Computational Methods

CMSC/AMSC/MAPL 460

Solving nonlinear equations and zero finding

Ramani Duraiswami,

Dept. of Computer Science

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?
- $\text{Cost}_{\text{Newton}}/\text{Cost}_{\text{Secant}} = 2n/s = 1.62 > 1$
  - 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

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

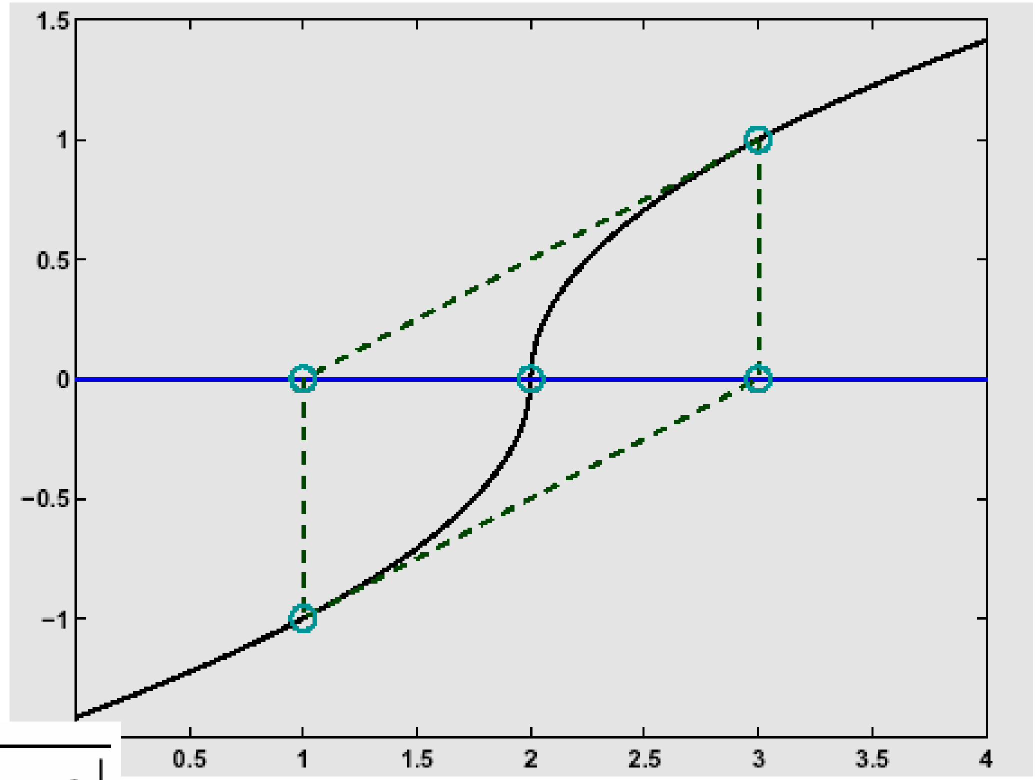
  – Rewrite as an ODE for f

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

  – Solution

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

  – 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

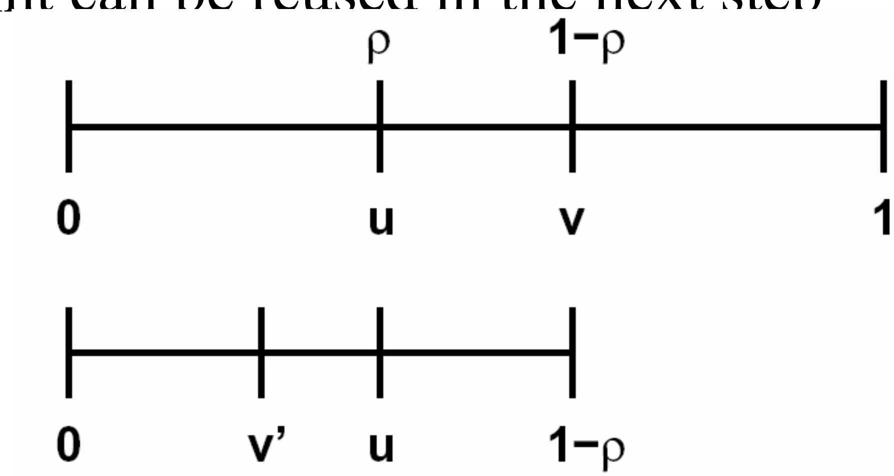
- Start with a and b so that $f(a)$ and $f(b)$ have opposite signs.
- Use a secant step to give c between a and b.
- Repeat until $|b - a| < \varepsilon\,|b|$ or $f(b) = 0$.
  - Arrange a, b, and c so that
    - $f(a)$ and $f(b)$ have opposite signs.
    - $|f(b)| < |f(a)|$
    - c is the previous value 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.

