# 2.29 Numerical Fluid Mechanics
# Spring 2015 – **Lecture 4**

## Review Lecture 3

- Truncation Errors, Taylor Series and Error Analysis
  - Taylor series: $f(x_{i+1}) = f(x_i) + \Delta x\, f'(x_i) + \frac{\Delta x^2}{2!} f''(x_i) + \frac{\Delta x^3}{3!} f'''(x_i) + \ldots + \frac{\Delta x^n}{n!} f^n(x_i) + R_n$

    $$R_n = \frac{\Delta x^{n+1}}{n+1!} f^{(n+1)}(\xi)$$
  - Use of Taylor series to derive finite difference schemes (first-order Euler scheme with forward, backward and centered differences)
  - General error propagation formulas and error estimation, with examples

    Consider $y = f(x_1, x_2, x_3, \ldots, x_n)$. If $\varepsilon_i$'s are magnitudes of errors on $x_i$'s, what is the error on $y$?
    - The Differential Formula: $\varepsilon_y \le \sum_{i=1}^{n} \left| \frac{\partial f(x_1, \ldots, x_n)}{\partial x_i} \right| \varepsilon_i$
    - The Standard Error (statistical formula): $E(\Delta_s y) \simeq \sqrt{\sum_{i=1}^{n} \left( \frac{\partial f}{\partial x_i} \right)^2 \varepsilon_i^2}$
  - Error cancellation (e.g. subtraction of errors of the same sign)
  - Condition number: $K_p = \frac{\bar{x}\, f'(\bar{x})}{f(\bar{x})}$
    - Well-conditioned problems vs. well-conditioned algorithms
    - Numerical stability

Reference: Chapra and Canale, Chapters 3 and 4

# 2.29 Numerical Fluid Mechanics
# Spring 2015 – **Lecture 4**

Reference: Chapra and Canale, Chapters 5 and 6

## REVIEW Lecture 3, Cont'd

- Roots of nonlinear equations $f(x) = 0$
  - Bracketing Methods:
    - Systematically reduce width of bracket, track error for convergence: $|\varepsilon_a| = \left| \frac{\hat{x}_r^n - \hat{x}_r^{n+1}}{\hat{x}_r^n} \right| \leq \varepsilon_s$
    - **Bisection:** Successive division of bracket in half
      - determine next interval based on sign of: $f(x_1^{n+1}) f(x_{\text{mid-point}}^{n+1})$
      - Number of Iterations: $n = \log_2 \left( \frac{\Delta x^0}{E_{a,d}} \right)$
    - **False-Position (Regula Falsi):** As Bisection, excepted that next $x_r$ is the "linearized zero", i.e. approximate f(x) with straight line using its values at end points, and find its zero:

$$x_r = x_U - \frac{f(x_U)\,(x_L - x_U)}{f(x_L) - f(x_U)}$$

  - "Open" Methods:
    - Systematic "Trial and Error" schemes, don't require a bracket $g(x) = x + c\,f(x)$
    - Computationally efficient, don't always converge
    - **Fixed Point Iteration (General Method or Picard Iteration):**

$$x_{n+1} = g(x_n) \quad \text{or}$$
$$x_{n+1} = x_n - h(x_n) f(x_n)$$

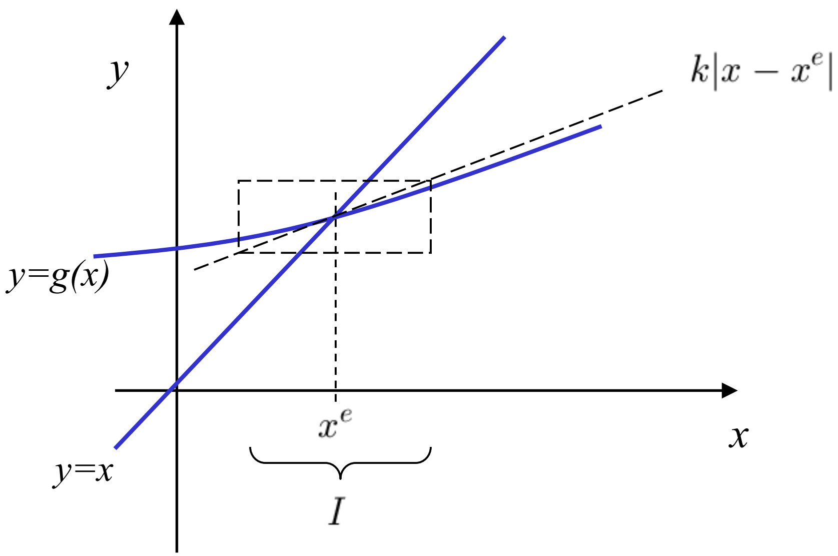
# Numerical Fluid Mechanics: **Lecture 4 Outline**

Reference: Chapra and Canale, Chapters 5 and 6

- Roots of nonlinear equations
  - Bracketing Methods
    - Example: Heron's formula
    - Bisection
    - False Position
  - "Open" Methods
    - Fixed-point Iteration (General method or Picard Iteration)
      - Examples
      - Convergence Criteria
      - Order of Convergence
    - Newton-Raphson
      - Convergence speed and examples
    - Secant Method
      - Examples
      - Convergence and efficiency
    - Extension of Newton-Raphson to systems of nonlinear equations
  - Roots of Polynomial (all real/complex roots)
    - Open methods (applications of the above for complex numbers)
    - Special Methods (e.g. Muller's and Bairstow's methods)
- Systems of Linear Equations

