Numerical Modeling

Unit 1: Solution of Equations in One Variable

Numerical Modeling

Intro

Series: X_n , n -> ∞

Limits: $\lim(X_n)$, n -> ∞

Continuity on [a, b]: $f \in C[a, b]$

Derivability on [a, b]: $\lim \left(f(x_n)-f(x_0)/(x_n-x_0)\right)$; $f \in C^1[a, b]$, $f \in C^2[a, b]$

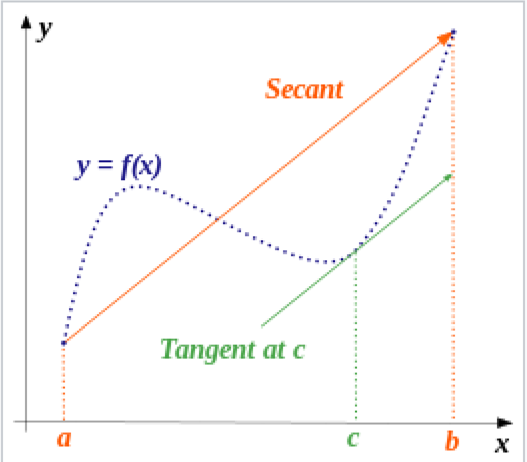
Integrals: $\lim \Sigma f(X_n)\Delta X_n$

Taylor's Theorem: if

- *$x_0 \in [a, b]$; $f \in C^n[a, b]$ and $f^{(n+1)}$*
- For every *$x \in [a, b]$* we can find a value *$g(x) \in [a, b]$* so that

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k + \frac{f^{(n+1)}(g(x))}{(n+1)!}(x - x_0)^{n+1}$$

Mean Value Theorem



For any function that is continuous on $[a, b]$ and differentiable on (a, b) there exists some c in the interval (a, b) such that the secant joining the endpoints of the interval $[a, b]$ is parallel to the tangent at c.

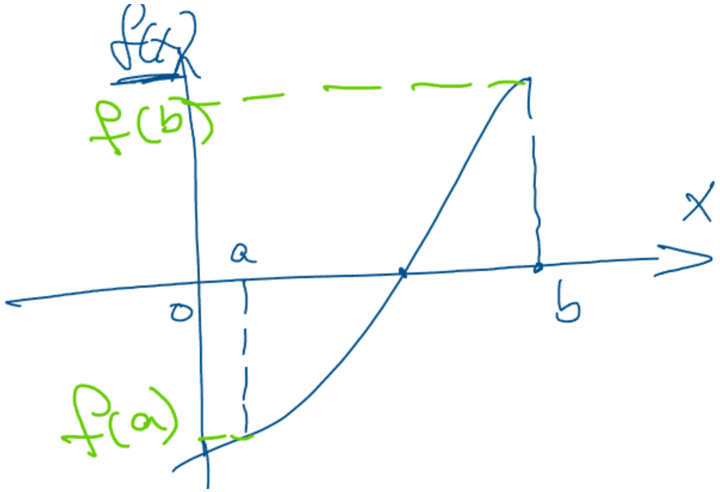
source: wikipedia

Solution of Equations in One Variable

Roots vs Fixed Points

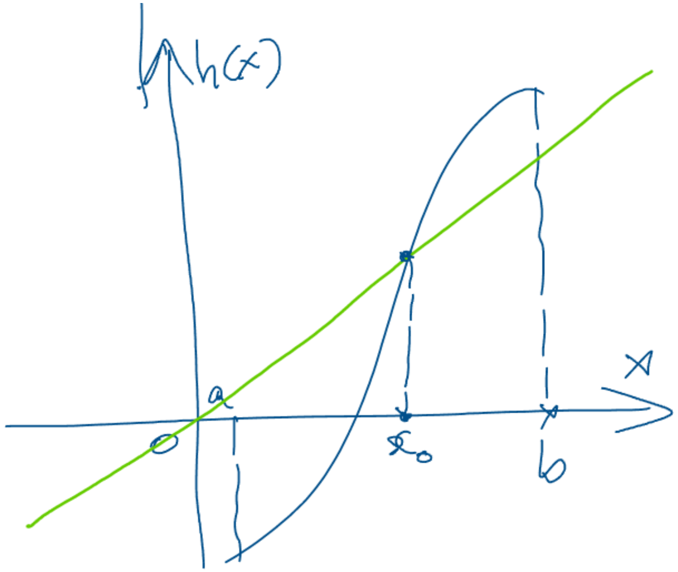
root of f.

$f(x) = 0$



fixed point

$f(x) = x$



Solution of Equations in One Variable

Bisection Method: finding the root of f [find x such that f(x) = 0]

If:

- f defined on the interval [a, b]
- f continuous on the full interval
- $f(a) * f(b) < 0$

