CE 205: Numerical Methods

Roots of Equations

What are roots?

Years ago you learnt: $x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$

to solve: $ax^2 + bx + c = 0$

Yet there are many more functions for which roots cannot be determined so easily

- The parameters to be determined may be implicit

<u>Example</u>: determine "*m*" when *v = 36 m/s, t = 4s* and c_d = 0.25 kg/m

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

Solution Methods

- Bisection/Half-interval Search
- Method of false position/Regula Falsi

} Bracketing Methods

- Secant Method
- Newton Raphson
- Iteration Method
- Many more….

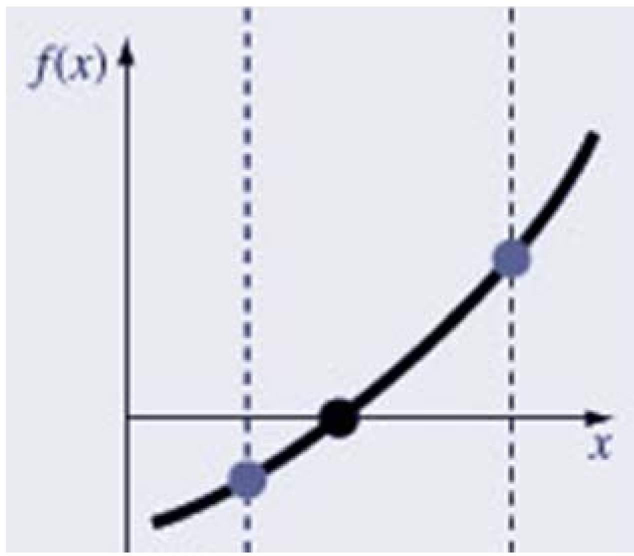
} Open Methods

Algebraic equation: $ax^2 + bx + c = 0$

Transcendental equation: $1 + \cos x - 5x = 0$

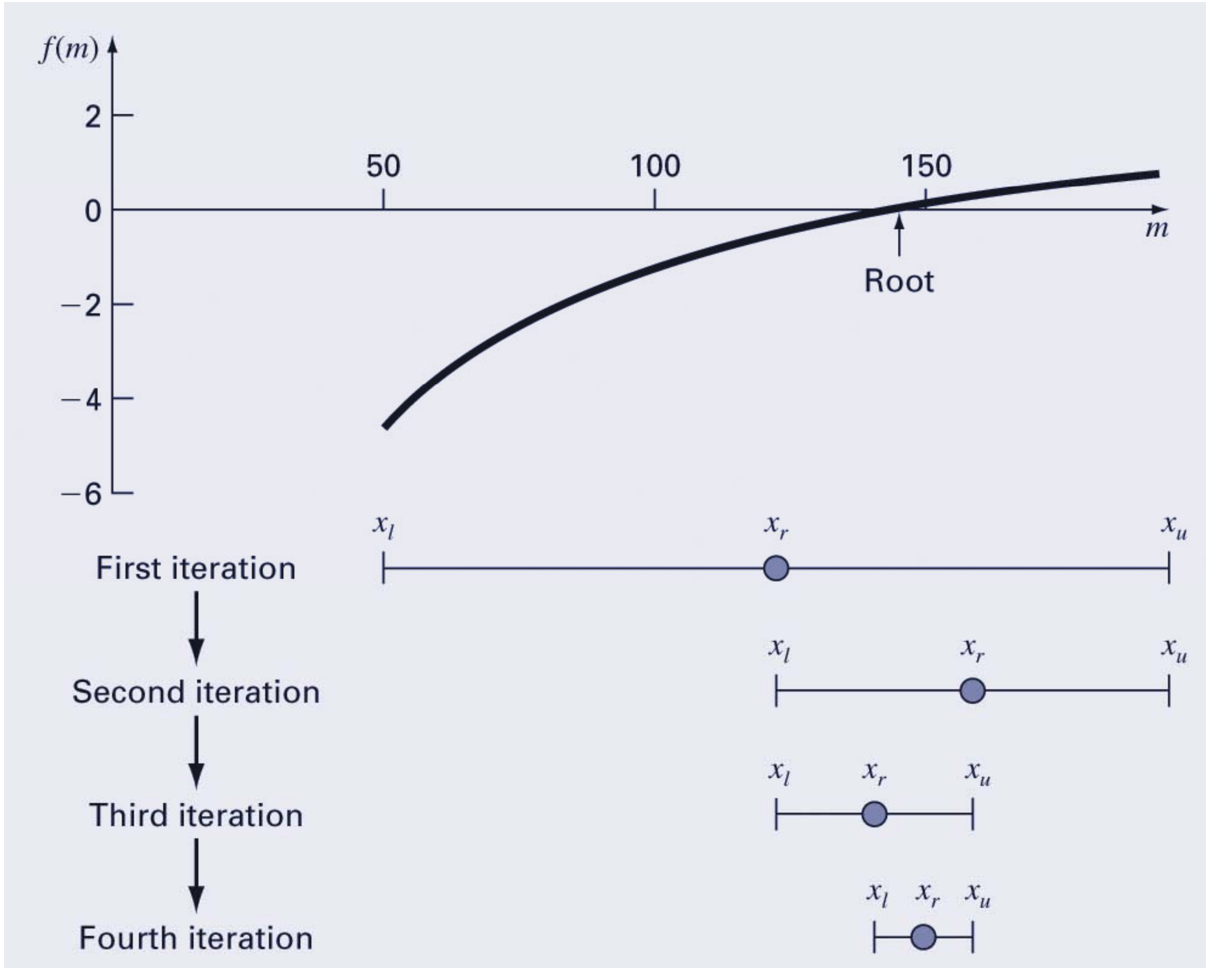
Bracketing Methods: incremental search

Brackets are formed by finding two guesses x_l and x_u where the sign of the function changes; that is, where $f(x_l)\, f(x_u) < 0$



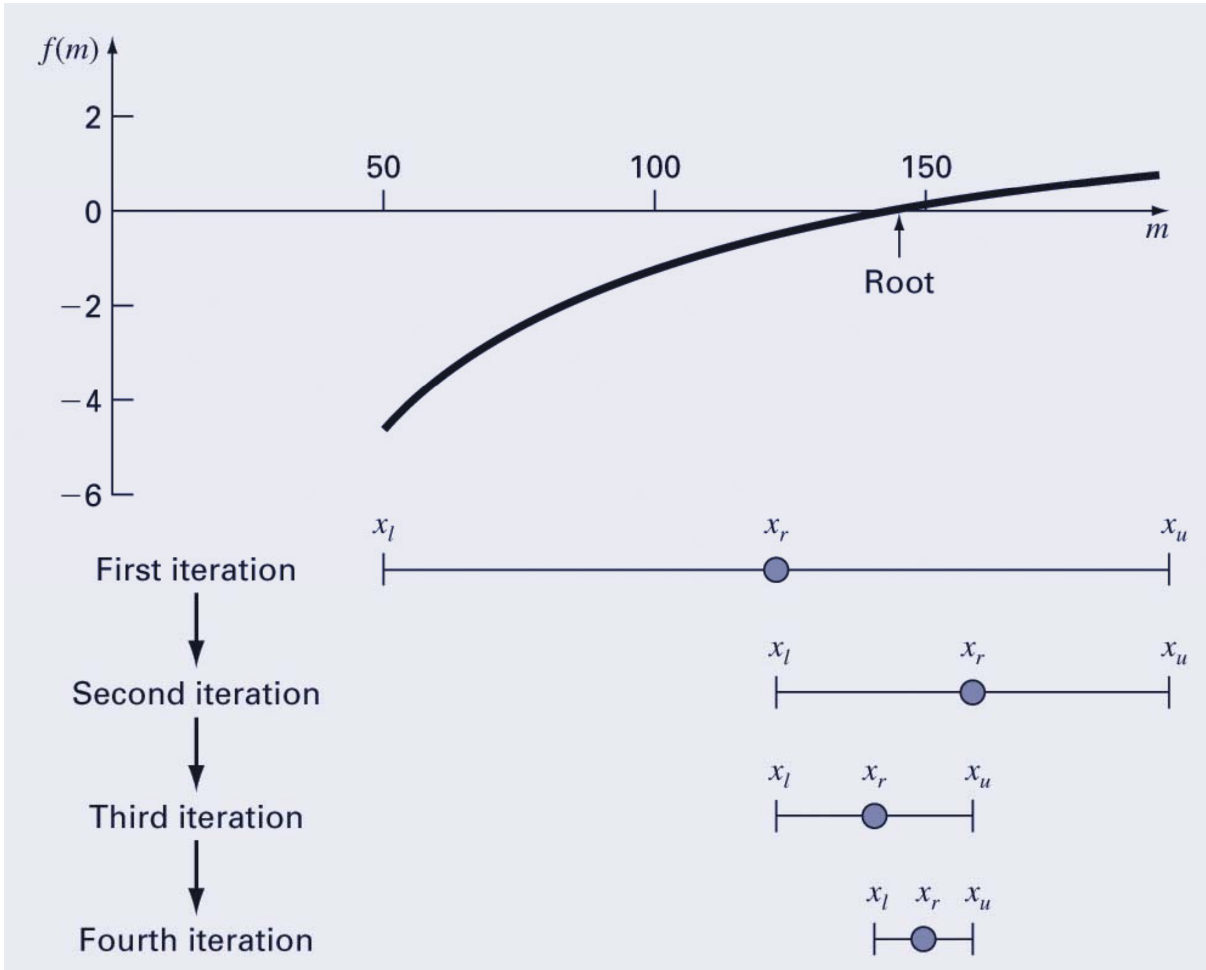
The *incremental search* method tests the value of the function at evenly spaced intervals

