Computational Methods
CMSC/AMSC/MAPL 460

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 = $\log e_0 - k \log 2$
  - 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

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

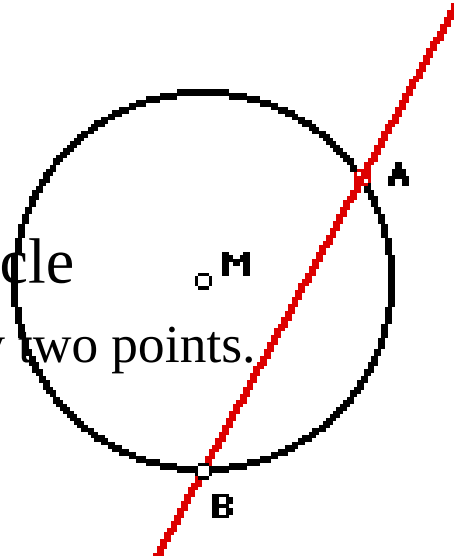
$$e_k = c\,(c e_{k-2}^{\,a})^a = C e_0^{-ka}$$

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

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

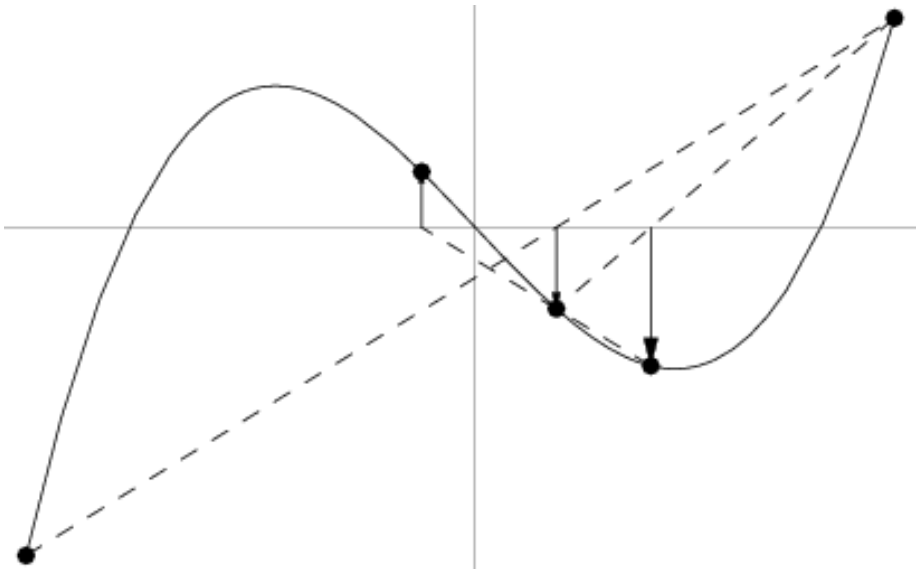
$$\sec(z) = 1/\cos(z)$$

  - 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

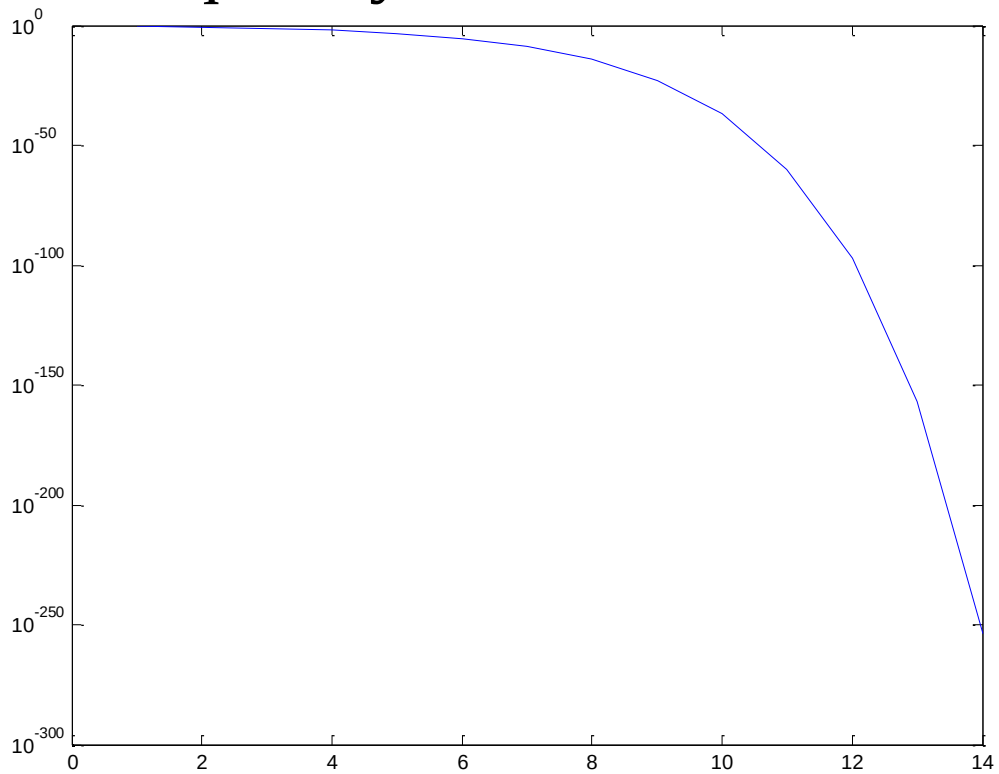
- In bisection and the modified secant method we were required to first bracket a zero