# Open Methods (**Fixed Point Iteration**)

# Convergence Theorem




**Hypothesis:**

*g(x)* satisifies the following Lipschitz condition:

There exist a $k$ such that if

$$x \in I$$

then

$$|g(x) - g(x^e)| = |g(x) - x^e| \leq k|x - x^e|$$

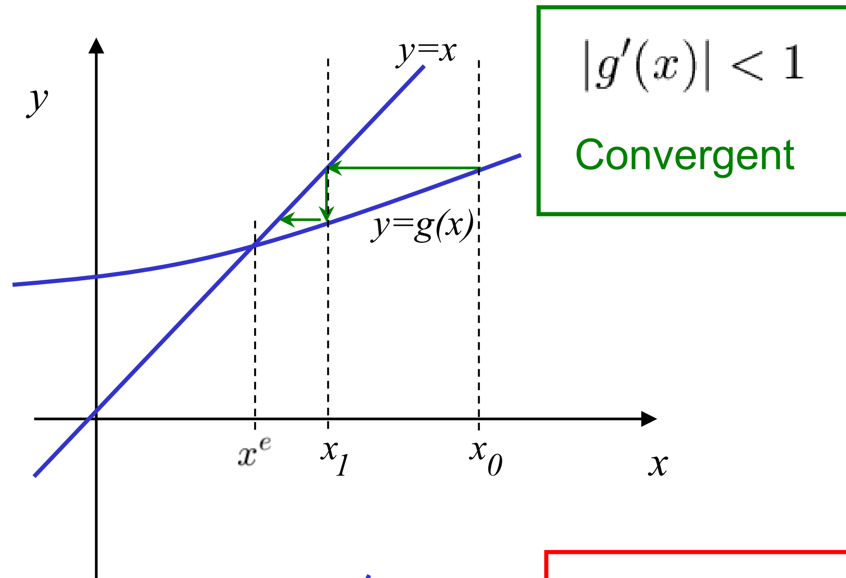
Then, one obtains the following Convergence Criterion: $x_{n-1} \in I \Rightarrow |x_n - x^e| = |g(x_{n-1}) - x^e| \leq k|x_{n-1} - x^e|$

Applying this inequality successively to $x_{n-1}$, $x_{n-2}$, etc: $|x_n - x^e| \leq k^n|x_0 - x^e|$

Convergence
$x_0 \in I, \quad k < 1$

# Open Methods (**Fixed Point Iteration)**

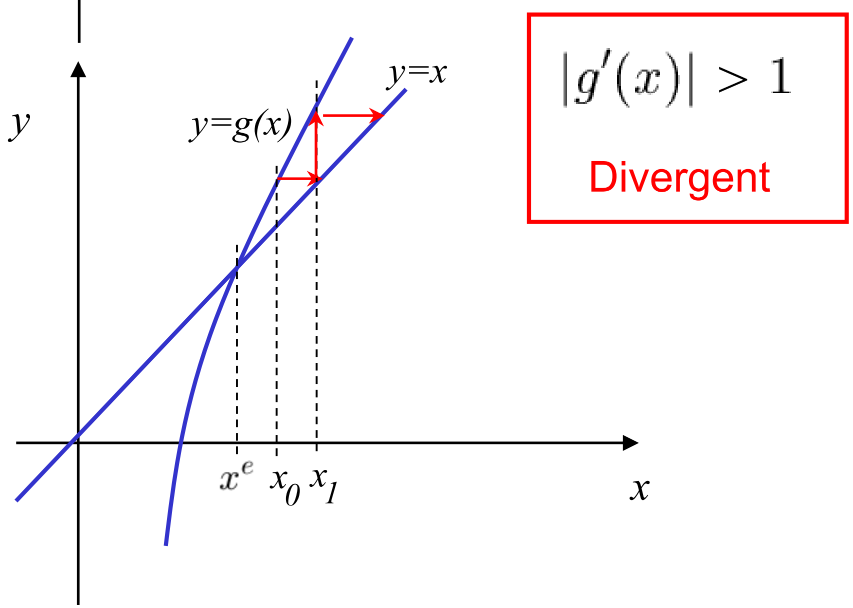
## Corollary Convergence Theorem




If the derivative of *g(x)* exists, then the Mean-value Theorem gives:

$$\{\exists \xi \in [x, x^e] \mid g(x) - g(x^e) = g'(\xi)(x - x^e)\}$$

$$\begin{cases} x < \xi < x^e \\ x^e < \xi < x \end{cases}$$




Hence, a Sufficient Condition for Convergence

If $|g'(x)|_{x \in I} \leq k < 1 \Rightarrow |g(x) - x^e| \leq k|x - x^e|$

# Open Methods (**Fixed Point Iteration**)

## Example: Cube root

$$x^3 - 2 = 0\ ,\quad x^e = 2^{1/3}$$

Rewrite

$$g(x) = x + C(x^3 - 2)$$

$$g'(x) = 3Cx^2 + 1$$

Convergence, for example in the 0<x<2 interval?