Bracketing Methods: Bisection



A variation of the incremental search method in which the interval is always divided by half

Bracketing Methods: Bisection



Location of the root lies within the interval where the sign change occurs

The absolute error is reduced by a factor of 2 for each iteration.

Bracketing Methods: Bisection

The absolute error of the bisection method is solely dependent on the absolute error at the start of the process (the space between the two guesses) and the number of iterations:

$$E_a^n = \frac{\Delta x^0}{2^n}$$

The required number of iterations to obtain a particular absolute error can be calculated based on the initial guesses:

$$n = \log_2\left(\frac{\Delta x^0}{E_{a,d}}\right)$$

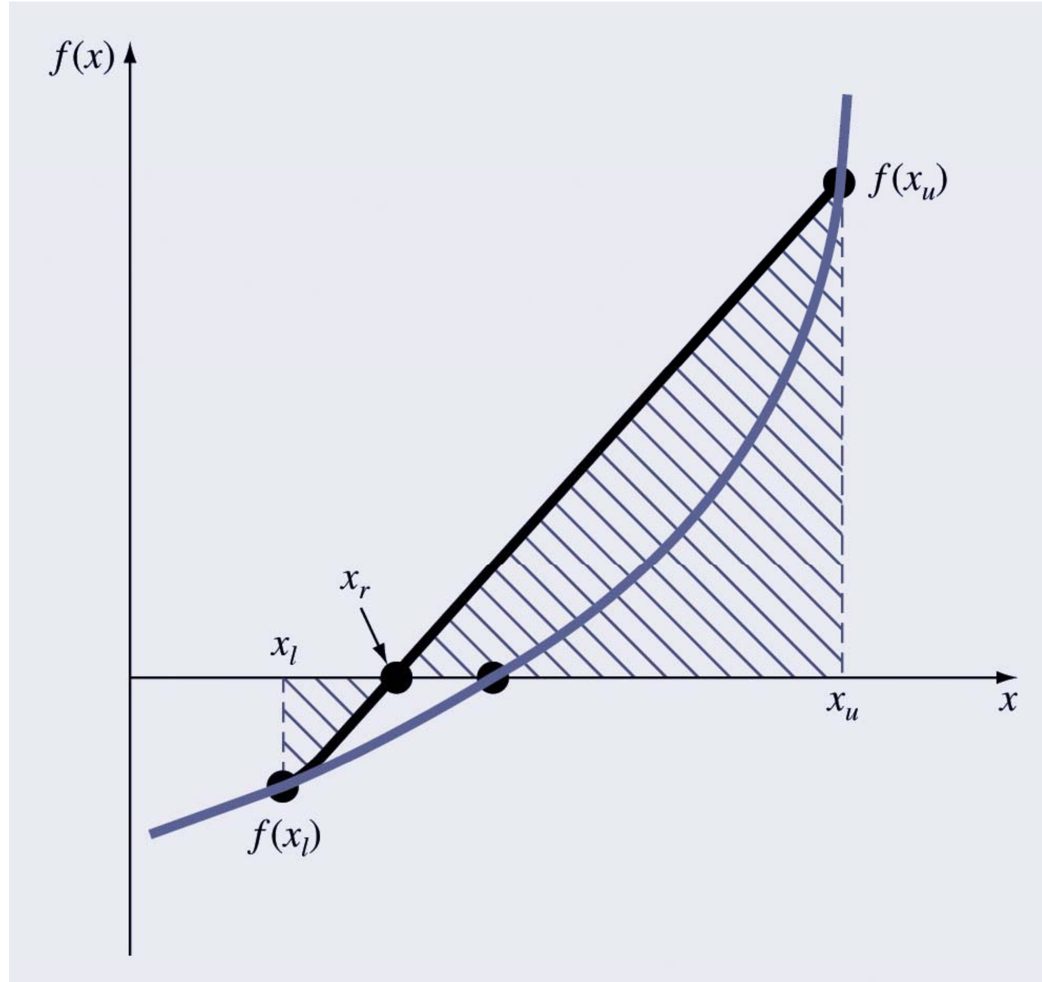
Choice of method depends on…

- Required accuracy
- Rate of convergence
- Inputs
  - How does initial approximation affect the computation?
- Often combination of multiple methods is the optimum
- Supplement these techniques with any other information that gives insight into the location of roots
  - Graphical methods
  - understanding the physical problem

Bracketing Methods: Regula Falsi

It determines the next guess by connecting the endpoints with a straight line and determining the location of the intercept of the straight line (x_r).

$$x_r = x_u - \frac{f(x_u)(x_l - x_u)}{f(x_l) - f(x_u)}$$



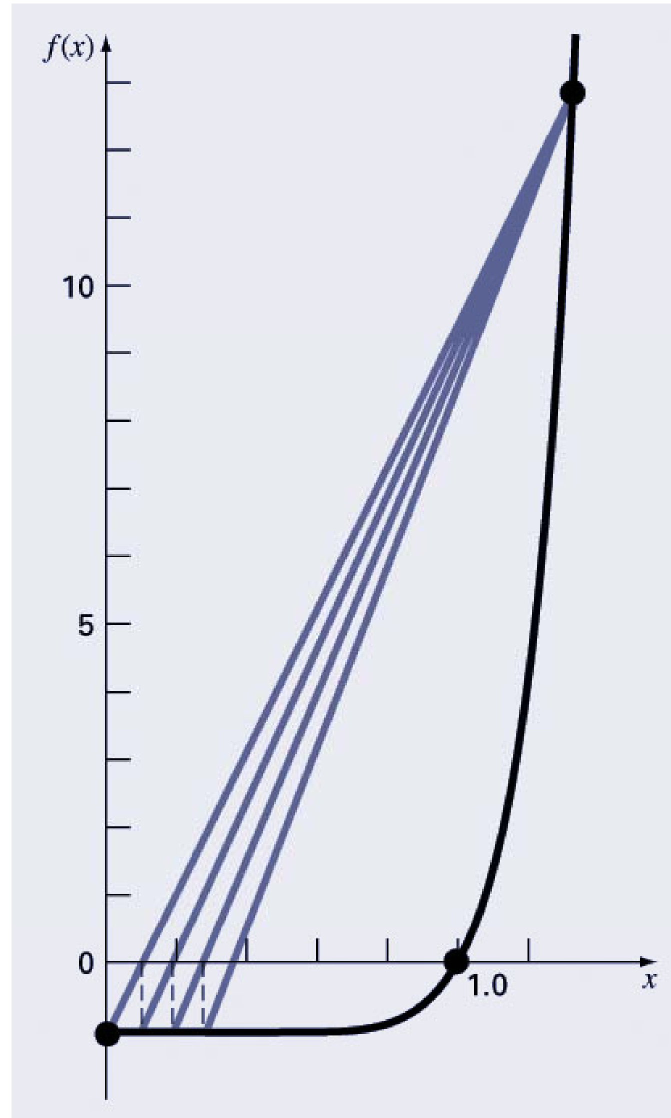
The value of x_r then replaces whichever of the two initial guesses yields a function value with the same sign as $f(x_r)$.