- This can be time consuming … and is indeed the hard part of minimization
- On the other hand once this is done we have ensured convergence
- Instead in the secant method choose two points
- Fit straight line and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

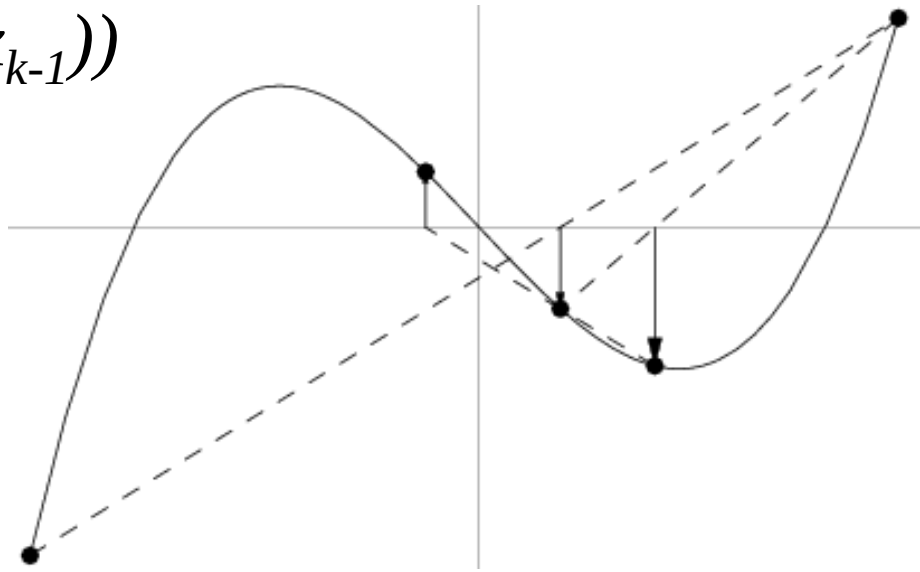
- Apply Newton method to square root
- X=sqrt(a)
- $f(x)=x^2 - a$
- $f'(x)=2x$
- $x_{k+1}=x_k+h=x_k-(x_k^2-a)/2x_k$
- *Guess sqrt(2) = 1*
- *1-(1-2)/2=1.5*
- *1.5-(2.25-2)/3 = 1.5-0.0833=1.4167*
- …
- *Converges rapidly*

Secant method

- Instead in the secant method choose two points
- Fit straight line and evaluate its zero