$$|g'(x)| < 1 \quad \Leftrightarrow \quad -2 < 3Cx^2 < 0$$

$$\text{For } 0 < x < 2 \Rightarrow \boxed{-1/6 < C < 0}$$

$$C = -\frac{1}{6} \Rightarrow x_{n+1} = g(x_n) = x_n - \frac{1}{6}(x_n^3 - 2)$$

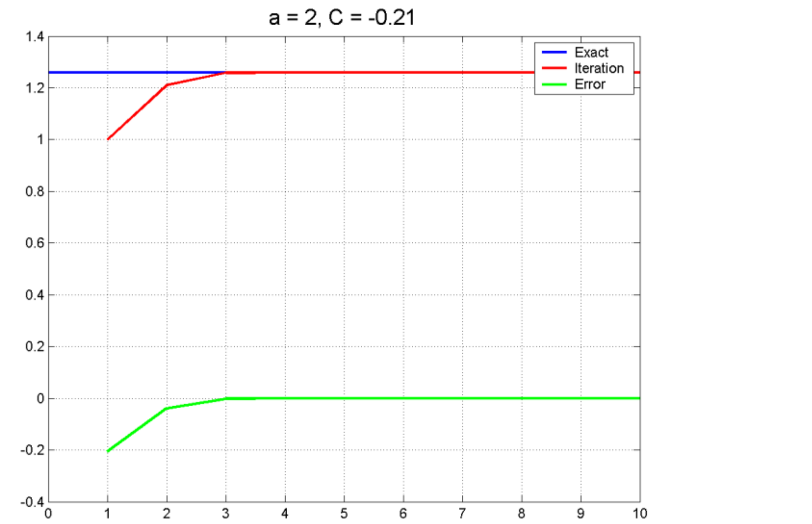
Converges more rapidly for small $|g'(x)|$

$$g'(1.26) = 3C \cdot 1.26^2 + 1 = 0 \Leftrightarrow \boxed{C = -0.21}$$

Ps: this means starting in smaller interval than 0<*x*<2 (smaller *x*'s)

cube.m

```
n=10;
g=1.0;
C=-0.21;
     sq(1)=g;
     for i=2:n
      sq(i)= sq(i-1) + C*(sq(i-1)^3 -a);
     end
     hold off
     f=plot([0 n],[a^(1./3.) a^(1./3.)],'b')
     set(f,'LineWidth',2);
     hold on
     f=plot(sq,'r')
     set(f,'LineWidth',2);
     f=plot( (sq-a^(1./3.))/(a^(1./3.)),'g')
     set(f,'LineWidth',2);
     legend('Exact','Iteration','Error');
     f=title(['a = ' num2str(a) ', C = ' num2str(C)])
     set(f,'FontSize',16);
     grid on
```



# Open Methods (**Fixed Point Iteration)**

## Converging, but how close: What is the error of the estimate?

Consider the Absolute error:

$$
\begin{aligned}
|x_{n-1} - x^e| &\leq |x_{n-1} - x_n| + |x_n - x^e| \\
&= |x_{n-1} - x_n| + |g(x_{n-1}) - g(x^e)| \\
&= |x_{n-1} - x_n| + |g'(\xi)||x_{n-1} - x^e| \\
&\leq |x_{n-1} - x_n| + k|x_{n-1} - x^e| \\
&\Rightarrow \\
|x_{n-1} - x^e| &\leq \frac{1}{1-k}|x_{n-1} - x_n| \qquad (0 \leq k < 1)
\end{aligned}
$$

Hence, at iteration n: $|x_n - x^e| \leq k|x_{n-1} - x^e| \leq \frac{k}{1-k}|x_{n-1} - x_n|$

**Fixed-Point Iteration Summary**

$$x_{n+1} = g(x_n)$$

Absolute error: $|x_n - x^e| \leq \frac{k}{1-k}|x_{n-1} - x_n|$

Convergence condition: $|g'(x)| \leq k < 1 \,, \quad x \in I$

Note: Total compounded error due to round-off is bounded by

$$\varepsilon_{r-o} / (1-k)$$

# Order of Convergence for an Iterative Method

- The speed of convergence for an iterative method is often characterized by the so-called **Order of Convergence**
- Consider a series $x_0, x_1, \ldots$ and the error $e_n = x_n - x^e$. If there exist a number $p$ and a constant $C \neq 0$ such that

$$\lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|^p} = C$$

  then $p$ is defined as the Order of Convergence or the Convergence exponent and $C$ as the asymptotic constant
  - $p=1$ linear convergence,
  - $p=2$ quadratic convergence,
  - $p=3$ cubic convergence, etc
- Note: Error estimates can be utilized to accelerate the scheme (Aitken's extrapolation, of order $2p$-$1$, if the fixed-point iteration is of order $p$)
- Fixed-Point: often linear convergence, $e_{n+1} = g'(\xi)\, e_n$
- "Order of accuracy" used for truncation err. (leads to convergence if stable)