Bisection vs. Regula Falsi

Bisection does not take into account the shape of the function

- this can be good or bad depending on the function!

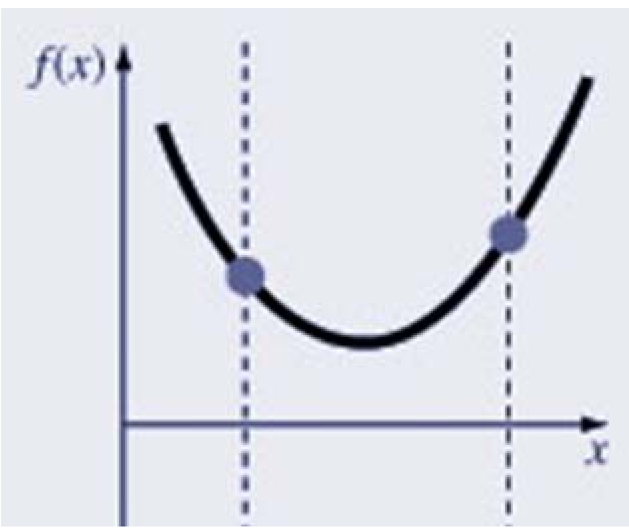
Try: $f(x) = x^{10} - 1$

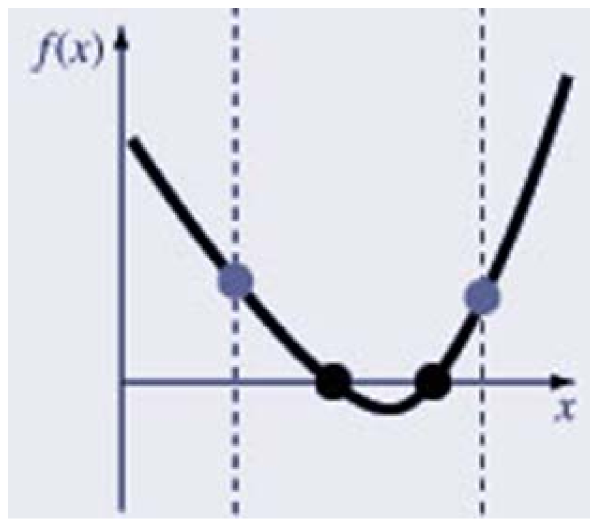


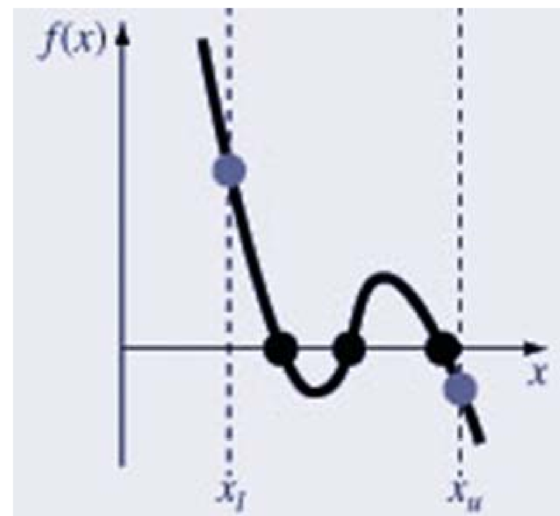
Problems with bracketing methods

Some root-finding methods may fail:

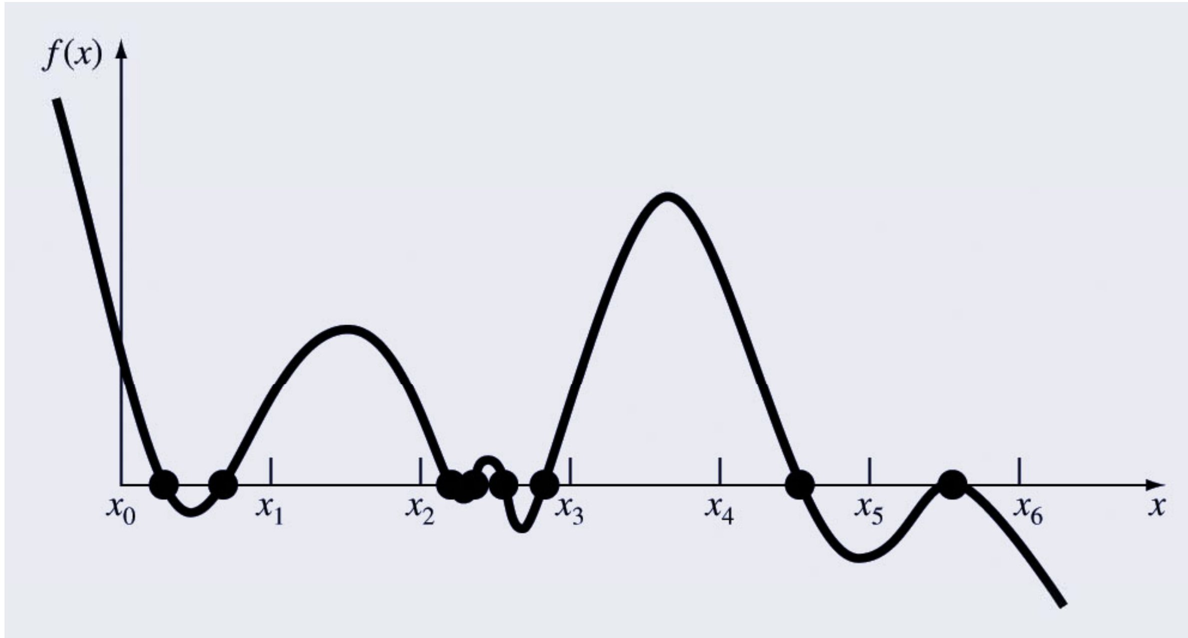
- Same sign, no roots
- Same sign, two roots
- Different sign, three roots







Incremental search is not foolproof!



Interval spacing choice

Short increments time consuming

Large increments may cause to miss some roots

Remedy:

Use graphical methods, taking derivatives at each intervals

Use personal judgment by analyzing the problem

Solution Methods

- Bisection/Half-interval Search
- Method of false position/Regula Falsi

} Bracketing Methods

- Secant Method
- Newton Raphson
- Iteration Method
- Many more….

} Open Methods

Open methods require one (or two) starting values which do not necessarily bracket a root.

