Computational Methods
CMSC/AMSC/MAPL 460

Splines Wrap Up
Solving nonlinear equations and zero finding

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Interpolation: wrap up

- Interpolation: Given a function at N points, find its value at other point(s)
- Polynomial interpolation
  - Monomial, Newton and Lagrange forms
- Piecewise polynomial interpolation
  - Linear, Hermite cubic and Cubic Splines
- Polynomial interpolation is good at low orders
- However, higher order polynomials "overfit" the data and do not predict the curve well in between interpolation points
- Cubic Splines are quite good in smoothly interpolating data

Finding zeroes of functions

- Where does it arise?
- Solving functional equations
  - Polynomials: Quadratic, cubic, quadric, quintic …
    - Galois in 1830 proved that there is no finite sequence of rational operations plus square/cube roots that can solve quintic or higher equations.
    - Aside: Galois died in a duel at a very young age (<21) http://www-groups.dcs.st-and.ac.uk/~history/Mathematicians/Galois.html
  - Minimization or maximization of a function
    - Recall if $f(x)$ has a minimum or maximum, $df/dx=0$
  - Intersection of curves
  - Others

The simplest algorithm: Bisection

- Suppose we know that
  - f is continuous in an interval $[a,b]$
  - $f(a) > 0$ and $f(b) < 0$ OR $f(a) < 0$ and $f(b) > 0$
- What does this tell us about f in the interval $[a,b]$?
  - By continuity, there must be at least one zero somewhere in between!
  - Hold on to this fact and squeeze the interval till we bracket the zero!
- Evaluate $f((a+b)/2)$.
  - If it has the same sign as $f(a)$, then the zero is in $[(a+b)/2, b]$
  - If it has the same sign as $f(b)$, then the zero is in $[a,(a+b)/2]$
- Repeat until the zero is obtained, or the interval is small enough.

Example

- Solve $x=2^{1/2}$;
  - Find x_* for which $f(x):x^2- 2$ has a zero
  - Evaluate $f(1)$ and $f(2)$
  - We know $f(1)<0$ and $f(2)>0$ $[1,2]$
  - Next guess 1½ : f(1½) >0 [1,1½]
  - Next guess 1¼ : f(1¼) <0 [1¼,1½]
  - Next guess 1 3/8 : f(1 3/8) <0 [1 3/8,1½]
  - …

$$1\frac{3}{8},\ 1\frac{5}{16},\ 1\frac{13}{32},\ 1\frac{27}{64},\ \ldots$$

- Will the algorithm ever stop?
  - Always will converge in floating point
  - After 52 steps a = 1.41421356237309 b = 1.41421356237310
  - Difference smaller than machine epsilon

- This algorithm needs one function evaluation per iteration

Convergence analysis

- For iterative algorithms, we want to know how the error decreases after each iteration
- Here the imprecision in locating the root (or the error), approximately halves each step
- What is the trend in convergence
- Error $=(x_k - x_*) = e_k$

$$e_k = e_{k-1}/2$$

$$e_k = e_0/2^k = e_0 2^{-k}$$

- So if we take logs
- Log error = log e_0 – k log2
  - Semilog plot shows linear rate
  - What is the slope here?
- This algorithm is said to have linear convergence

Another algorithm

- Note that in bisection we take the half-way point no matter how close $f(a)$ or $f(b)$ maybe to zero
- Instead let us fit a straight line joining $f(a)$ and $f(b)$
- Find where it becomes zero
- Recall the straight line is

$$g(x)=f(a)+(x-a)\,(f(b)-f(a))/(b-a)$$

$$g(a)=f(a) \qquad g(b)=f(a)+f(b)-f(a)=f(b)$$

- Set $g(x)=0$

$$x_{*}= a-f(a)(b-a)/(f(b)-f(a))$$

Evaluate $f(x_{*})$

Depending on sign of $f(x_{*})$ replace a or b with x_{*}

Modified secant method

- Algorithm is a modified secant method
- Requires one function evaluation per iteration
  - Convergence is superlinear

$$e_k = c\, e_{k-1}^{a}$$

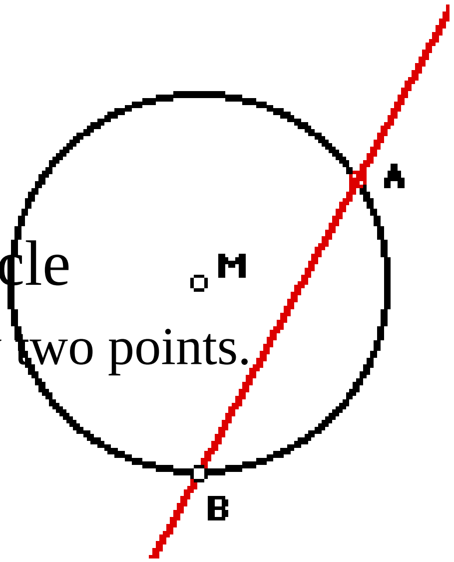
$$e_k = c\,(c e_{k-2}^{a})^{a} = C e_0^{-ka}$$