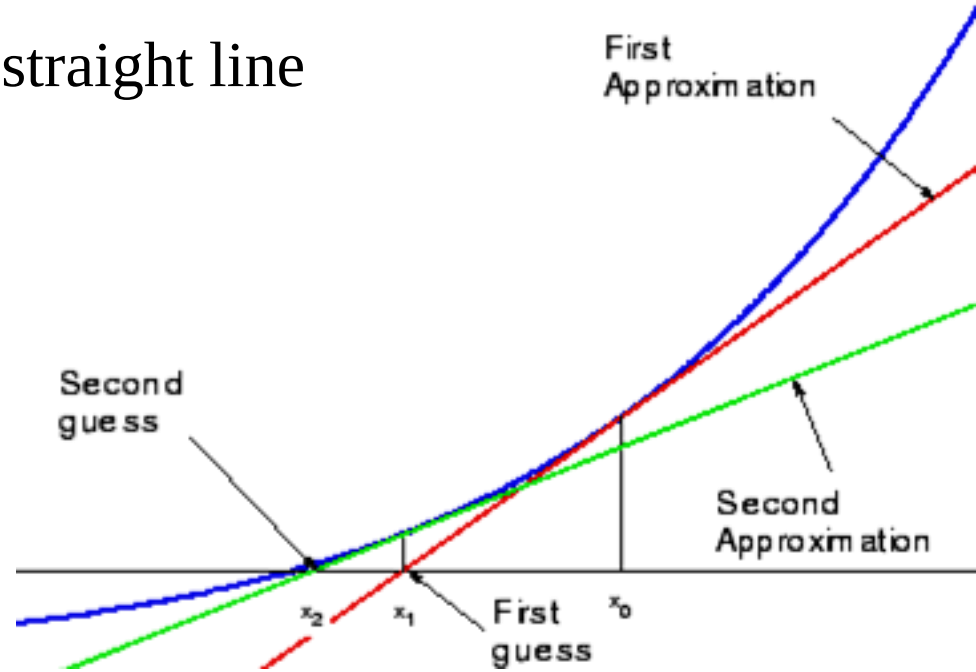
$x_{k+1} = x_k - f(x_k)(x_k - x_{k-1})/(f(x_k) - f(x_{k-1}))$

- Choose next point and repeat
- Convergence is superlinear
- $e_{k+1} = c.\ e_k^{\phi}$
- $\phi = (5^{1/2} + 1)/2 = 1.62 \ldots$



Newton's method

- Several ways to derive: We choose Taylor series
- 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
- $f(x_k+h)=f(x_k)+hf'(x_k)+O(h^2)$
- Ignore terms of $O(h^2)$
  - Approximate curve locally as straight line
  - When will this not work?
- Solve $f(x_k)+hf'(x_k)=0$ for h
- 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



Convergence analysis

- For iterative algorithms, we want to know how the error decreases after each iteration
- We also want to check how much each iteration costs
- Optimal algorithm is the one that achieves a given error for a given cost

Algorithm	convergence	function evaluations per step
Bisection	Linear	One
Secant	Superlinear	One
Newton	Quadratic	Two

- Which method is better?
- Define better:
- Bisection guaranteed to converge, but slow
- Secant one evaluation per step Newton: two
- Newton quadratic convergence Secant super linear
- Newton needs derivative, which may be unavailable

Comparing convergence

- Suppose cost of function evaluations for derivative and function are similar
- Then let Newton method converge in n steps to error τ
- So $e_0^{2n} \leq \tau$
  - Take logs: $2n \log e_0 \leq \log \tau$
  - So $2n \geq |\log \tau| / |\log e_0|$ $\quad n \geq (2)^{-1} (|\log \tau| / |\log e_0|)$
- Secant will require s steps to ensure $e_0^{1.62s} \leq \tau$
  - For secant: $s \geq (1.62)^{-1}(|\log \tau| / |\log e_0|)$
- Cost of Newton is $2n$ while that of secant is s
- Which is larger?
- $\text{Cost}_{\text{Newton}}/\text{Cost}_{\text{Secant}} = 2n/s = 1/(1.62)^{-1} = 1.62 > 1$
  - So Secant is cheaper!

Infinite cycles

- Newton's method could iterate forever!