- May diverge or converge
- if they converge they do so at a faster rate

Method of iteration

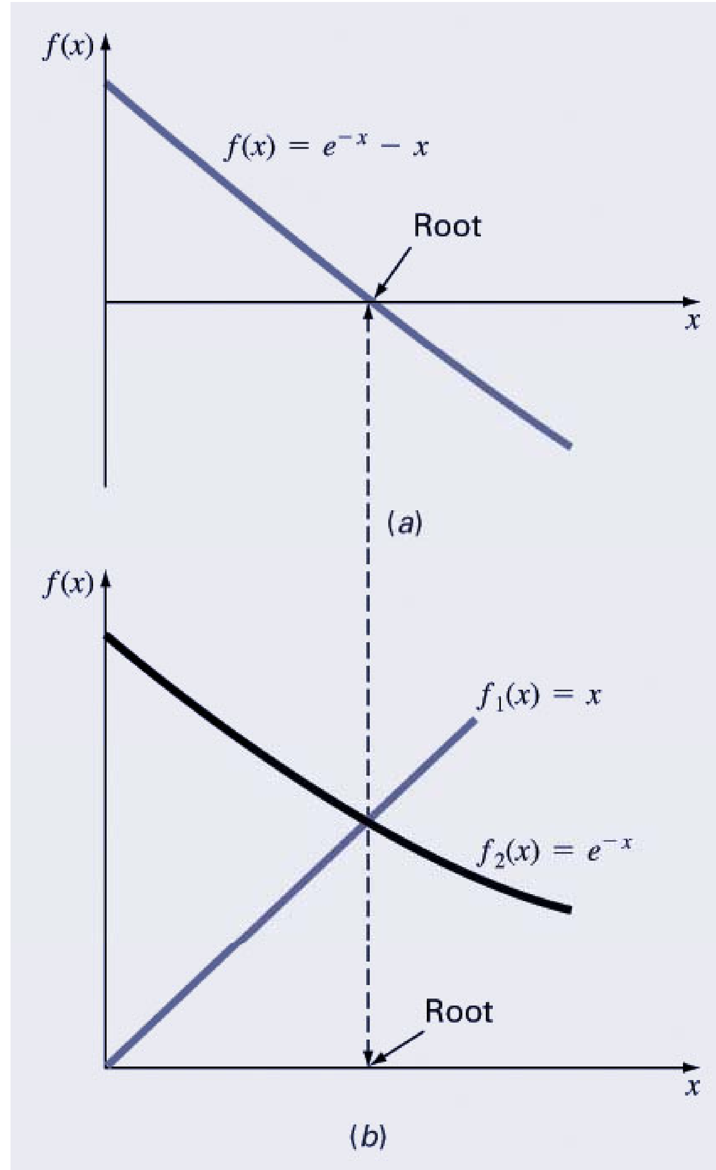
Rearrange the function $f(x)=0$ so that x is on the left-hand side of the equation: $x=g(x)$

- To Solve $f(x)=e^{-x}-x$, rewrite as $x=e^{-x}$

Use the new function g to predict a new value of x - that is, $x_{i+1}=g(x_i)$

The approximate error is given by:

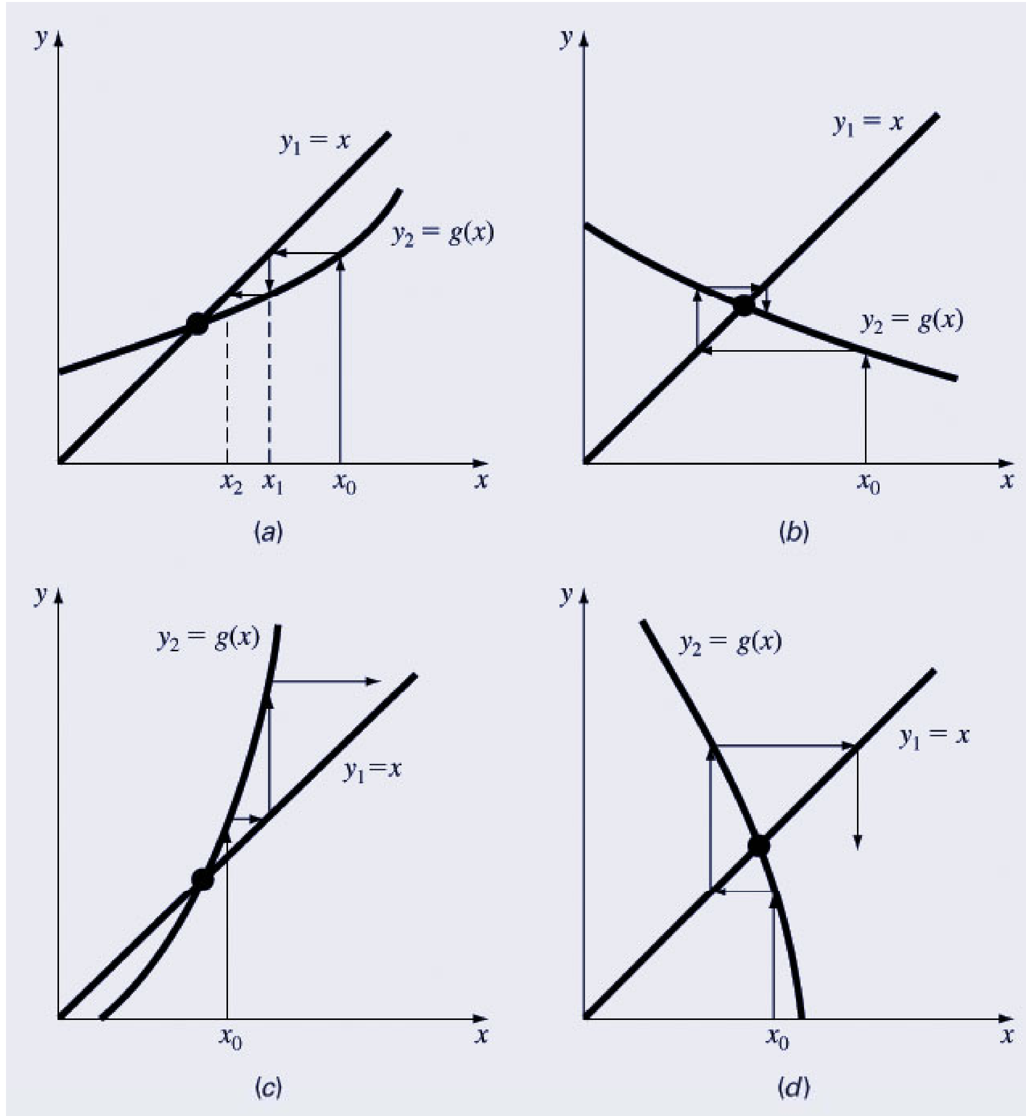
$$\varepsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| 100\%$$



Convergence

Convergence of the simple fixed-point iteration method requires that the derivative of g(x) near the root has a magnitude less than 1.

a) Convergent, $0 \le g' < 1$
b) Convergent, $-1 < g' \le 0$
c) Divergent, $g' > 1$
d) Divergent, $g' < -1$