Here a is the golden ratio (1+sqrt(5))/2

- What is a secant?
  - In trigonometry it is the function defined as

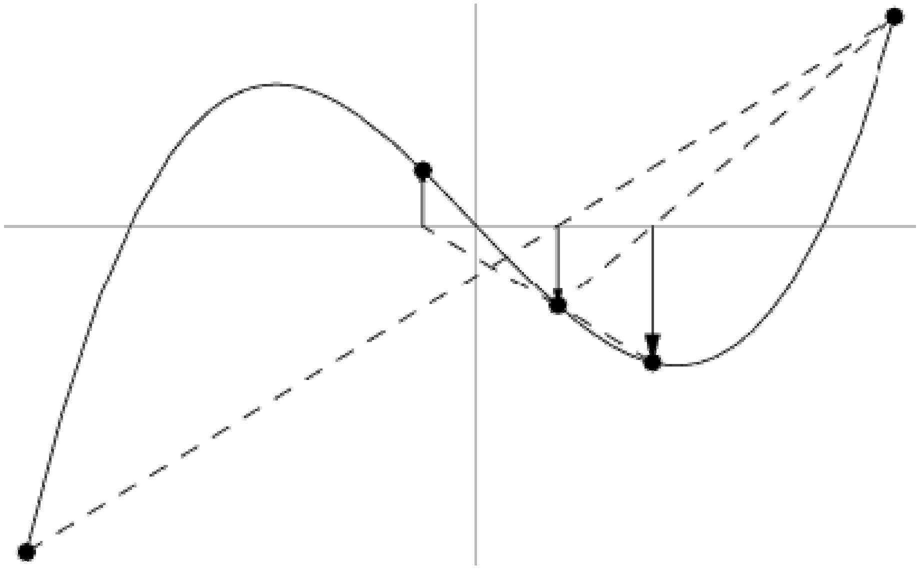
$$\sec(z) = 1/\cos(z)$$

  - Here the use is more from the geometry of a circle
    - A SECANT is a line that intersects a circle in exactly two points.
    - Every secant forms a chord.



Secant method

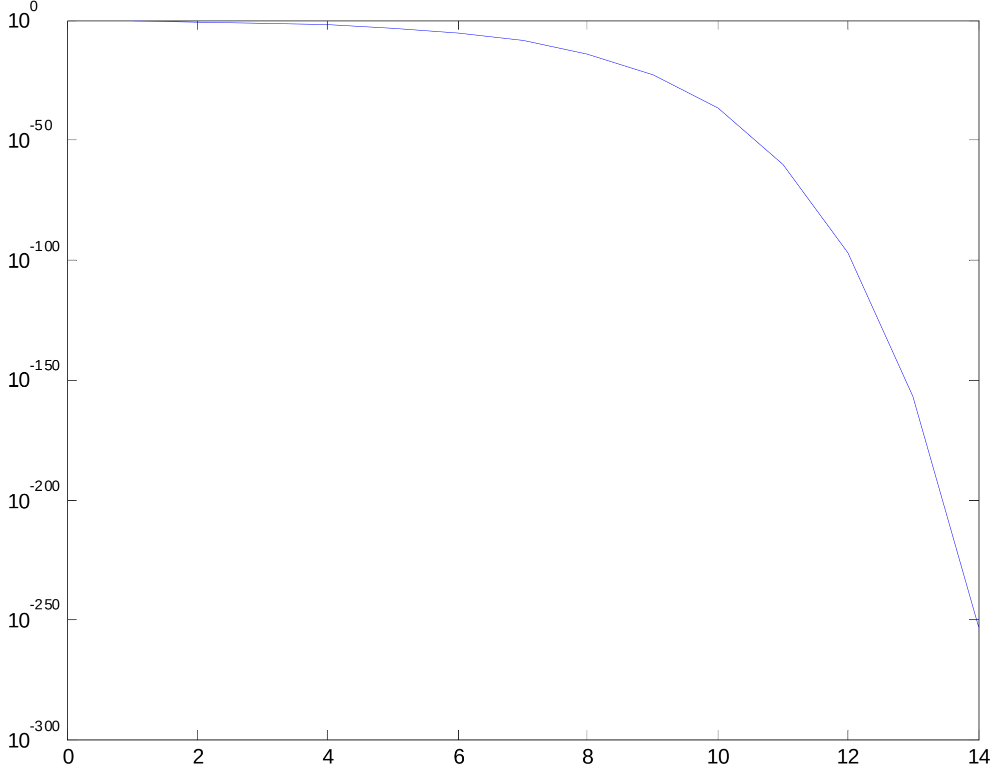
- In bisection and the modified secant method we were required to first bracket a zero
- This can be time consuming … and is indeed the hard part of minimization
- On the other hand once this is done we have ensured convergence
- Instead in the secant method choose two points
- Fit straight line and evaluate its zero
- Choose next point and repeat



Secant method

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

- When it converges, the convergence is super linear
- Each step the error is raised to a power >1
- Convergence to zero occurs quickly
- But, convergence is not guaranteed till we are near the zero



Newton’s method

- Several ways to derive
  - Taylor series
  - Take secant to tangent …
- I want $f(x_*)=0$
- But I have $f(x_k)$ which is not zero
- Let me guess that $f(x_k+h)$ will be zero
- $f(x_k+h)=f(x_k)+hf'(x_k)=0$
- So $h=-f(x_k)/f'(x_k)$
- *So* $x_{k+1}=x_k+h=x_k-f(x_k)/f'(x_k)$
- Repeat until convergence

- Apply Newton method to square root
- X=sqrt(a)
- $f(x)=x^2 - a$
- $f'(x)=2x$
- $x_{k+1}=x_k+h=x_k-(x_k^2-a)/2x_k$
- *Guess sqrt(2) = 1*
- *1-(1-2)/2=1.5*
- *1.5-(2.25-2)/3 = 1.5-0.0833=1.4167*
- …
- *Converges rapidly*