2.29 Numerical Fluid Mechanics
Fall 2011 – 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 and 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 ε_i's are magnitudes of errors on x_i's, what is the error on y?
    - The Differential Formula: $\varepsilon_y \leq \sum_{i=1}^{n} \left| \frac{\partial f(x_1, \ldots, x_n)}{\partial x_i} \right| \varepsilon_i$
    - The Standard Error (statistical formula): $E(\Delta_s y) \approx \sqrt{\sum_{i=1}^{n} \left(\frac{\partial f}{\partial x_i} \right)^2 \varepsilon_i^{\,2}}$
  - 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, Chaps 3, 4 and 5

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REVIEW Lecture 3

- Roots of nonlinear equations
  - Bracketing Methods:
    - Systematically reduce width of bracket, track error for convergence: $|\varepsilon_a| = \left|\frac{\hat{x}_r^n - \hat{x}_r^{n+1}}{\hat{x}_r^n}\right| \le \varepsilon_s$
    - **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 function 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
    - Computationally efficient, don't always converge
    - **Fixed Point Iteration (General Method or Picard Iteration):**

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

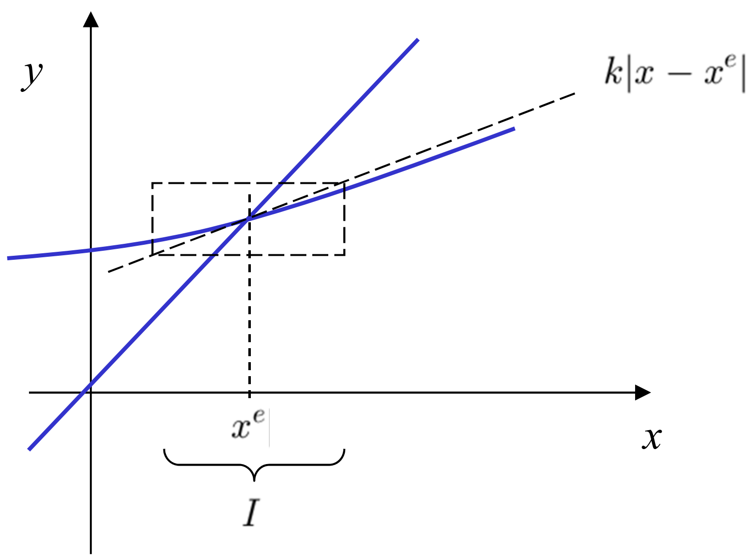
Numerical Fluid Mechanics: **Lecture 4 Outline**

Reference: Chapra and Canale, Chaps 3, 4 and 5

- Roots of nonlinear equations
  - Bracketing Methods
    - Example: Heron's formula
    - Bisection
    - False Position
  - "Open" Methods
    - Open-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)