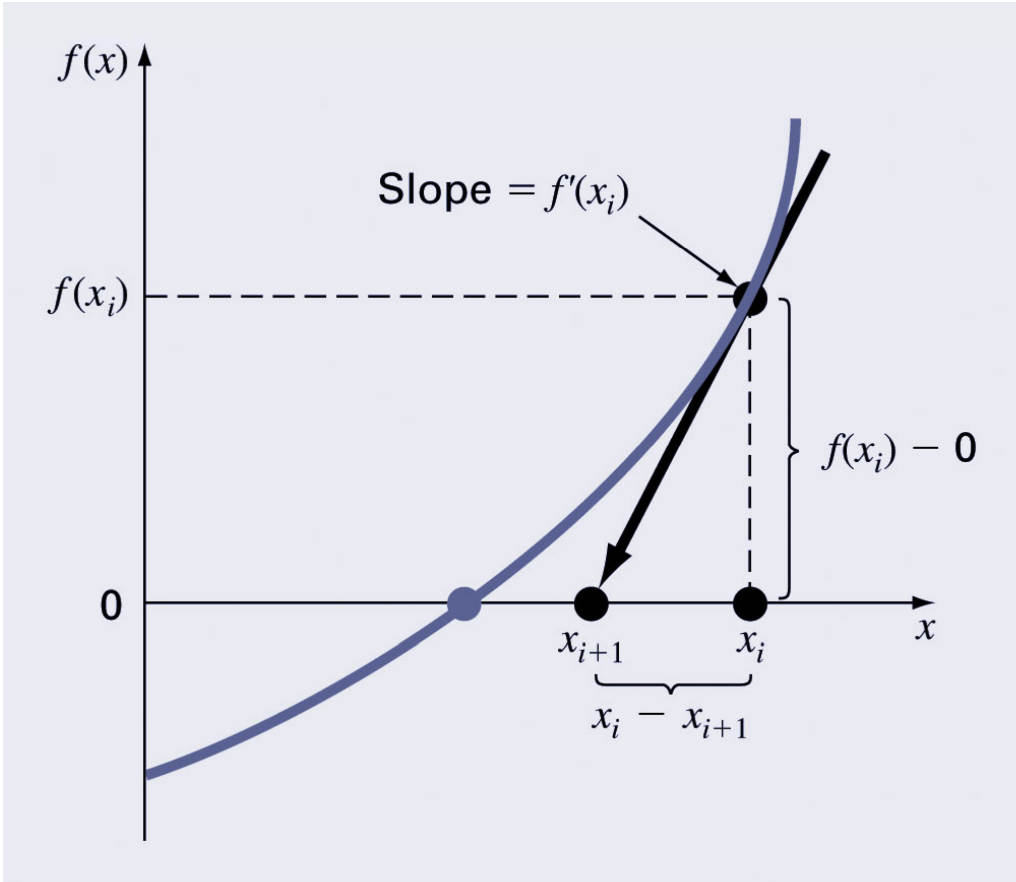


Newton-Raphson Method

Based on forming the tangent line to the $f(x)$ curve at some guess x, then following the tangent line to where it crosses the x-axis.

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

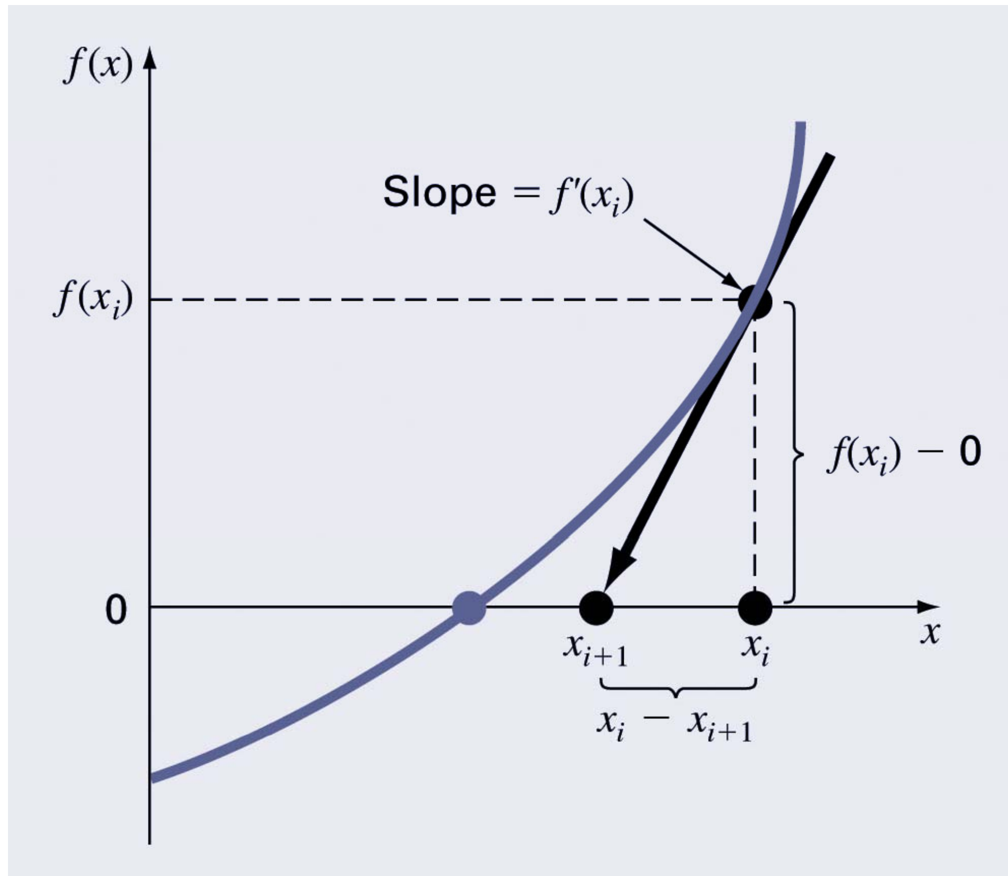
$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$



Quadratic convergence in Newton-Raphson

The error is roughly proportional to the square of the previous error.