# “Open” Iterative Methods: Newton-Raphson

- So far, the iterative schemes to solve $f(x)=0$ can all be written as

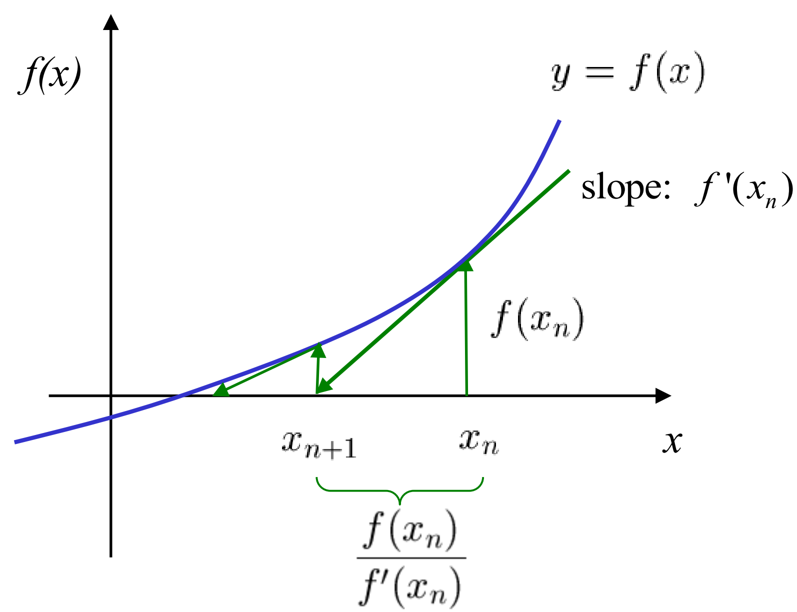
$$x_{n+1} = g(x_n) = x_n - h(x_n) f(x_n)$$

- Newton-Raphson: one of the most widely used scheme
- Extend the tangent from current guess $x_n$ to find point where $x$ axis is crossed:

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

or truncated Taylor-series:

$$f(x_{n+1}) = f(x_n) + f'(x_n)(x_{n+1} - x_n) = 0 \quad \Rightarrow$$



# Newton-Raphson Method:
## Its derivation based on local derivative and “fast” rate of convergence

Non-linear Equation

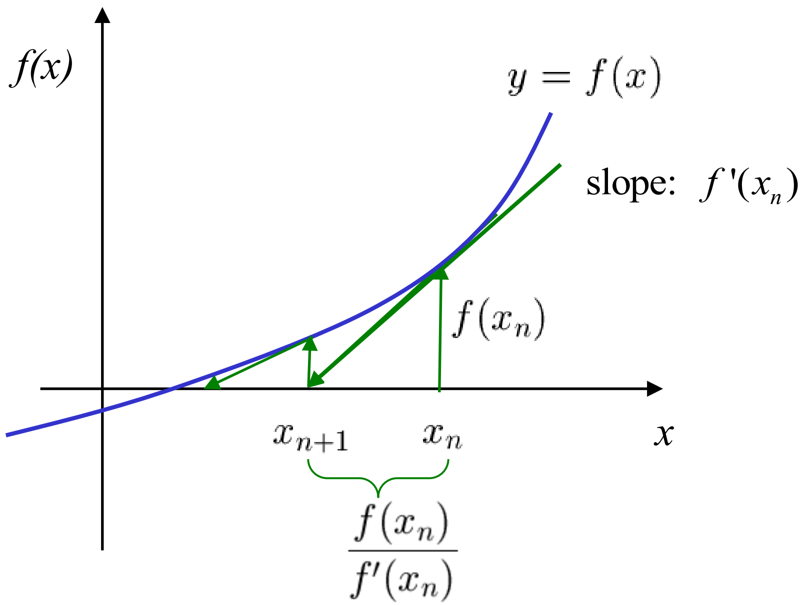
$$f(x) = 0 \Leftrightarrow x = g(x)$$

Convergence Crit., use Lipschitz condition & $x_n = g(x_{n-1})$

$$|g'(x_n)| < k < 1 \Rightarrow |x_n - x^e| \leq k|x_{n-1} - x^e|$$

Fast Convergence

$$|g'(x^e)| = 0$$




$$g(x) = x + h(x)f(x)\ , \quad h(x) \neq 0$$

$$\begin{aligned} g'(x^e) &= 1 + h(x^e)f'(x^e) + h'(x^e)f(x^e) \\ &= 1 + h(x^e)f'(x^e) \end{aligned}$$

$$g'(x^e) = 0 \Leftarrow h(x) = -\frac{1}{f'(x)}$$

**Newton-Raphson Iteration**

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

# Newton-Raphson Method: Example

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

Example – Square Root

$$x = \sqrt{a} \Leftrightarrow f(x) = x^2 - a = 0$$

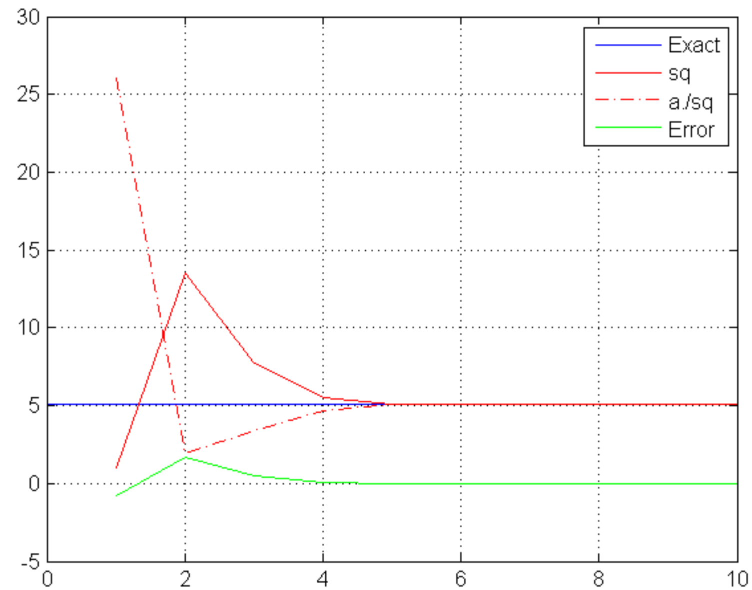
Newton-Raphson

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

Same as Heron's formula !

