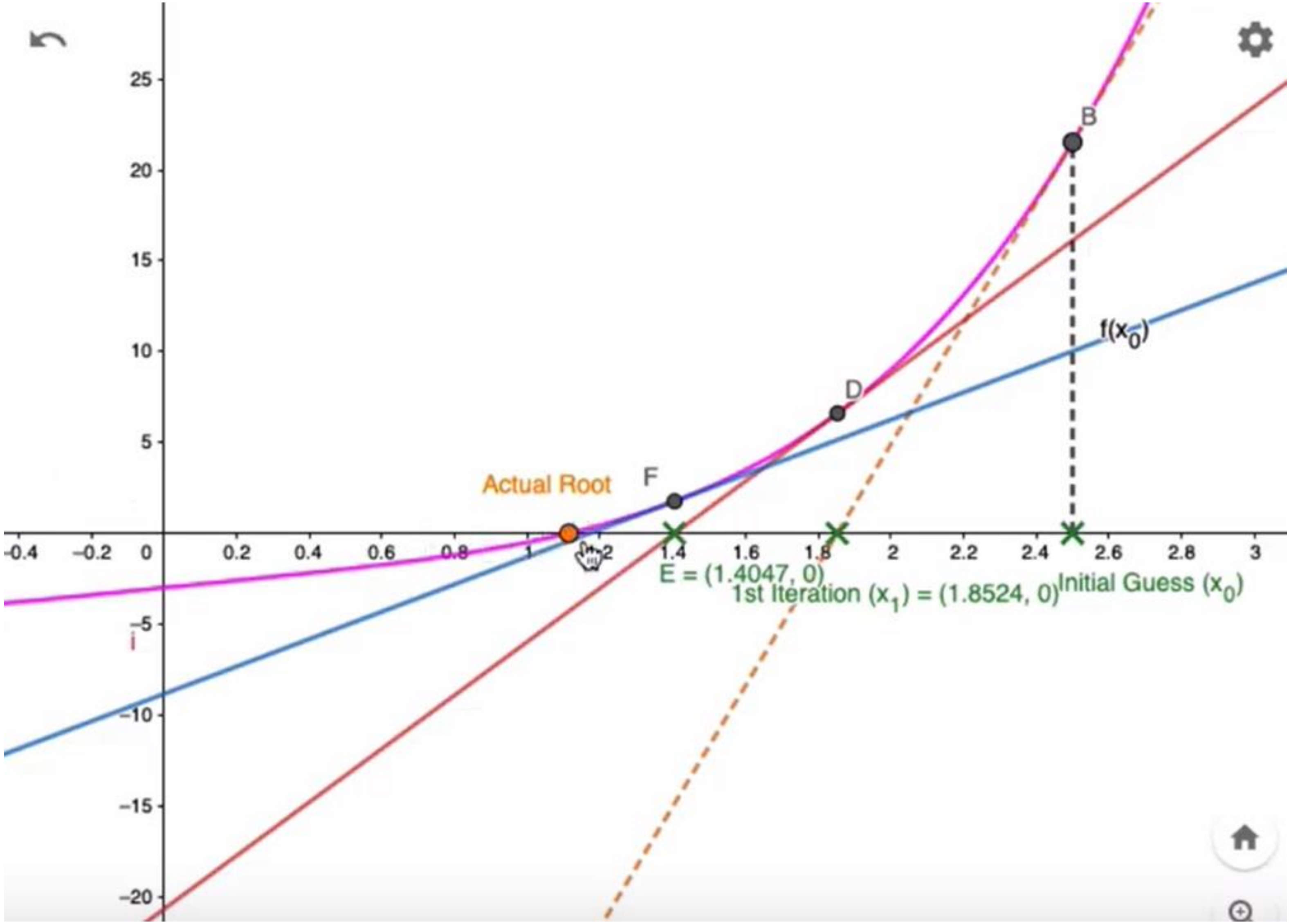
Repeat
  Set $x_2 = x_1 - f(x_1)\frac{x_1 - x_0}{f(x_1) - f(x_0)}$
  If $f(x_2) * f(x_0) < 0$ Then
    Set $x_1 = x_2$
    Else Set $x_0 = x_2$
  End if
Until $|f(x_2)| < tolerance$