$$E_{t,i+1} \cong \frac{-f''(x_r)}{2f'(x_r)} E_{t,i}^2$$

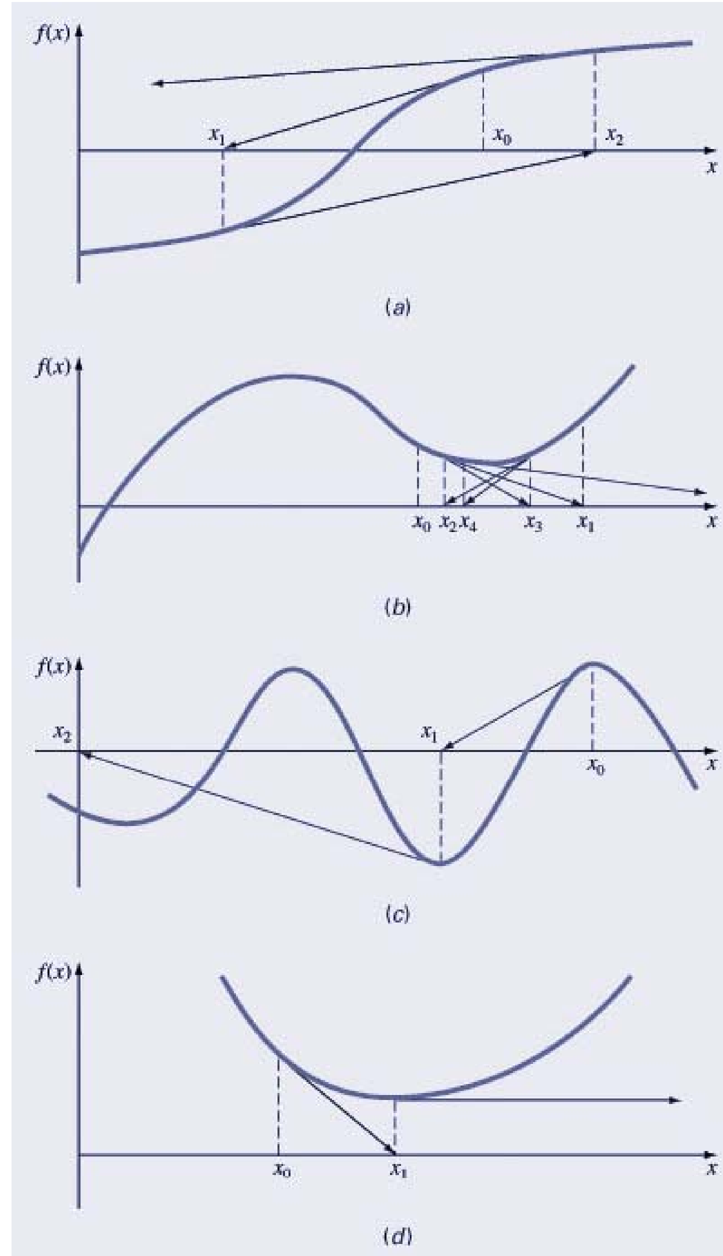


Pitfalls of Newton-Raphson Method

Inflection point at the vicinity of the root

Tendency to oscillate around a local maxima/minima

Encountering near zero slopes can the send the next guess far away from the root



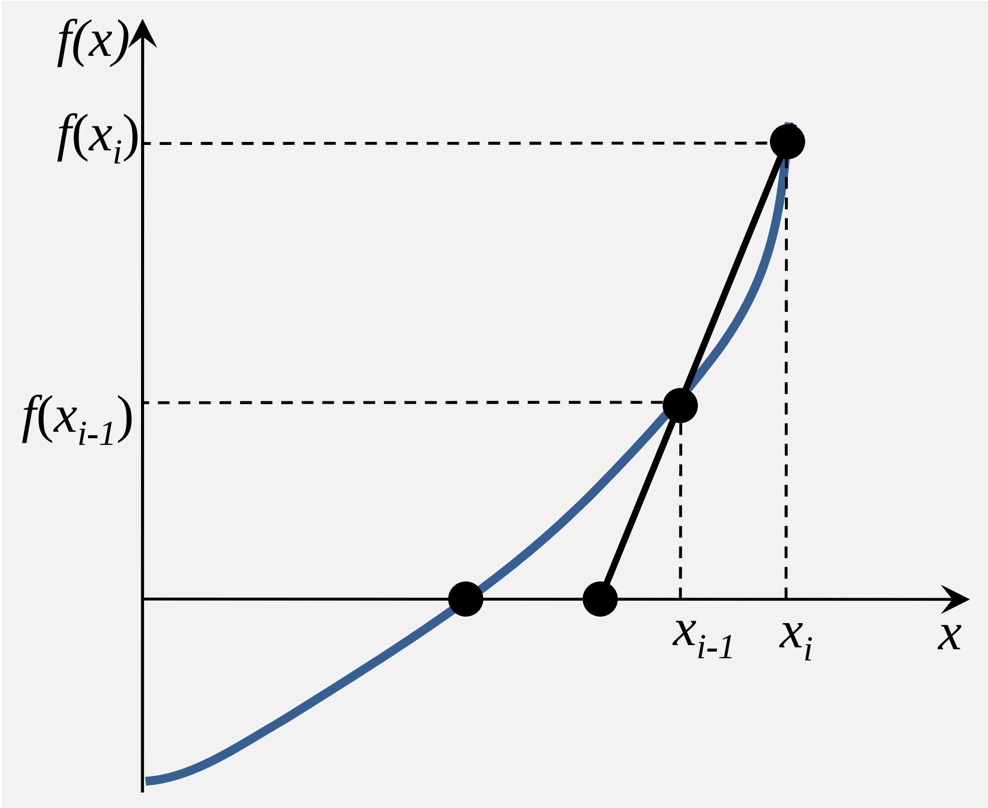
Secant Method

there are certain functions whose derivatives may be difficult or inconvenient to evaluate.

the derivative can be approximated by a <u>backward finite divided difference</u>:

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

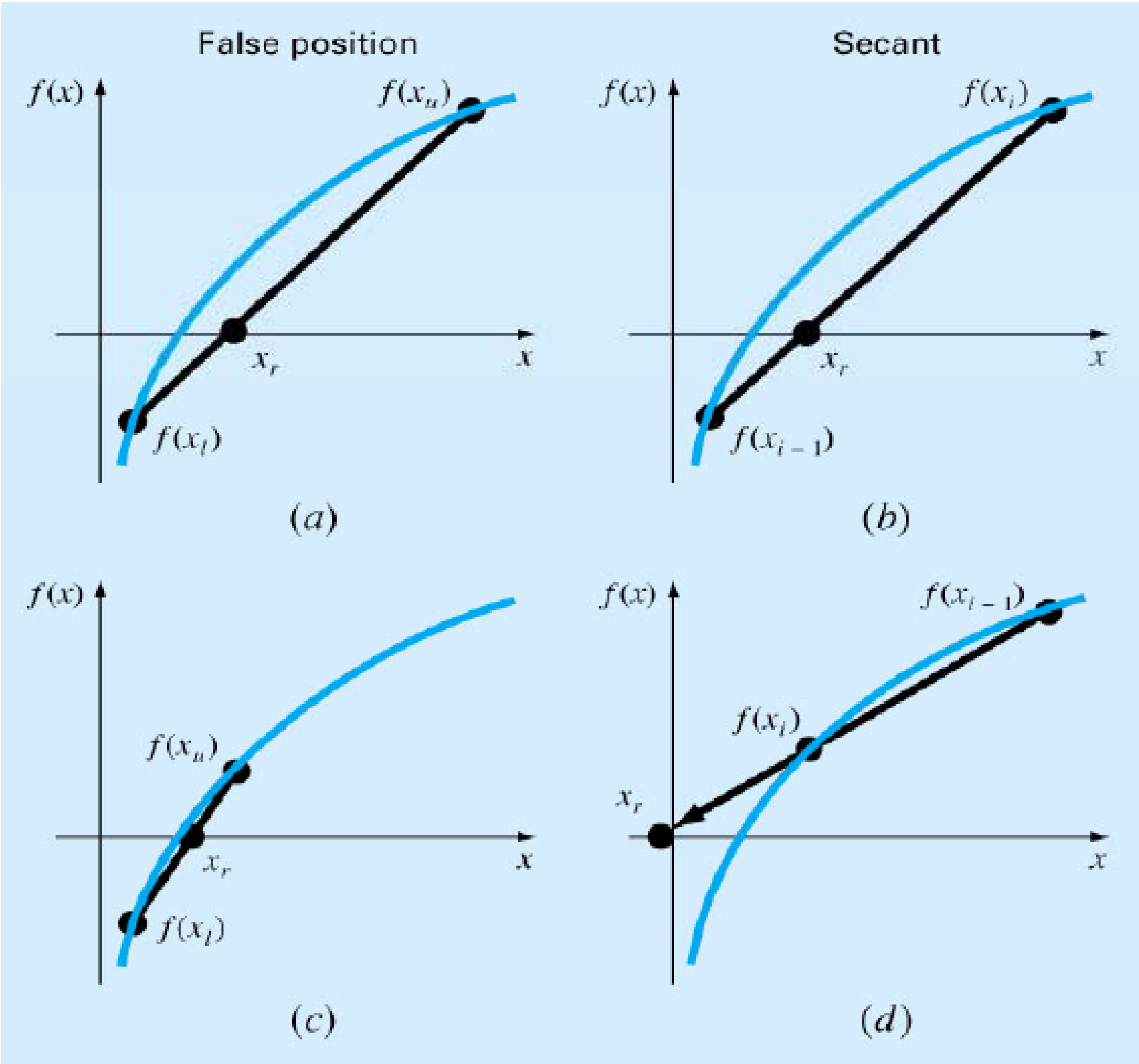
$$x_{i+1} = x_i - \frac{f(x_i)(x_{i-1} - x_i)}{f(x_{i-1}) - f(x_i)}$$