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

- cycles back and forth around a point *a* if

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

- This happens if

$$x - a - \frac{f(x)}{f'(x)} = -(x-a)$$

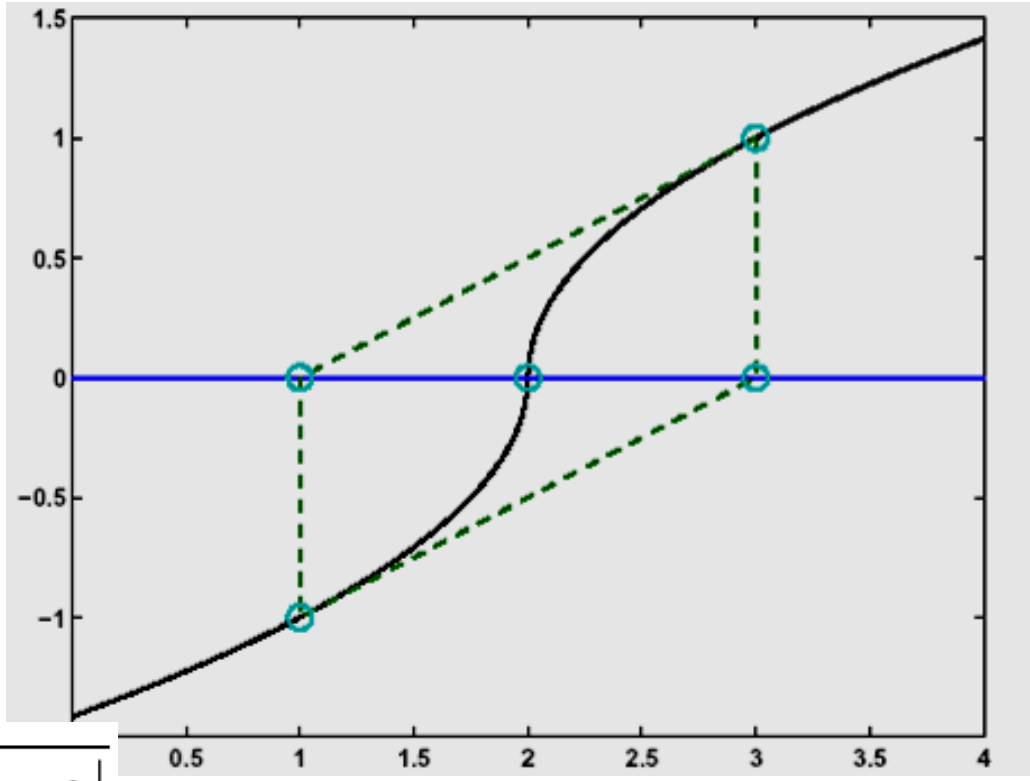
  – Rewrite as an ODE for *f*

$$\frac{f'(x)}{f(x)} = \frac{1}{2(x-a)}$$

  – Solution

$$f(x) = \mathrm{sign}(x-a)\sqrt{|x-a|}$$

  – Such cycles could exist with secant methods as well.



Inverse Quadratic Interpolation

- Secant method fits a straight line to predict zero from two previous values
- We could instead fit a parabola to predict the zero from three values!
- However parabola may not intersect x axis (straight line will always)
  - In this case roots will be complex
- Idea of inverse quadratic interpolation
  - Fit a parabola $x=f(y^2)$ instead of a parabola $y=f(x^2)$
  - Evaluate it at 0
- Problem: polynomial interpolation needs the points (here function values) to be distinct
- Cannot guarantee this!
- So method may not converge
- However near solution it converges very rapidly

```
k = 0;
fa=f(a)
fb=f(b)
fc=f(c)
while abs(c-b) > eps*abs(c)
    x = polyinterp([fa,fb,fc],[a,b,c],0)
    a = b;fa=fb;
    b = c;fb=fc;
    c = x;fc=f(x);
    k = k + 1;
end
```

Guaranteed methods: Zeroin

- Start with a and b so that $f(a)$ and $f(b)$ have opposite signs.
- Use a secant step to give c between a and b.
- Repeat until $|b - a| < \varepsilon |b|$ or $f(b) = 0$.
  - Arrange a, b, and c so that
    - $f(a)$ and $f(b)$ have opposite signs.
    - $|f(b)| < |f(a)|$
    - c is the previous value of b.
- If $c \neq a$, consider an IQI step.
- If $c = a$, consider a secant step.
- If the IQI or secant step is in the interval [a,b], take it.
- If the step is not in the interval, use bisection.