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

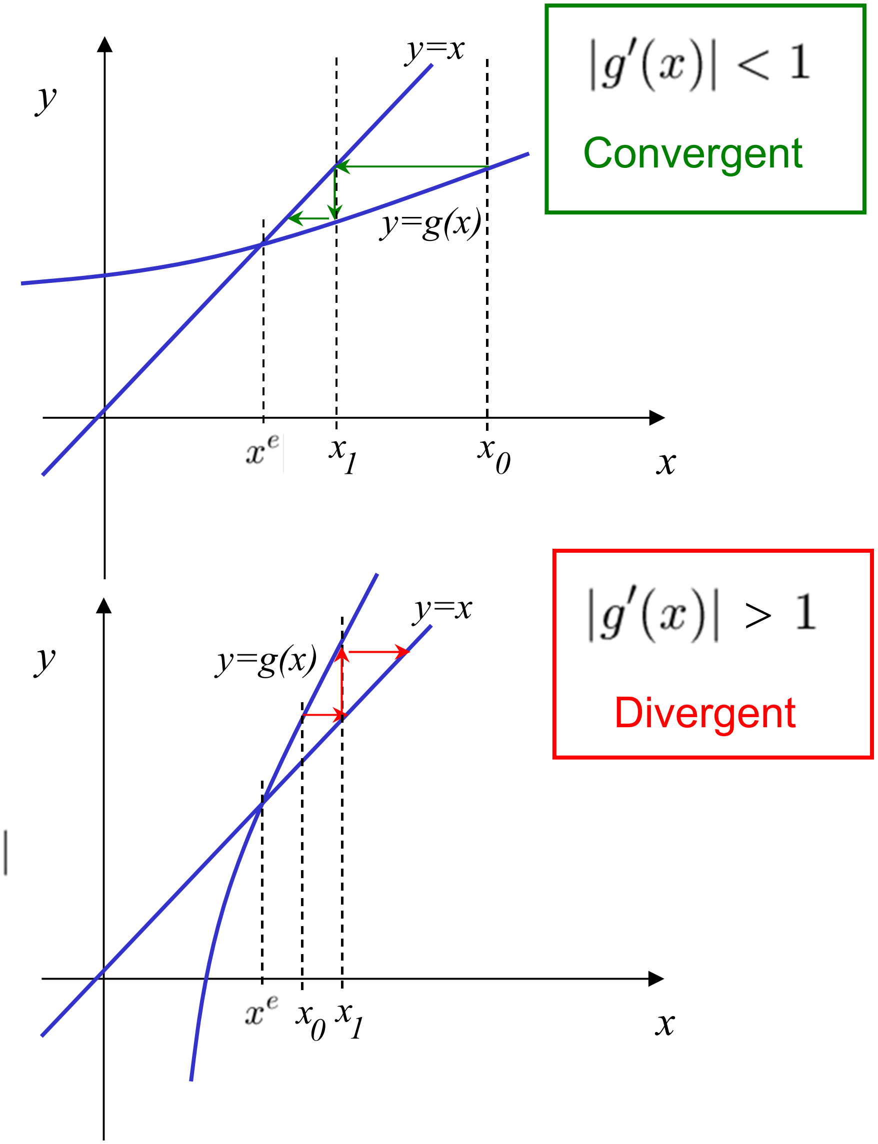
If the derivative of *g(x)* exists, then
the Mean-value Theorem gives:

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

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

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?

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

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

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

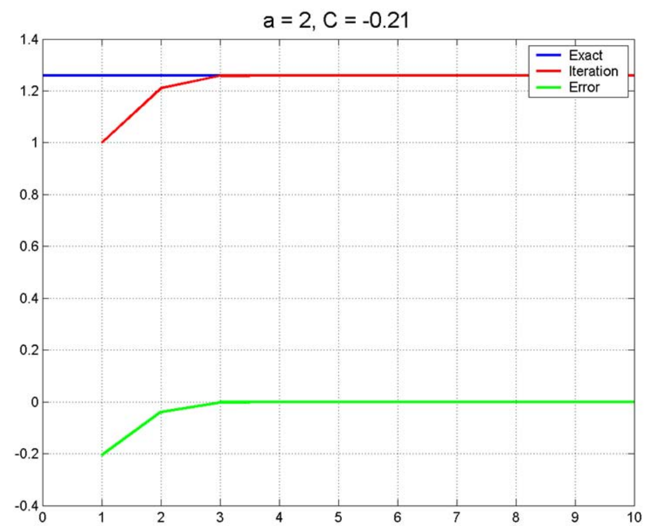
Converges more rapidly for small $|g'(x)|$

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

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:

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

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

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

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, $e_{n+1} = g'(\xi)\, e_n$

"Open" Iterative Methods: Newton-Raphson

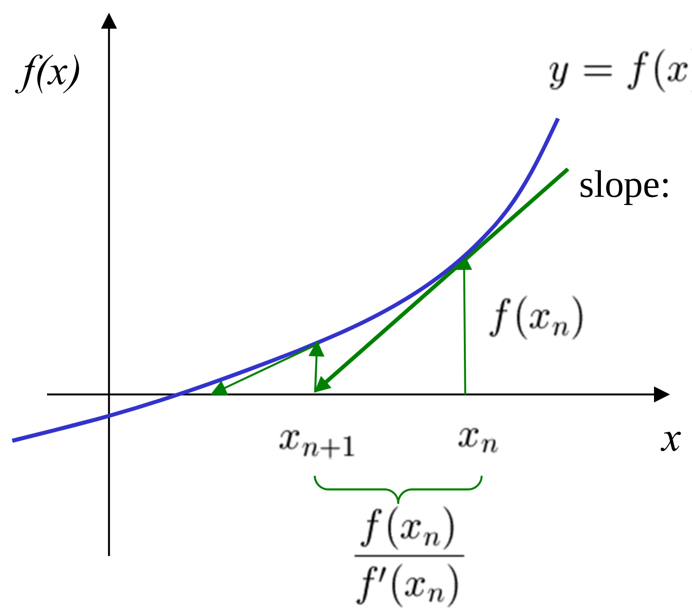
- So far, the iterative schemes to solve $f(x)=0$ can all be written as

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

- 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:

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

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



Newton-Raphson Method:
Its derivation based on the local derivative and the rate of convergence

Non-linear Equation

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

Convergence Criteria

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

Fast Convergence

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

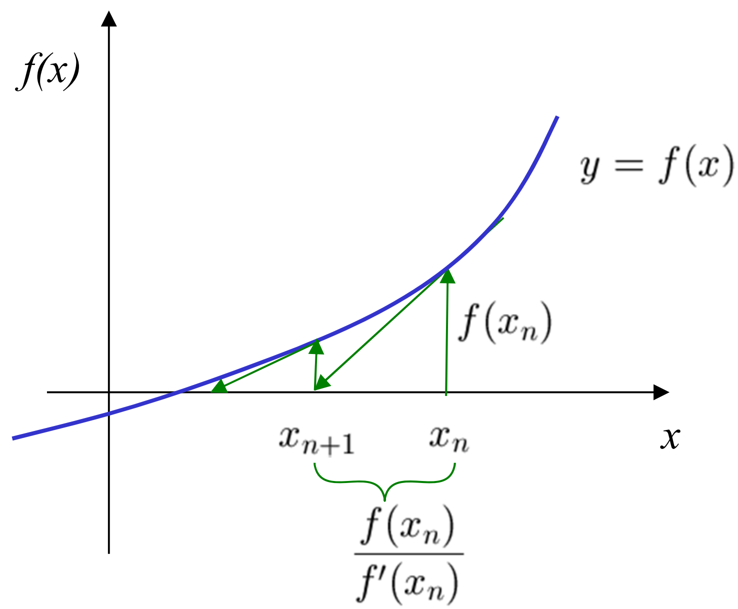
$$g(x) = x + h(x)f(x)\ , \quad h(x) \neq 0$$