sqr.m

```
a=26;
n=10;
g=1;
     sq(1)=g;
     for i=2:n
      sq(i)= 0.5*(sq(i-1) + a/sq(i-1));
     end
     hold off
     plot([0 n],[sqrt(a) sqrt(a)],'b')
     hold on
     plot(sq,'r')
     plot(a./sq,'r-.')
     plot((sq-sqrt(a))/sqrt(a),'g')
     grid on
```



# Newton-Raphson Example: Its use for divisions

$$x = \frac{1}{a}$$

$$f(x) = ax - 1 = 0$$

$$f'(x) = a$$

$$\frac{f(x)}{f'(x)} = \frac{ax-1}{a} = x^e(ax-1) \simeq x(ax-1)$$

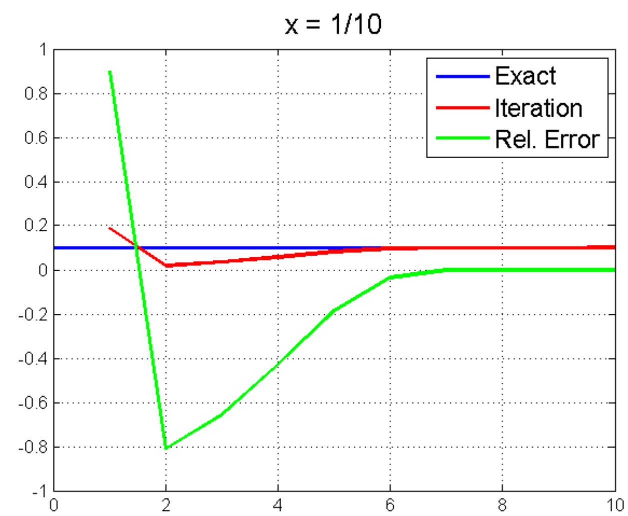
which is a good approximation if $\frac{|x - x^e|}{|x^e|} \ll 1$

Hence, Newton-Raphson for divisions:

$$x_{n+1} = x_n - x_n(ax_n - 1)$$

div.m

```
a=10;
n=10;
g=0.19;
sq(1)=g;
      for i=2:n
       sq(i)=sq(i-1) - sq(i-1)*(a*sq(i-1) -1) ;
      end
      hold off
      plot([0 n],[1/a 1/a],'b')
      hold on
      plot(sq,'r')
      plot((sq-1/a)*a,'g')
      grid on
      legend('Exact','Iteration','Rel Error');
      title(['x = 1/' num2str(a)])
```



# Newton-Raphson: Order of Convergence

Define: $\epsilon_n = x_n - x^e$

Taylor Expansion: $g(x_n) = g(x^e) + \epsilon_n g'(x^e) + \frac{1}{2}\epsilon_n^2 g''(x^e) \cdots$

Since $g'(x_e) = 0$, truncating third order terms and higher, leads to a second order expansion:

$$g(x_n) - g(x^e) \simeq \frac{1}{2}\epsilon_n^2 g''(x^e)$$

$$\Rightarrow$$

$$\epsilon_{n+1} = x_{n+1} - x_e \simeq \frac{1}{2}\epsilon_n^2 g''(x^e)$$

Quadratic Convergence

Relative Error: $$\frac{\epsilon_{n+1}}{|x^e|} \simeq \frac{1}{2}|x^e| g''(x^e) \left(\frac{\epsilon_n}{|x^e|}\right)^2 = A(x^e)\left(\frac{\epsilon_n}{|x^e|}\right)^2$$

$$\epsilon_{n+1} \simeq \epsilon_n^m A$$

Convergence Exponent/Order

Note: at $x_e$, one can evaluate $g''$ in terms of $f'$ and $f''$ using

$$g(x) = x - \frac{f}{f'} \quad , \quad g'(x) = \frac{f\, f''}{f'^2} \text{ and } g''(x) = \frac{f''}{f'} + \frac{f\, f'''}{f'^2} + f(\ldots)$$