Newton's method

- **Key idea**
  - Make a initial guess, say x_i
  - A tangent can be drawn from the point $[x_i, f(x_i)]$
  - The point where this tangent crosses the x axis usually represents an improved estimate of the root



Newton's method



https://www.youtube.com/watch?v=R0no1yo-ckQ

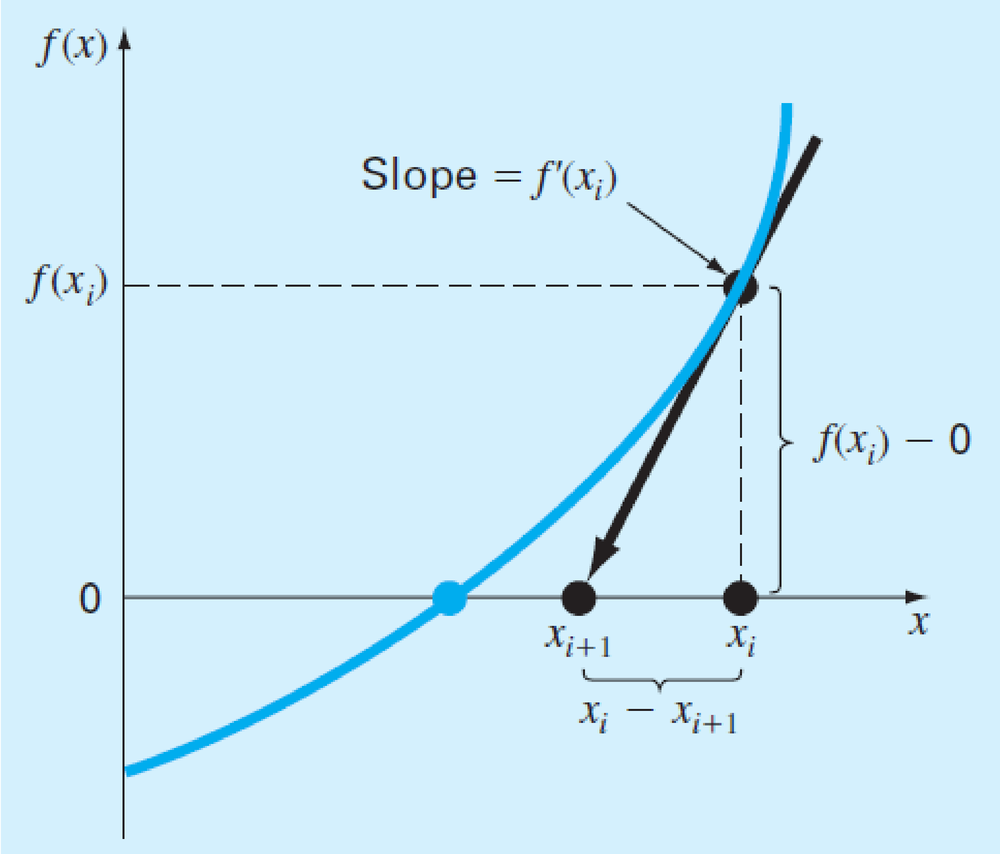
Newton's method

- We know that

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

Rearranging this gives

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



Newton's method by Taylor Series Interpretation

- Let us write Taylor series expansion of $f(x)$ around the point x_i

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

- Retaining only the first order term

$$f(x) = f(x_i) + f'(x_i)(x - x_i)$$

Good approximation of $f(x)$ at x_i and in the vicinity of x_i

- Consider x = r (root)

$$f(r) = f(x_i) + f'(x_i)(r - x_i)$$

Newton's method by Taylor Series Interpretation

- But $f(r) = 0$

$$0 = f(x_i) + f'(x_i)(r - x_i)$$

- This implies

$$r = x_i - \frac{f(x_i)}{f'(x_i)}$$

- In general

$$x^{[n+1]} = x^{[n]} - \frac{f\left(x^{[n]}\right)}{f'(x^{[n]})}$$

Newton's method: algorithm

- To determine a root of $f(x) = 0$, given x_0 reasonably close to the root,

Compute $f(x_0)$, $f'(x_0)$.
If $f(x_0) \neq 0$ And $f'(x_0) \neq 0$ Then
    Repeat
    Set $x_1 = x_0$.
    Set $x_0 = x_0 - \frac{f(x_0)}{f'(x_0)}$
    Until $(|x_1 - x_0|) <* tol1$ Or $|f(x_1)| < tol2$.
End If.