Based on Intermediate Value Theorem $\Rightarrow$ there is a $x \in [a, b]$ so that $f(x) = 0$

err very small number .. precision

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Step 1: sol_min = a;      sol_max =  b;
Step 2: mid = sol_min/2 + sol_max/2;
Step 3: if     abs(   f(mid)    ) < err
                      return mid;
Step 4: if      f(sol_min) * f(mid) < 0
                      sol_max = mid;
                      jump [Step 2]
Step 5: sol_min = mid;
Step 6: jump [Step 2]
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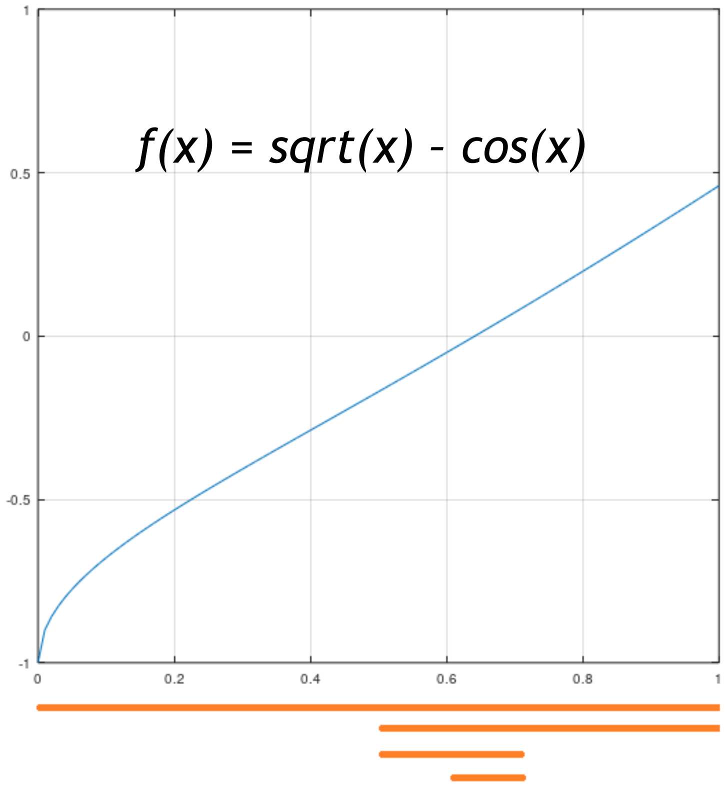
Attention should be given to limit number of steps



Solution of Equations in One Variable

Fixed Point Iteration Methods: find x so that f(x) = x

Method 1: (Bisection) Convert the problem to $g(x) = f(x) - x = 0$ and solve using bisection method
- If bisection conditions verified => method will always find a solution
- Bisection method can be slow

Method 2: (Iteration) use a sequence $x_n=g(x_{n-1})$ starting from a good approximation for x_0
- this method can diverge
- can converge faster than bisection method

Theorem: If $f \in C[a,b]$; $f(x) \in [a, b]$, $0 < \text{abs}(f'(x)) < 1$ for any $x \in [a,b]$

$\Rightarrow$ the iteration method converges for any starting point in [a,b]

Prof: Assume $p \in [a, b]$ is the fixed-point solution:

$$|x_n - p| = |f(x_{n-1}) - f(p)| = [\text{MeanValueTheorem}] = |f'(c)|\,|x_{n-1} - p| < |x_{n-1} - p|$$

Step 1: x = x0;
Step 2: x = f(x); step = step + 1;
Step 3: if (abs(x – f(x) < err) return x;
Step 4: if(step > MaxSteps) return FAIL;
Step 5: jump [Step 2]

Attention should be given to limit number of steps

Solution of Equations in One Variable

Newton Method: find x so that f(x) = 0

Taylor's Theorem: if

- $x_0 \in [a, b]$; $f \in C^n[a, b]$ and $f^{(n+1)}$
- For every $x \in [a, b]$ we can find a value $g(x) \in [a, b]$ so that

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k + \frac{f^{(n+1)}(g(x))}{(n+1)!}(x - x_0)^{n+1}$$

For $n = 1$ we get: $f(x) = f(x_0)+(x-x_0)f'(x_0)+(1/2)(x-x_0)^2 f''(g(x))$

Simplification 1: We try to find a root so $f(x) = 0$

Simplification 2: The Newton method works for small $(x-x_0)$. In this case $(x-x_0)^2$ is very small and can be ignored

With these simplifications we get $f(x_0)+(x-x_0)f'(x_0) =\sim 0$

or: $x =\sim x_0 - f(x_0)/ f'(x_0)$

$$x_{k+1} = x_k - f(x_k)/f'(x_k)$$

Solution of Equations in One Variable

Newton Method: find x so that f(x) = 0

$x \approx x_0 - f(x_0)/ f'(x_0)$

Step 1: Set $x_n = x_{n-1} - f(x_{n-1})/ f'(x_{n-1})$
Step 2: If (abs(f(xn-1)- f(xn)) < err) return x
Step 3: $x_{n-1} = x_n$;
Step 4: Jump to Step 1

If (abs(f(x_n*) < err) return x*

Attention should be given to limit number of steps

Solution of Equations in One Variable

Secant Method: find x so that f(x) = 0

Approximate *f*' s derivative in (x_n) using $f(X_n) - f(X_{n-1})/(Xn - Xn\text{-}1)$

Newton: $x_n =\sim x_{n-1} - f(x_{n-1})/\ f'(x_{n-1})$
Secant: $x_n =\sim x_{n-1} - f(x_{n-1})/\ [\ (f(x_{n-1})-f(x_{n-2}))/(x_{n-1}-x_{n-2}\ )]$

Step 1: Set $x_n =\sim x_{n-1} - f(x_{n-1})/\ [\ (f(x_{n-1})-f(x_{n-2}))/(x_{n-1}-x_{n-2}\ )]$
Step 2: If (abs(f(x_n*)) < err) return x*
Step 3: $x_{n-2} = x_{n-1};x_{n-1} = x_n;$
Step 4: Jump to Step 1

Attention should be given to limit number of steps

Solution of Equations in One Variable

Seminar using Octave/Matlab

Implement bisection method
Implement fixed point method
Implement Newton Method

Example solutions using bisection method (demo)
Example solutions using fixed point method
Example solutions using Newton Method