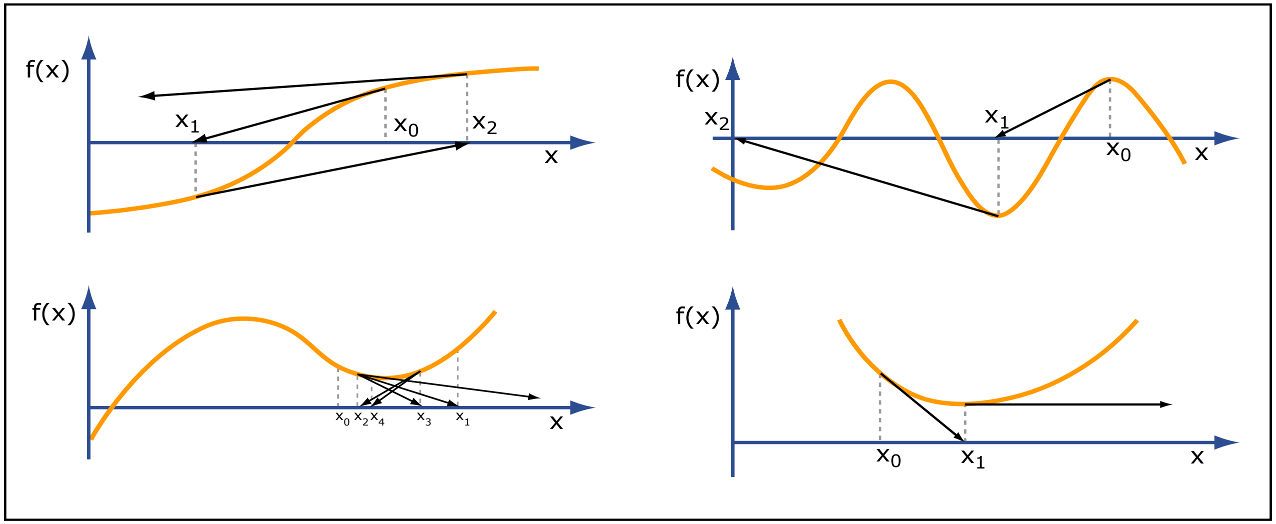
# Newton-Raphson: Issues

a) Inflection points in the vicinity of the root, i.e. $f''(x^e) = 0$

b) Iterations can oscillate around a local minima or maxima

c) Near-zero slope encountered

d) Zero slope at the root

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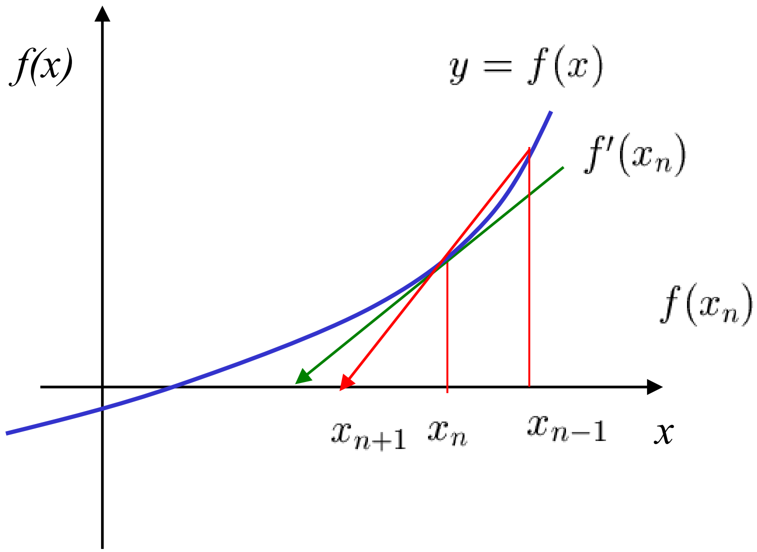
Four cases in which there is poor convergence with the Newton-Raphson method.

# Roots of Nonlinear Equations:
# Secant Method

1. In Newton-Raphson we have to evaluate 2 functions: $f(x_n),\ f'(x_n)$

2. $f(x_n)$ and $f'(x_n)$ may not be given in closed, analytical form: e.g. in CFD, even $f(x_n)$ is often a result of a numerical algorithm




Approximate Derivative:

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

Secant Method Iteration:

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

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

- Only 1 function call per iteration! : $f(x_n)$

- It is the open (iterative) version of False Position

# Secant Method: Order of convergence

Absolute Error $\epsilon_n = x_n - x^e$

$$\epsilon_{n+1} = x_{n+1} - x^e = \frac{f(x^e+\epsilon_n)(x^e+\epsilon_{n-1}) - f(x^e+\epsilon_{n-1})(x^e+\epsilon_n)}{f(x^e+\epsilon_n) - f(x^e+\epsilon_{n-1})} - x^e$$

Using Taylor Series, up to 2nd order

Absolute Error $\epsilon_{n+1} \simeq \frac{1}{2}\epsilon_{n-1}\epsilon_n \frac{f''(x^e)}{f'(x^e)}$

Relative Error $\frac{\epsilon_{n+1}}{|x^e|} \simeq \frac{\epsilon_{n-1}}{|x_e|}\frac{\epsilon_n}{|x_e|}\frac{f''(x^e)}{2f'(x^e)}x^e$

Convergence Order/Exponent

By definition:

$$\epsilon_n = A(x^e)\epsilon_{n-1}^m \Rightarrow \epsilon_{n-1} = \left(\frac{1}{A}\epsilon_n\right)^{1/m} = B(x^e)\epsilon_n^{1/m}$$

Then:

$$\epsilon_{n+1} = C(x^e)\epsilon_n\epsilon_{n-1} = D(x^e)\epsilon_n\epsilon_n^{1/m} = D(x^e)\epsilon_n^{1+1/m}$$

$$\Rightarrow \quad 1 + \frac{1}{m} = m \Leftrightarrow m = \frac{1}{2}(1+\sqrt{5}) \simeq 1.62$$

Error improvement for each function call

Secant Method $\epsilon_{n+1}^* \simeq \epsilon_n^{1.62}$

Newton-Raphson $\epsilon_{n+1}^* = \epsilon_n^{2}$

# Roots of Nonlinear Equations
# Multiple Roots

p-order Root

$$f(x) = (x - x^e)^p f_1(x)\ ,\ f_1(x^e) \neq 0$$

Newton-Raphson

$$x_{n+1} = g(x_n) = x_n - \frac{(x_n - x^e)^p f_1(x_n)}{p(x_n - x^e)^{p-1} f_1(x_n) + (x_n - x^e)^p f'(x_n)}$$