Extended Newton's method

- When we derived Newton's method from Taylor series expansion, we retained only the first order term
- We can retain both linear and quadratic terms, it is called extended Newton's method

$$f(x) = f(x_i) + f'(x_i)(x - x_i) + \frac{f''(x_i)(x - x_i)^2}{2}$$

- Consider x = r (root)

$$f(r) = f(x_i) + f'(x_i)(r - x_i) + \frac{f''(x_i)(r - x_i)^2}{2}$$

Extended Newton's method

- But $f(r) = 0$

$$0 = f(x_i) + f'(x_i)(r - x_i) + \frac{f''(x_i)(r - x_i)^2}{2}$$

$$\rightarrow \quad f(x_i) + (r - x_i)\left[f'(x_i) + \frac{f''(x_i)(r - x_i)}{2}\right] = 0$$

The $(r - x_i)$ term inside the square braces may be replaced by the results of the Newton Method

$$r = x_i - \frac{f(x_i)}{f'(x_i)}$$

$$\rightarrow \quad f(x_i) + (r - x_i)\left[f'(x_i) - \frac{f''(x_i)\, f(x_i)}{2f'(x_i)}\right] = 0$$

Extended Newton's method

$$(r - x_i) = \frac{-f(x_i)}{\left[f'(x_i) - \frac{f''(x_i)\, f(x_i)}{2f'(x_i)}\right]}$$

$$\rightarrow \quad r = x_i - \frac{f(x_i)}{\left[f'(x_i) - \frac{f''(x_i)\, f(x_i)}{2f'(x_i)}\right]}$$

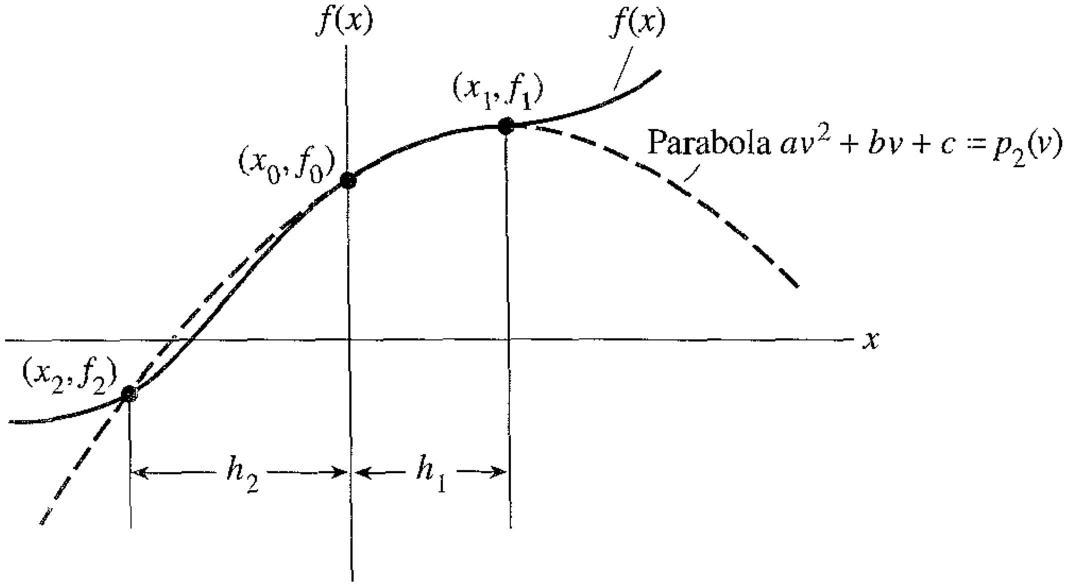
$$\rightarrow \quad x^{[n+1]} = x^{[n]} - \frac{f\left(x^{[n]}\right)}{\left[f'(x^{[n]}) - \frac{f''(x^{[n]})\, f(x^{[n]})}{2f'(x^{[n]})}\right]}$$

Muller's method

- <u>Key idea</u>: approximate the function $f(x)$ with a quadratic polynomial for x.