Optimization analog of bisection

- Optimization involves finding maximum and minimum of functions
- At these point first derivative vanishes
- So optimization typically involves use of differential methods
- Here we consider an algorithm like bisection
- Suppose we are given an interval $[a,b]$ and have to find the minimum in this interval
- We could look at $f(a)$, $f(b)$ and $f((a+b)/2)$
- Even if $f((a+b)/2) < f(a)$ and $f((a+b)/2) < f(b)$ don't know if $[a,(a+b)/2]$ or $[(a+b)/2,b]$ contains the minimum
- Could divide domain into three regions
- $f(a)$, $f(b)$, $f((a+b)/3)$, and $f(2(a+b)/3)$.
- Then we know which interval $[a,2(a+b)/3]$ or $[(a+b)/3, b]$ contains the minimum

Golden Search

- Let [0,2/3] be the reduced domain
- At next step we cannot reuse our function evalution at 1/3 (which is the mid-point of our interval)
- Instead we must evaluate the function at 2/9 and 4/9.
- Thus each iteration requires two function evaluations.
- Can we instead choose points (not at 1/3 and 2/3) but at some other points ρ and $1-\rho$, so that the point can be reused in the next step



- So $\rho/(1-\rho) = (1-\rho)/1$
- $1-2\rho + \rho^2 = \rho$
- $\rho^2 - 3\rho + 1 = 0$
- $\rho = (3 \pm (9-4)^{1/2})/2$
- $\rho = 1 + (1-5^{1/2})/2 = 2-\phi = 0.382..$
- Length of interval is reduced by a factor of $\phi - 1 \simeq 0.618$ each step
  - So to converge to machine epsilon we require $52/0.618 \simeq 75$ steps

Improved Golden Search: `fminbd`

- As the search proceeds, we will have three points in the interval with the minimum
- Fit a parabola and find the minimum
- If the minimum is within the interval, we can choose it as the next point
- To stop: recall near a minimum derivative vanishes
- So $f(x)=f(x_*)+b(x-x_*)^2$
- Let $x-x_*=\delta$ and $f(x_*)=a$ $\qquad f(x)=a+b\delta^2$
- If the interval δ is as small as machine ε, then the change in the value of f will of the order of machine ε^2.
- SO it is not computable
- Rather change can at most be about the square root of machine ε
- This is employed in Matlab function `fminbd` and in the book software function `fmintx`

Systems of Nonlinear equations

- Analog for 1d bisection: Too hard to find bracketed zero
- Analog for Newton is what is used
- Derivative is now ∇ f

Example: Let the function $f(x)$ be defined by

$$\begin{aligned} f_1(x_1, x_2) &= x_1^3 + \cos(x_2) \\ f_2(x_1, x_2) &= x_1 x_2^2 - x_2^3 . \end{aligned}$$

Then in solving $f(x) = 0$, we look for a point x_1, x_2 where both f_1 and f_2 are zero.

The derivative of the function is called the **Jacobian matrix**. It is a matrix $J(x)$ defined by

$$J(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 3x_1^2 & -\sin(x_2) \\ x_2^2 & 2x_1x_2 - 3x_2^2 \end{bmatrix}$$

Multidimensional Newton's Method

- $f_1(\mathbf{x})=f_1(x_1, x_2, \ldots, x_N)$
- $f_2(\mathbf{x})=f_2(x_1, x_2, \ldots, x_N)$
- ...
- $f_M(\mathbf{x})=f_M(x_1, x_2, \ldots, x_N)$

- $f_1(\mathbf{x}+\mathbf{h})=f_1(x_1, x_2, \ldots, x_N)+\nabla f_1 \cdot \mathbf{h}$
- …
- $f_M(\mathbf{x}+\mathbf{h})=f_1(x_1, x_2, \ldots, x_N)+\nabla f_M \cdot \mathbf{h}$

- $\nabla f_1 = [\partial f_1/\partial x_1 \; \partial f_1/\partial x_1 \ldots \partial f_1/\partial x_N]$
- ...
- $\nabla f_M = [\partial f_M/\partial x_1 \; \partial f_M/\partial x_1 \ldots \partial f_M/\partial x_N]$

- $\mathbf{f}(\mathbf{x}+\mathbf{h})=\mathbf{f}(\mathbf{x})+\mathbf{J}\mathbf{h}=\mathbf{0}$
- Solve $\mathbf{J}\mathbf{h}=-\mathbf{f}$ to find the step
- $\mathbf{x}_{k+1}=\mathbf{x}_k+\mathbf{h}$