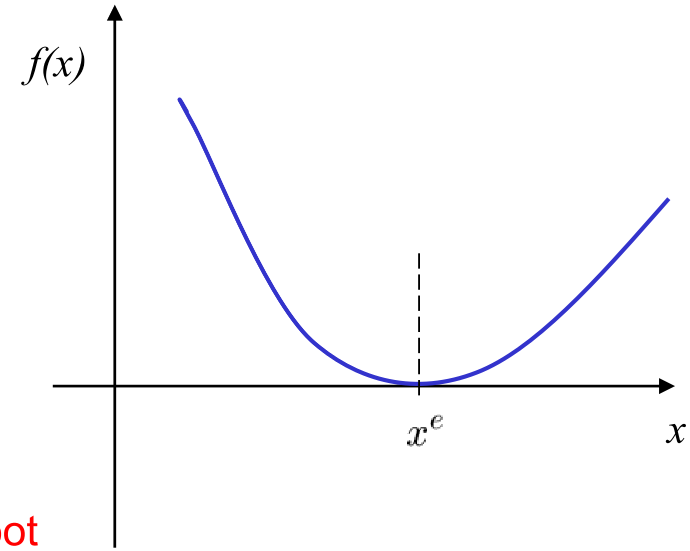
=>

$$x_{n+1} = x_n - \frac{(x_n - x^e) f_1(x_n)}{p f_1(x_n) + (x_n - x^e) f'(x_n)}$$

Convergence

$$|x_{n+1} - x^e| \leq k|x_n - x^e| \simeq |g'(x^e)|\ |x_n - x^e|$$

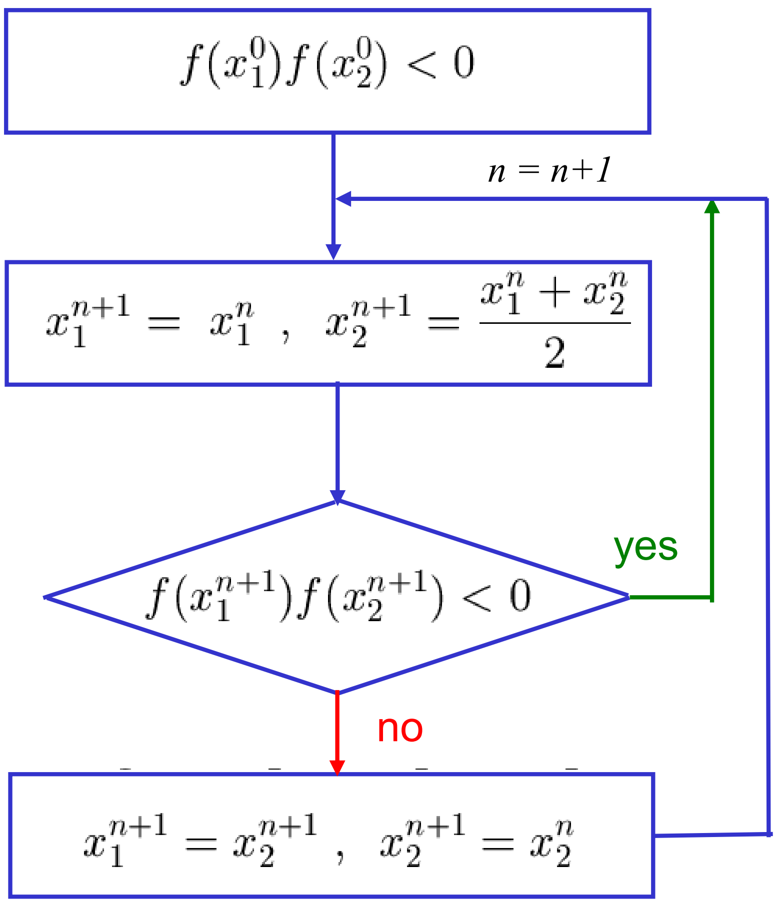
$$g'(x^e) = 1 - \frac{1}{p}$$

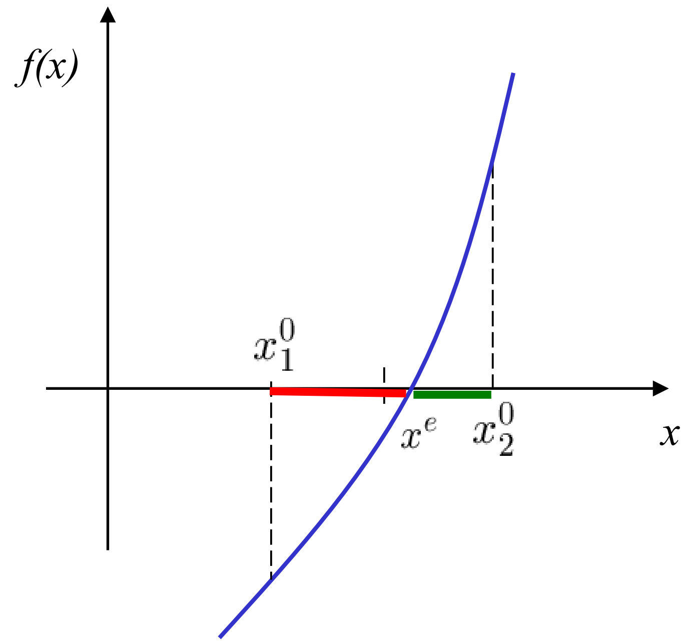



Slower convergence the higher the order of the root

# Roots of Nonlinear Equations
# Bisection

Algorithm




Less efficient than Newton-Raphson and Secant methods, but often used to isolate interval with root and obtain approximate value. Then followed by N-R or Secant method for accurate root.

