Computational Methods
CMSC/AMSC/MAPL 460

Splines Wrap Up
Solving nonlinear equations and zero finding

Ramani Duraiswami,
Dept. of Computer Science
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 $1 \frac{1}{2} : f(1 \frac{1}{2}) > 0$ [1,1\frac{1}{2}]
  – Next guess $1 \frac{1}{4} : f(1 \frac{1}{4}) < 0$ [1\frac{1}{4},1\frac{1}{2}]
  – Next guess $1 \frac{3}{8} : f(1 \frac{3}{8}) < 0$ [1\frac{3}{8},1\frac{1}{2}]
  – …
  \[
  \begin{array}{cccc}
    \frac{3}{8} & \frac{5}{16} & \frac{13}{32} & \frac{27}{64} \\
    1\frac{3}{8} & 1\frac{5}{16} & 1\frac{13}{32} & 1\frac{27}{64} \\
  \end{array}
  \]

• 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 = \( (x_k - x_*) = e_k \)

\[
e_k = e_{k-1}/2
\]

\[
e_k = e_0/2^k = e_02^{-k}
\]

• 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
  \[
  g(x) = f(a) + (x - a) \frac{(f(b) - f(a))}{(b - a)}
  \]
  \[
  g(a) = f(a) \quad g(b) = f(a) + f(b) - f(a) = f(b)
  \]
- Set \( g(x) = 0 \)
  \[
  x^* = a - f(a) \frac{(b - a)}{(f(b) - f(a))}
  \]
  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

\[ x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})} \]

- 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

\[ X = \sqrt{a} \]

\[ f(x) = x^2 - a \]

\[ f'(x) = 2x \]

\[ x_{k+1} = x_k + h = x_k - \frac{(x_k^2 - a)}{2x_k} \]

Guess \( \sqrt{2} = 1 \)

\[ 1 - (1 - 2)/2 = 1.5 \]

\[ 1.5 - (2.25 - 2)/3 = 1.5 - 0.0833 = 1.4167 \]

... 

Converges rapidly