- We need three initial guesses

- Similar to secant method

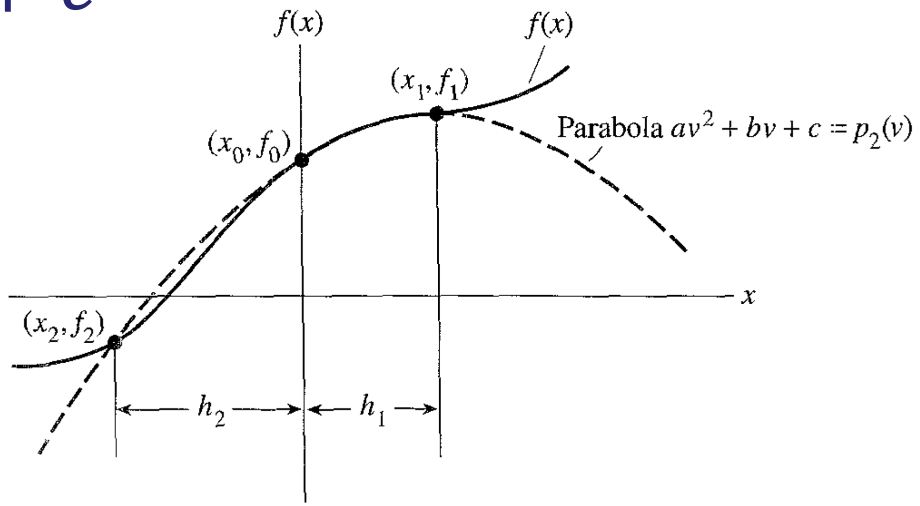


Muller's method

- Let the three initial guesses be (x_0, x_1, x_2). Let the function values at these three points be denoted by (f_0, f_1, f_2).
- Define $v = x - x_0$
- We construct a 2nd degree polynomial as

$$P_2(v) = av^2 + bv + c$$

- Let $h_1 = x_1 - x_0$ and $h_2 = x_0 - x_2$



Muller's method

- We estimate the coefficients (a, b and c) by evaluating $P_2(v)$ at the 3 points

$$v = 0: \quad a(0)^2 + b(0) + c = f_0;$$

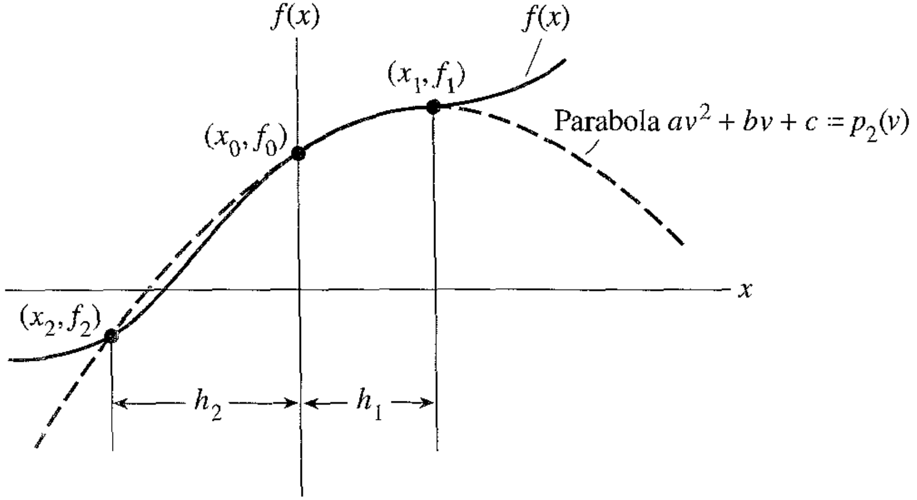
$c = f_0$

$$v = h_1: \quad ah_1^2 + bh_1 + c = f_1;$$
$$v = -h_2: \quad ah_2^2 - bh_2 + c = f_2.$$

2 eqns and 2 unknowns

$$a = \frac{f_2 + \gamma f_1 - f_0(1+\gamma)}{\gamma h_1^2 (1+\gamma)} \quad \text{and} \quad b = \frac{f_1 - f_0 - ah_1^2}{h_1}$$

where $\gamma = \dfrac{h_2}{h_1}$



Muller's method

- We have now obtained the values of a, b & c

- The roots of the equation $P_2(v) = 0$ are given by (analytical expression for quadratic equation)

$$v = \tilde{r} - x_0 = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$\tilde{r} = x_0 + \left[\frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \right]$$

$\tilde{r}$ is a better guess for the root of $f(x) = 0$