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

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

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

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

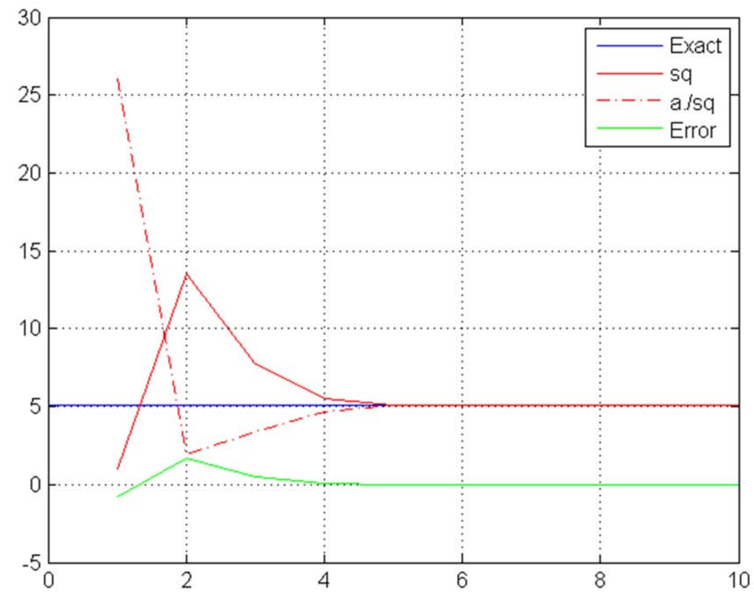
Newton-Raphson

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

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

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

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

$$f'(x) = a$$

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

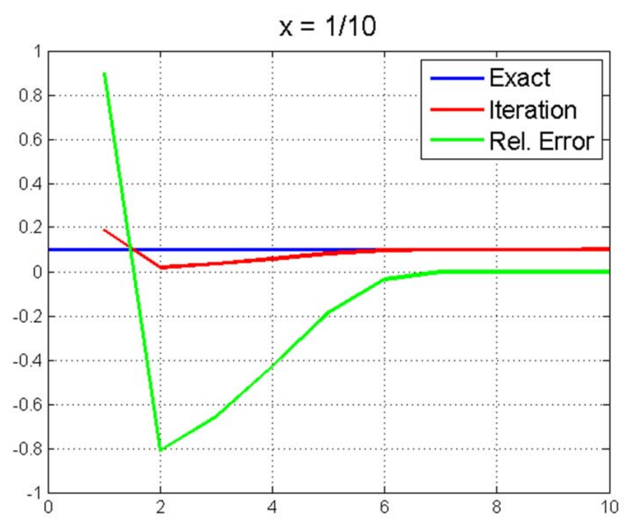
which is a good approximation if $\frac{|x - x^e|}{|x^e|} \ll 1$

Hence, Newton-Raphson for divisions:

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

```
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)])
```

div.m



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:

$$\begin{aligned} g(x_n) - g(x^e) &\simeq \frac{1}{2}\epsilon_n^2 g''(x^e) \\ &\Rightarrow \\ \epsilon_{n+1} = x_{n+1} - x_e &\simeq \frac{1}{2}\epsilon_n^2 g''(x^e) \end{aligned}$$

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: $g(x) = x - \frac{f}{f'}$, $g'(x) = \frac{f\,f''}{f'^2}$ and $g''(x) = \frac{f''}{f'} + \frac{f\,f'''}{f'^2} + f(...)$