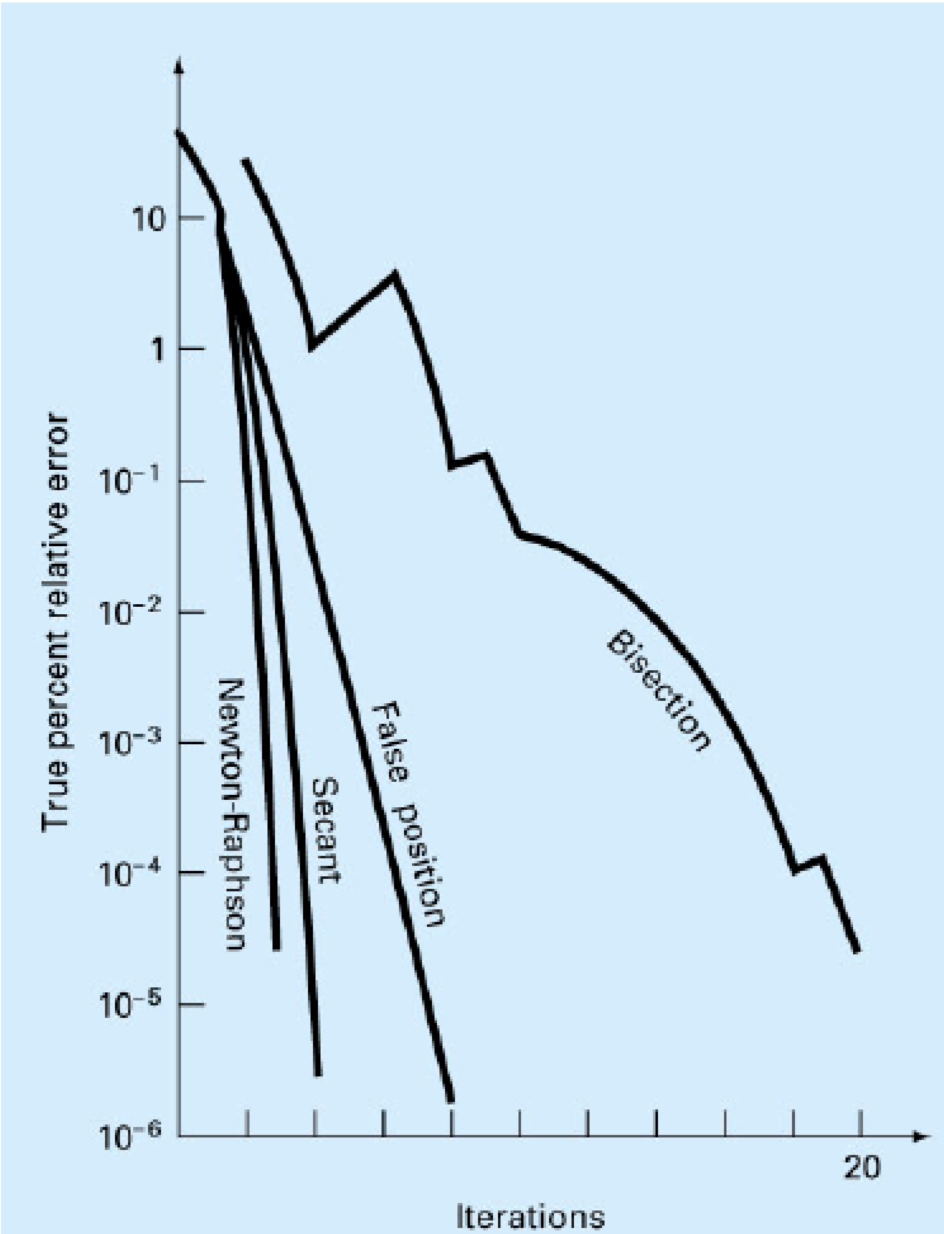
<u>Note:</u> Requires two initial guesses for *x*

Secant Method vs. Regula Falsi

Both of them uses two initial guesses to obtain the next estimate
The difference is in how the initial value is replaces by the new estimate.



Performance comparison



Newton-Raphson and Secant method, in general converges more rapidly

Comparison of the true percent relative errors to find the root of $f(x)=e^{-x}-x$

Multiple roots

Problems:

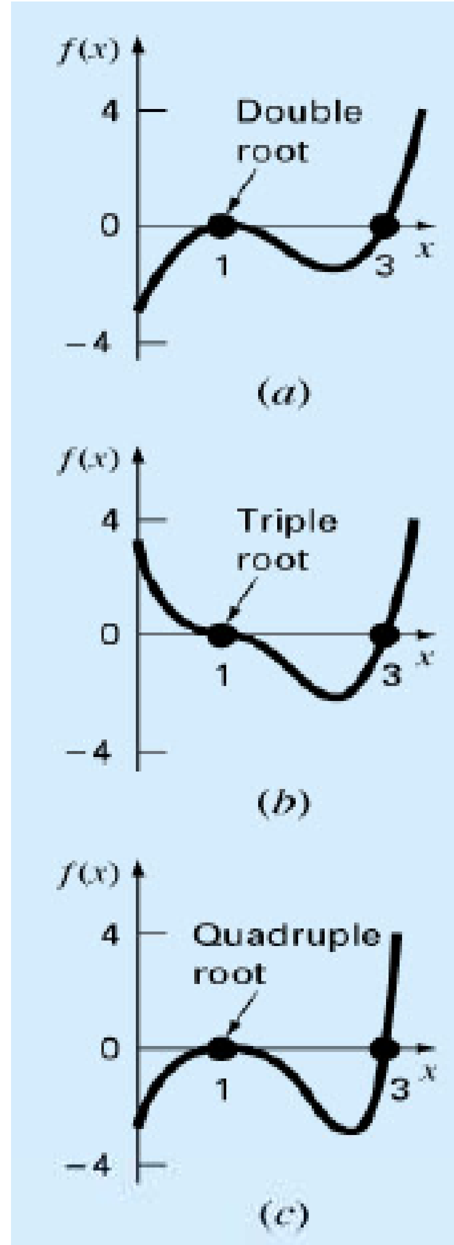
Function does not change sign at even roots

-can use only open methods

f'(x) goes to zero (at the root)

- division by zero!!

None of the methods can deal with multiple roots efficiently.



Modifications to Newton Raphson

Replace *f(x)* with *u(x)* in Newton-Raphson formula, where

$$u(x) = \frac{f(x_i)}{f'(x_i)}$$

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

$$u'(x) = \frac{f'(x_i)f'(x_i) - f(x_i)f''(x_i)}{[f'(x_i)]^2}$$

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

Roots of Polynomials

$$f_n(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$$

General Rules:

- For an nth order equation, there are n real or complex roots.
- If n is odd, there is at least one real root.
- If complex root exist in conjugate pairs (that is, λ+μi and λ-μi), where i=sqrt(-1).

Roots of Polynomials: conventional methods

$$f_n(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$$

The efficacy of bracketing and open methods depends on whether the problem being solved involves complex roots. **If only real roots exist, these methods could be used.**

– Finding good initial guesses complicates conventional methods
- open methods could be susceptible to divergence.

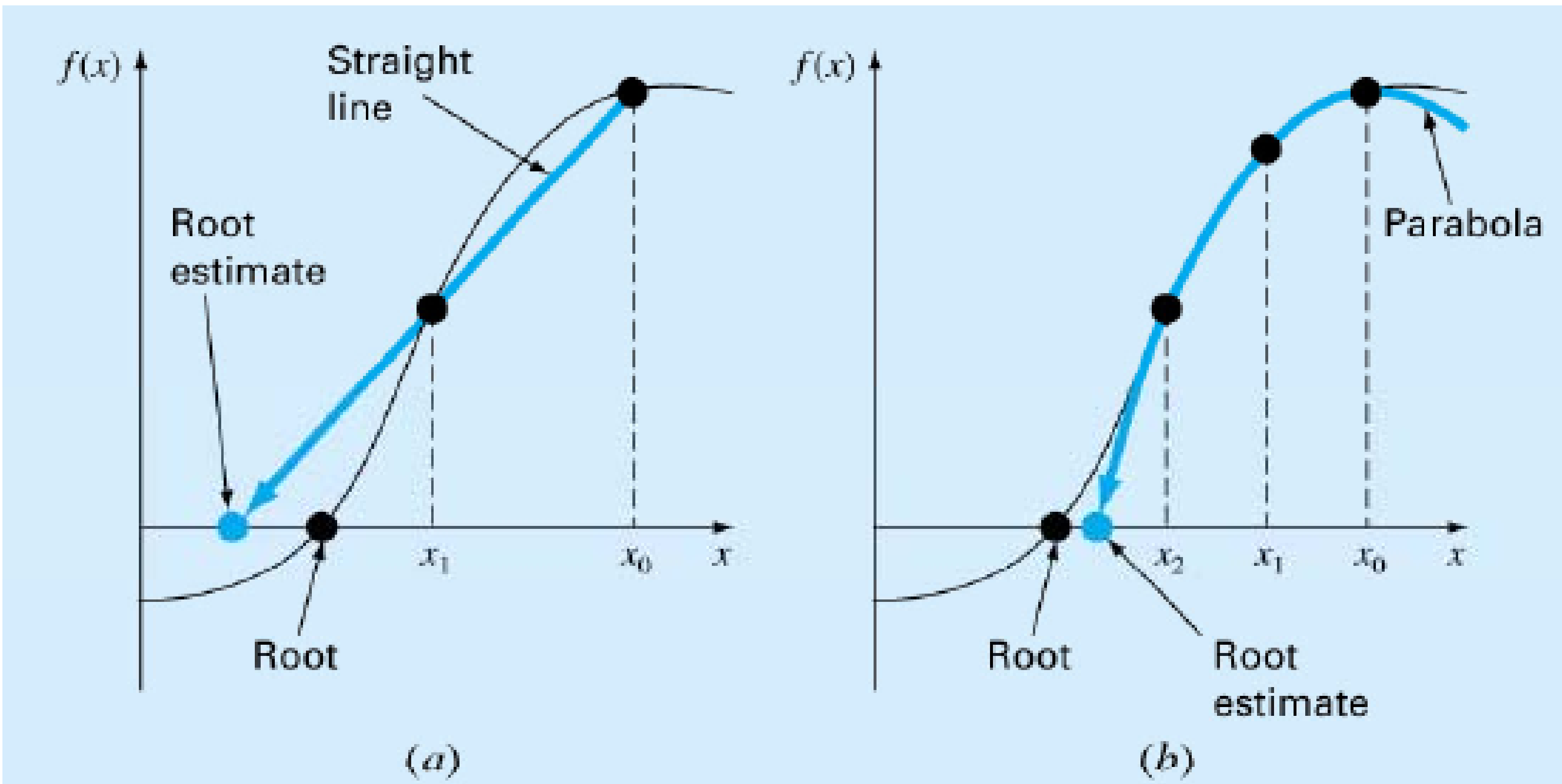
Special methods have been developed to find the real and complex roots of polynomials