Table removed due to copyright restrictions. Useful reference tables for this material: Tables PT2.3 on p.212 and PT2.4 on p. 214 in Chapra, S., and R. Canale. *Numerical Methods for Engineers*. 6th ed. McGraw-Hill Higher Education, 2009. ISBN: 9780073401065.

Chapra and Canale, ed. 7th,
pg 226

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# Systems of Linear Equations

- **Motivation and Plans**
- **Direct Methods for solving Linear Equation Systems**
  - Cramer's Rule (and other methods for a small number of equations)
  - Gaussian Elimination
  - Numerical implementation
    - Numerical stability
      - Partial Pivoting
      - Equilibration
      - Full Pivoting
    - Multiple right hand sides, Computation count
    - LU factorization
    - Error Analysis for Linear Systems
      - Condition Number
    - Special Matrices: Tri-diagonal systems
- **Iterative Methods**
  - Jacobi's method
  - Gauss-Seidel iteration
  - Convergence

# Motivations and Plans

- Fundamental equations in engineering are conservation laws (mass, momentum, energy, mass ratios/concentrations, etc)
  - Can be written as " *System Behavior (state variables) = forcing* "
- Result of the discretized (volume or differential form) of the Navier-Stokes equations (or most other differential equations):
  - System of (mostly coupled) algebraic equations which are linear or nonlinear, depending on the nature of the continuous equations
  - Often, resulting matrices are sparse (e.g. banded and/or block matrices)
- Lectures 3 and earlier today:
  - Methods for solving $f(x)=0$ or $\mathbf{f}(\mathbf{x})=\mathbf{0}$
  - Can be used for systems of equations: $\mathbf{f}(\mathbf{x})=\mathbf{b}$, i.e: $\mathbf{f} = \left( f_1(\mathbf{x}), f_2(\mathbf{x}), ..., f_n(\mathbf{x}) \right) = \mathbf{b}$
- Here we first deal with solving Linear Algebraic equations:

$$\mathbf{A}\,\mathbf{x} = \mathbf{b} \quad \text{or} \quad \mathbf{A}\,\mathbf{X} = \mathbf{B}$$

# Motivations and Plans

- Above 75% of engineering/scientific problems involve solving linear systems of equations
  - As soon as methods were used on computers => dramatic advances
- Main Goal: Learn methods to solve systems of linear algebraic equations and apply them to CFD applications

- Reading Assignment
  - Part III and Chapter 9 of "Chapra and Canale, Numerical Methods for Engineers, 2010."
  - For Matrix background, see Chapra and Canale (ed. 7th. pg 233-244) and other linear algebra texts (e.g. Trefethen and Bau, 1997)
- Other References :
  - Any chapter on "Solving linear systems of equations" in CFD references provided.
  - For example: chapter 5 of "J. H. Ferziger and M. Peric, Computational Methods for Fluid Dynamics. Springer, NY, 3rd edition, 2002"

# Direct Numerical Methods
## for Linear Equation Systems

$$\mathbf{A}\,\mathbf{x} = \mathbf{b} \quad \text{or} \quad \mathbf{A}\,\mathbf{X} = \mathbf{B}$$

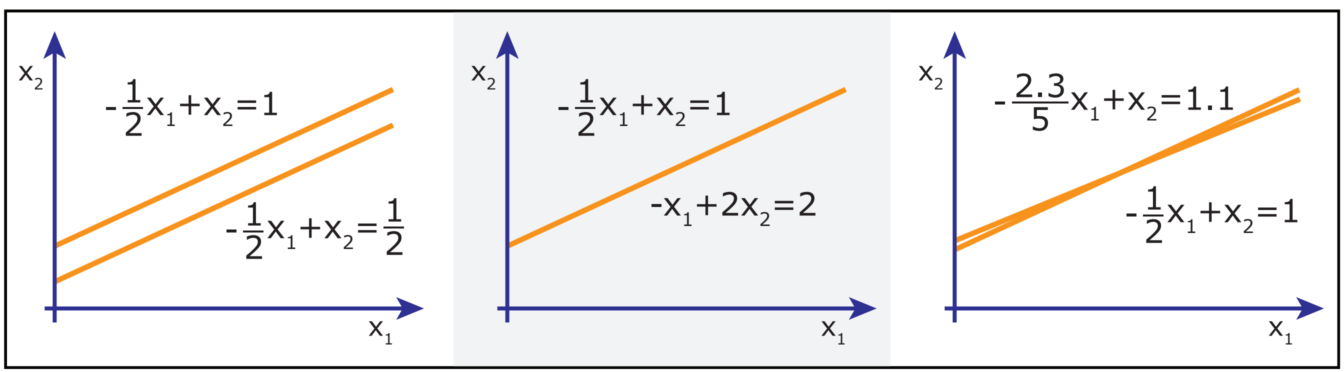
- Main Direct Method is: Gauss Elimination

  Key idea is simply to "combine equations so as to eliminate unknowns"

- First, let's consider systems with a small number of equations
  - Graphical Methods
    - Two equations (2 var.): intersection of 2 lines
    - Three equations (3 var.): intersection of 3 planes
    - Useful to illustrate issues:

      no solution or infinite solutions (singular) or ill-conditioned system

Fig 9.2 Chapra and Canale

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