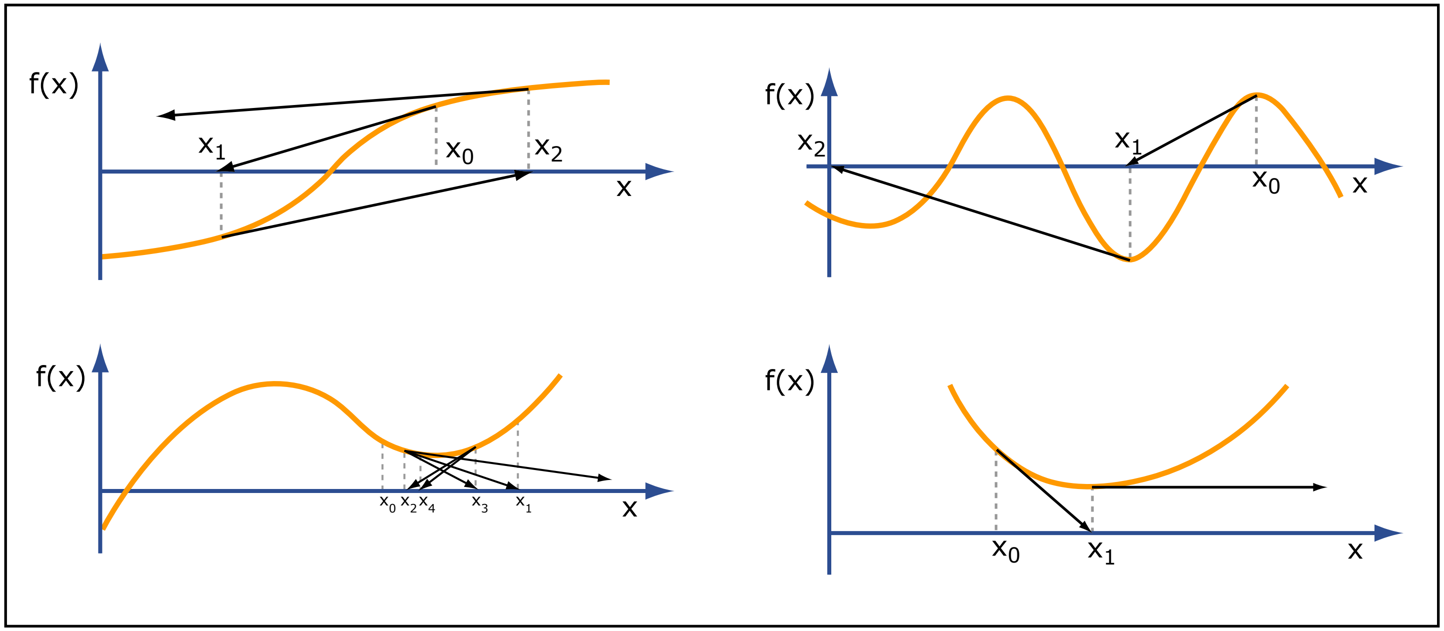
Newton-Raphson: Issues

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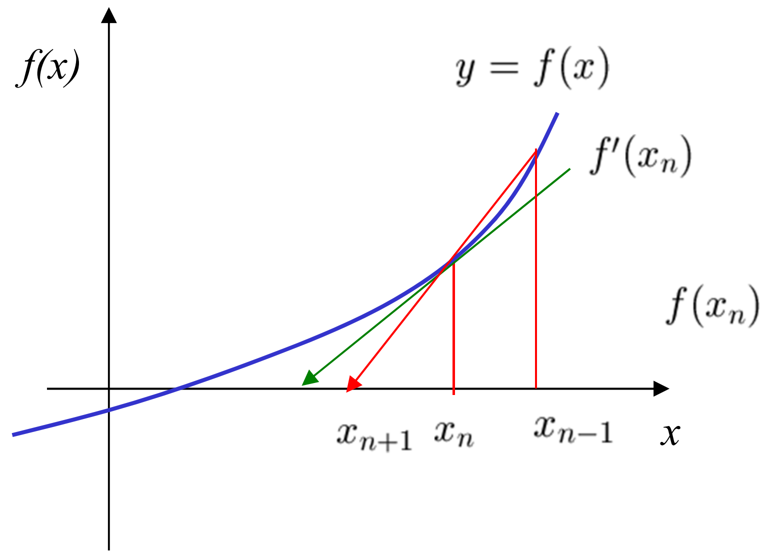
Four cases in which there is poor convergence with the Newton-Raphson method.

Roots of Nonlinear Equations: Secant Method

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

2. $f(x_n)$ may not be given in closed, analytical form, i.e. in CFD, it 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:

$$\begin{aligned} x_{n+1} &= x_n - \frac{f(x_n)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})} \\ &= \frac{f(x_n)x_{n-1} - f(x_{n-1})x_n}{f(x_n) - f(x_{n-1})} \end{aligned}$$