–Müller and Bairstow methods.

Müller’s Method

Müller’s method obtains a root estimate by projecting a parabola to the x axis through three function values.

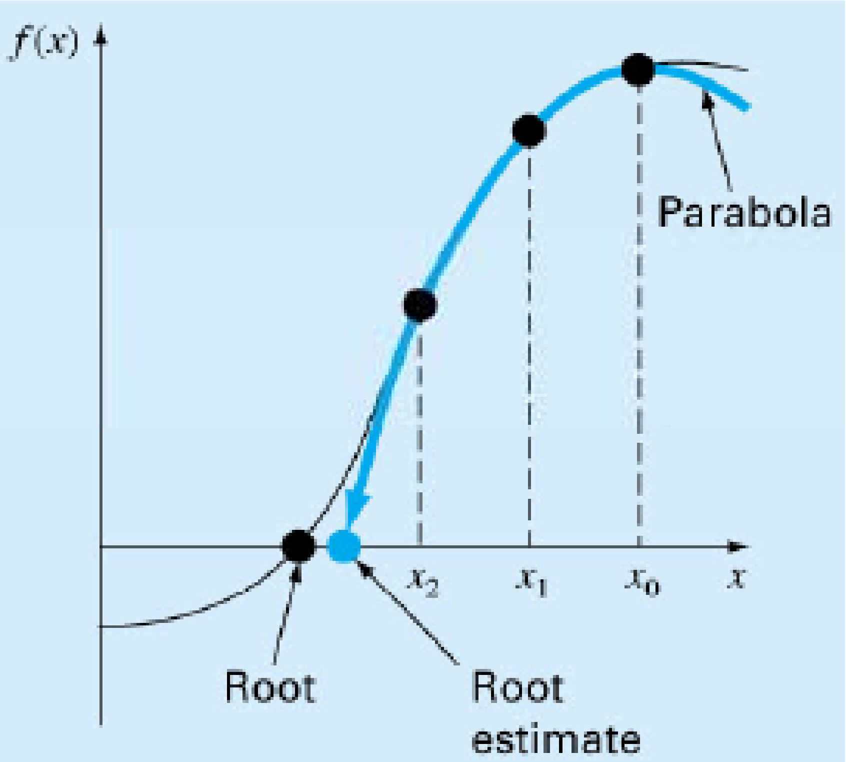
- Note the similarity with the Secant method



Müller's Method: steps

1. The parabolic equation in convenient form

$$f_2(x) = a(x - x_2)^2 + b(x - x_2) + c$$



2. Evaluate a, b, c by making the parabola intersect [x_0, $f(x_0)$], [x_1, $f(x_1)$] and [x_2, $f(x_2)$],

$$f(x_o) = a(x_o - x_2)^2 + b(x_o - x_2) + c$$
$$f(x_1) = a(x_1 - x_2)^2 + b(x_1 - x_2) + c$$
$$f(x_2) = a(x_2 - x_2)^2 + b(x_2 - x_2) + c$$

$$f(x_o) - f(x_2) = a(x_o - x_2)^2 + b(x_o - x_2)$$
$$f(x_1) - f(x_2) = a(x_1 - x_2)^2 + b(x_1 - x_2)$$

Müller's Method: steps

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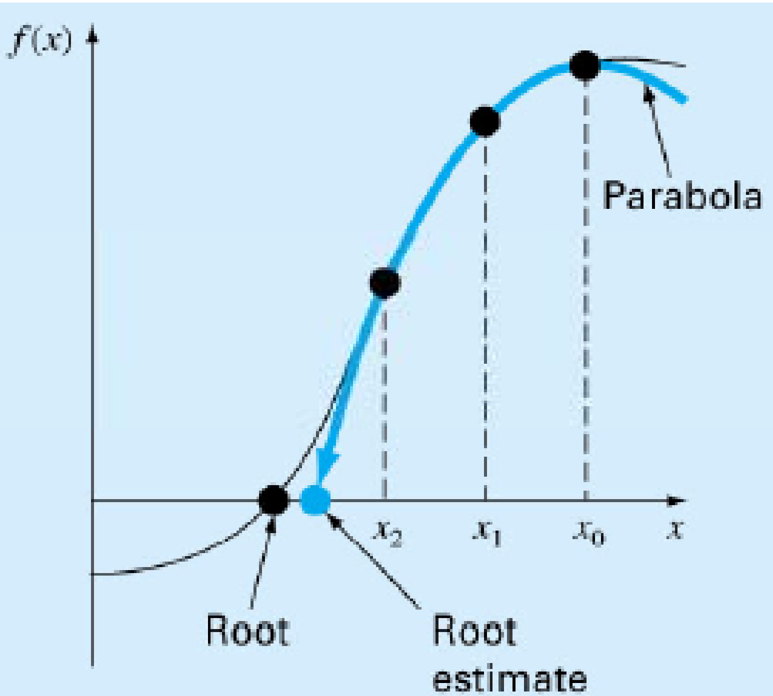

$$f(x_o) - f(x_2) = a(x_o - x_2)^2 + b(x_o - x_2)$$
$$f(x_1) - f(x_2) = a(x_1 - x_2)^2 + b(x_1 - x_2)$$

$$c = f(x_2)$$

If

$$h_o = x_1 - x_o \qquad h_1 = x_2 - x_1$$

$$\delta_o = \frac{f(x_1) - f(x_o)}{x_1 - x_o} \qquad \delta_1 = \frac{f(x_2) - f(x_1)}{x_2 - x_1}$$

$$a = \frac{\delta_1 - \delta_o}{h_1 + h_o} \qquad b = ah_1 + \delta_1 \qquad c = f(x_2)$$

Müller's Method: steps

3. Obtain the new estimate x_3 by using the quadratic formula

$$x_3 = x_2 + \frac{-2c}{b \pm \sqrt{b^2 - 4ac}}$$

4. Choose x_3 which gives the value closest to x_2

5. Repeat the process using the following guidelines:

- If only real roots are being located, choose the two original points that are nearest to the new root estimate, x_3.
- If both real and complex roots are estimated, employ a sequential approach just like in secant method, x_1, x_2 *and* x_3 *to replace* x_0, x_1 *and* x_2.