ECE 595, Section 10
Numerical Simulations
Lecture 6: Finding Special Values

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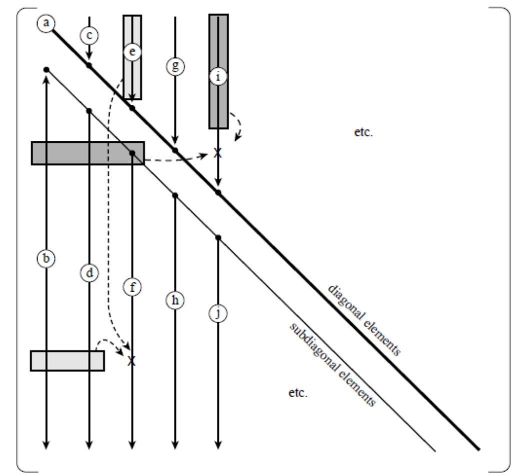
Outline

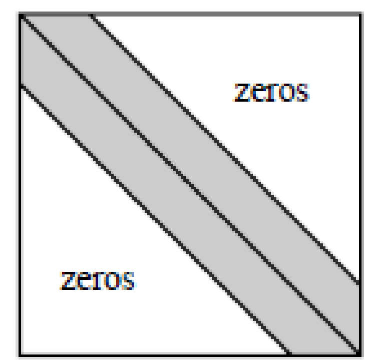
- Recap from Wednesday
- Root Finding
  - Bisection
  - Newton-Raphson method
  - Brent's method
- Optimization
  - Golden Section Search
  - Brent's Method
  - Downhill Simplex
  - Conjugate gradient methods
  - Multiple level, single linkage (MLSL)

Recap from Wednesday

- Solve linear algebra problems A^{-1} and $A \cdot x = b$
- Gauss-Jordan method $(A' \cdot x = b')$
- Gaussian Elimination $(U \cdot x = b')$
- LU Decomposition $(A = L \cdot U)$
- Singular Value Decomposition $(A = U \cdot W \cdot V^T)$
- Sparse Matrices
- Iterative improvement (subtract $A^{-1}(b' - b)$ from x')
- QR Decomposition $(A = \prod Q_i \cdot R)$



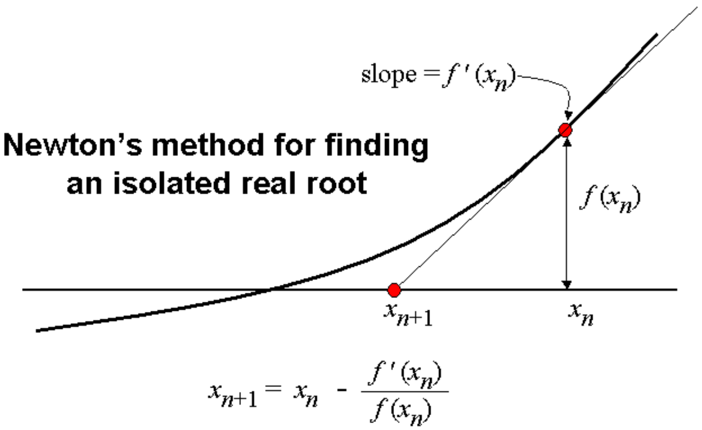
Crout's algorithm



Band diagonal sparse matrix

Finding Zeros

- Relevance in micro & nano research
- Key concept: bracketing
- Bisection – continuously halve intervals
- Newton-Raphson method – uses tangent
- Laguerre's method – for polynomials
- Brent's method – adds inverse quadratic interpolation

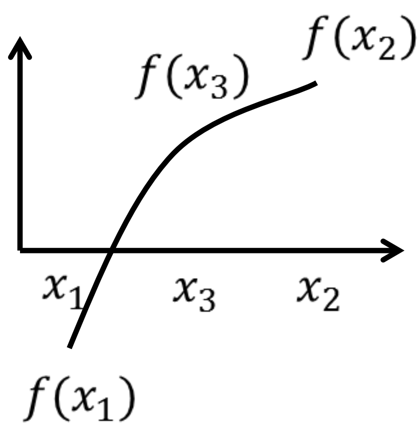


Importance of Bracketing

- Critically important for both root finding and optimization
- Can always guarantee at least one solution for continuous functions with sign change in 1D
- If more than one solution present, may not be able to guarantee which one is reached – method-dependent