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

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

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

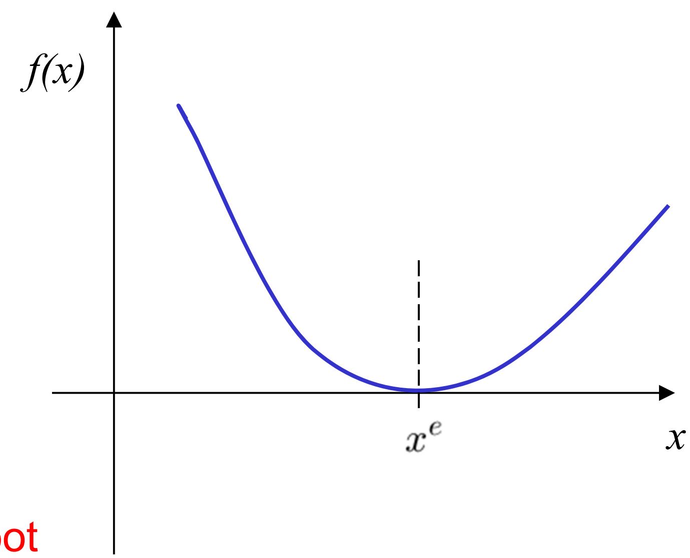
=>

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

Convergence

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

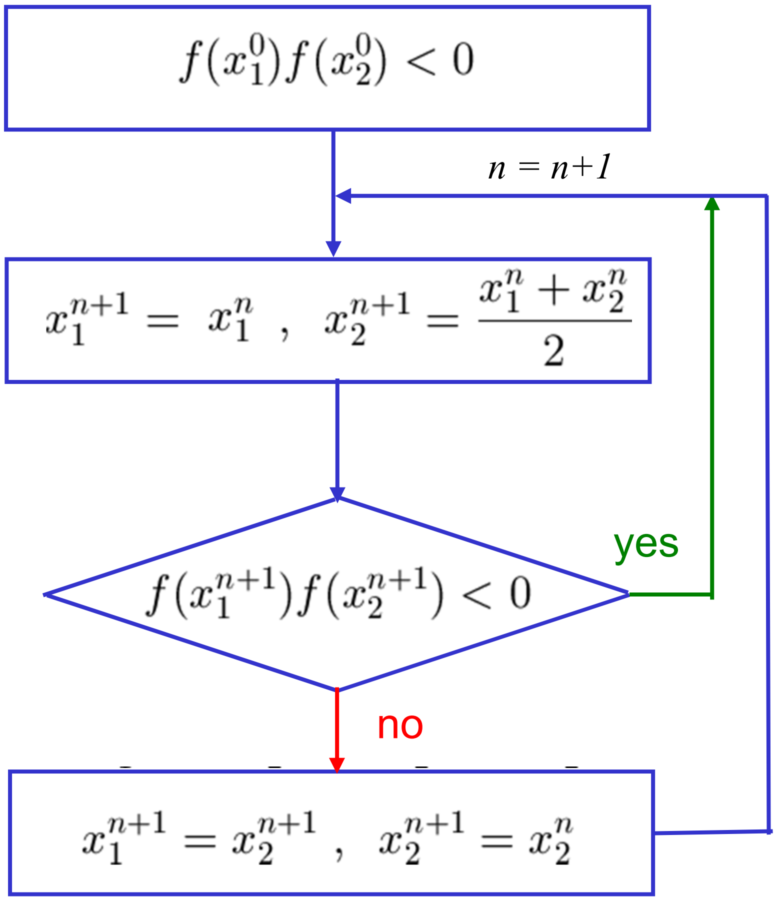
$$g'(x^e) = 1 - \frac{1}{p}$$

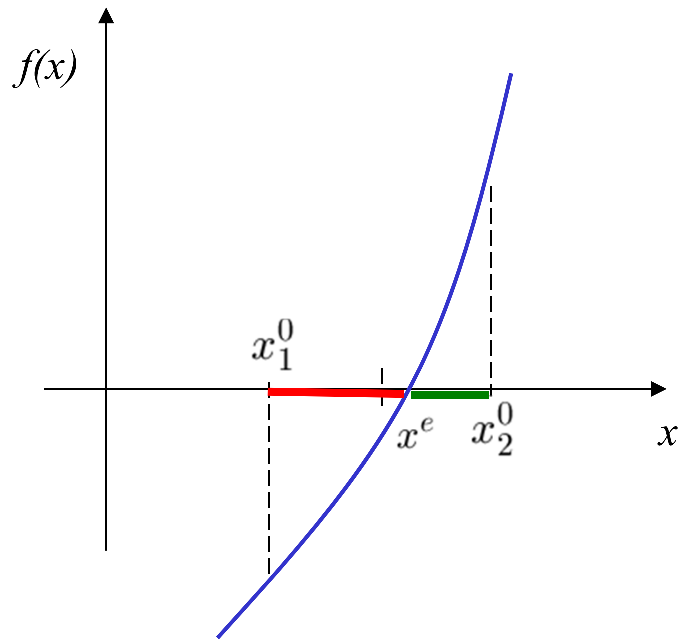


Slower convergence the higher the order of the root

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.

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.

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