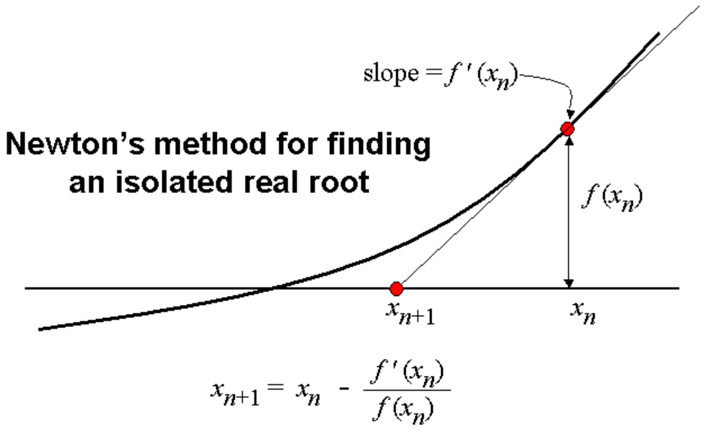
Bisection

- Most stable and reliable approach
- Algorithm:
  - Choose point x_3 in the middle of the bracket with sign change: $[x_1, x_2]$
  - Check sign of $f(x_3)$
  - If non-zero, construct new bracket from midpoint and original point with opposite sign
  - Repeat previous steps



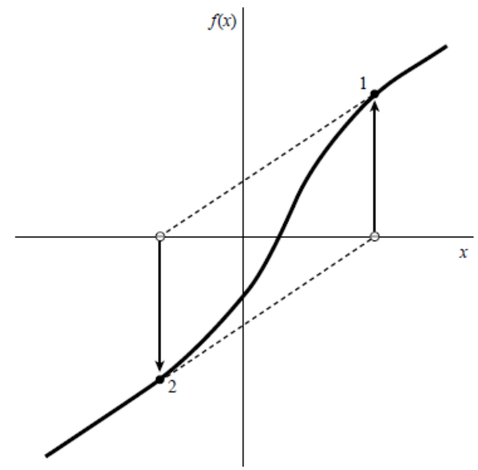
Newton-Raphson Method

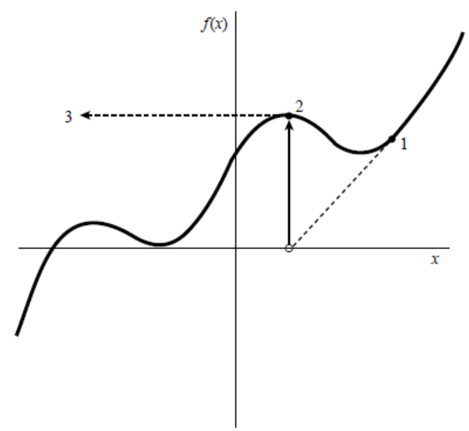
- Key assumption: system is nearly linear in region between starting point and root
- When sufficiently close, converge quadratically on correct value (from Taylor expansion)



NR Method Failures

- Getting stuck in a limit cycle is possible
- Can even get worse – certain locally flat curves can send you into outer space!





Laguerre's Method

- Specifically for polynomials
- Algorithm
  - Calculate quantities G and H
  - Assume far roots a distance b; one root is a distance a away
  - Iterate solution as $a \to 0$

$$P_n(x) = \prod_i (x - x_i)$$

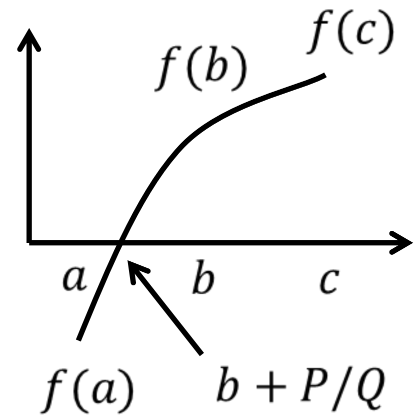
$$G = \frac{d \ln|P_n(x)|}{dx}$$

$$H = -\frac{d^2 \ln|P_n(x)|}{dx^2}$$

$$a = \frac{n}{G \pm \sqrt{(n-1)(nH - G^2)}}$$

Brent's Method: Finding Roots

- Combines bracketing, bisection, and inverse quadratic interpolation
- Guaranteed to converge, but speed can vary with function and quality of initial guess
- Algorithm:
  - Calculate $f(a)$, $f(b)$, $f(c)$
  - Calculate *R*, *S*, *T*, *P*, *Q*
  - Let $b \to b + P/Q$
  - Repeat as $f(b) \to 0$



$$R = \frac{f(b)}{f(c)}$$

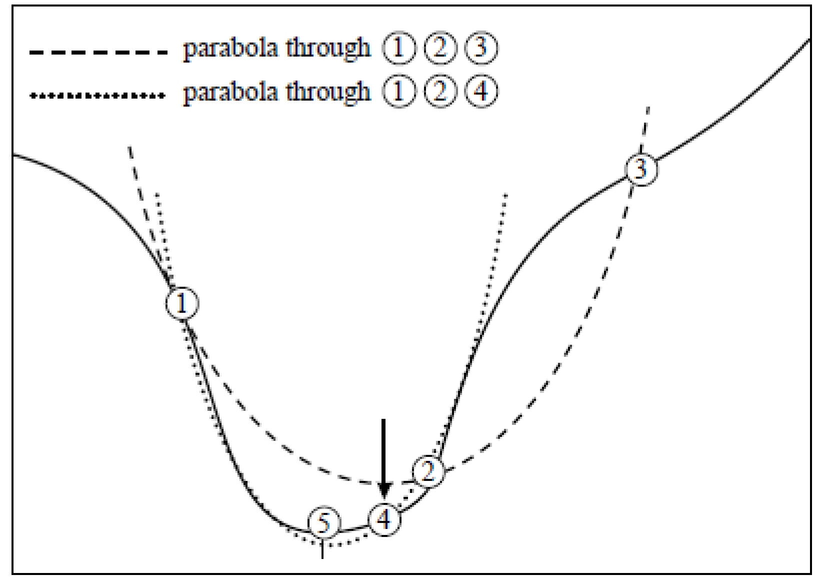
$$S = \frac{f(b)}{f(a)}$$

$$T = \frac{f(a)}{f(c)}$$

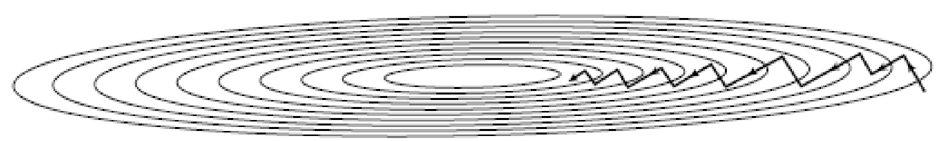
$$P = S[T(R-T)(c-b) - (1-R)(b-a)]$$
$$Q = (T-1)(R-1)(S-1)$$

Optimization

- Relevance in micro & nano research
- Convexity
- Search classifications
- Techniques:
  - Brent's Method
  - Golden Section Search
  - Downhill Simplex
  - Conjugate gradient methods
  - Multiple level, single linkage (MLSL)

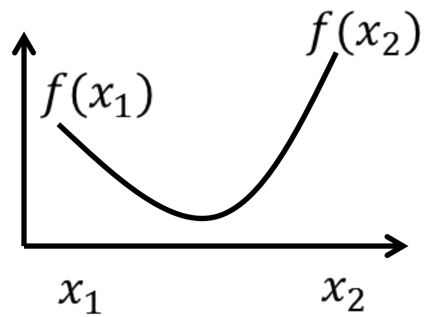


These and further images from "Numerical Recipes," by WH Press *et al*.



Convexity

- Convex functions have certain properties that aid in finding an optimum:
  - Precisely one optimum in an open set of values
  - Continuous and at least twice differentiable
  - Midpoints always lower than edges – i.e., $f[\delta x_1 + (1-\delta)\delta x_2] < \delta f(x_1) + (1-\delta) f(x_2)$
- Examples include x^2, sinh(x)

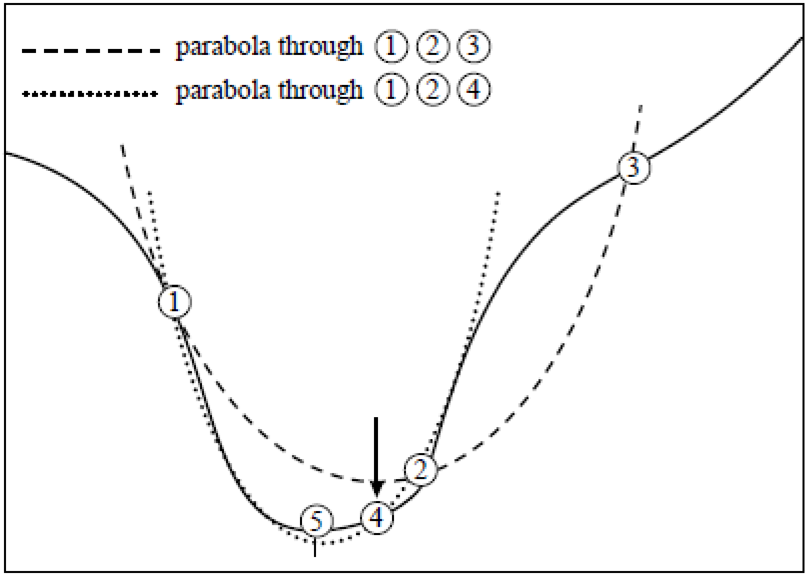


Search Types

- Local – assumes convex/concave problem
- Global – uses heuristics to deal with multiple optima
- Non-derivative based – no specific assumptions about best search direction
- Derivative based – incorporates derivatives to determine search direction

Brent's Method: Finding Optima

- Assumes a concave function
- Algorithm:
  - Evaluate function at bracket endpoints & center
  - Fit parabola
  - Find x_{min} & $f(x_{min})$
  - Keep two closest points for bracket and repeat until bracket is around $\sqrt{\varepsilon}$
- Infer optimum based



Next Class

- Is on Wednesday, Jan. 23 (because of Martin Luther King, Jr. Day)
- Discussion of optimization and eigenproblems
- Please read Chapter 11 of "Numerical Recipes" by W.H. Press *et al*.