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

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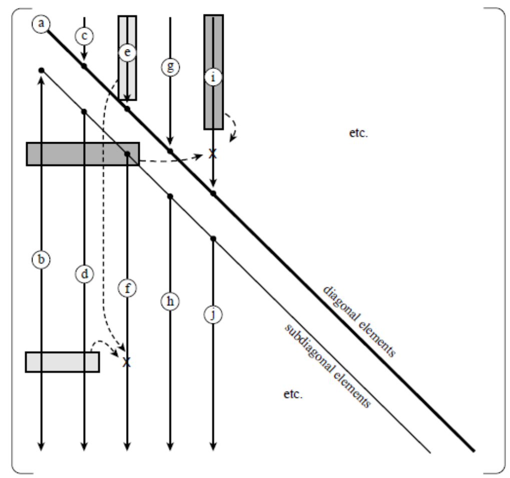
Outline

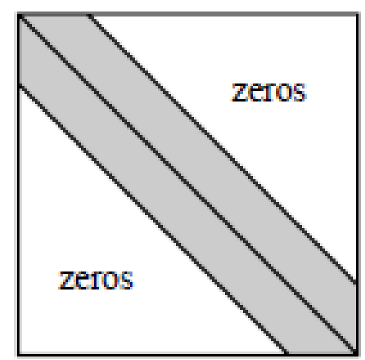
- Recap from Wednesday
- Root Finding
  - Bisection
  - Newton-Raphson method
  - Brent's method
- Optimization
  - Golden Section Search
  - Brent's Method
  - Downhill Simplex
  - Conjugate gradient methods
  - Multiple level, single linkage (MLSL)

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 ($A = \prod Q_i \cdot R$)



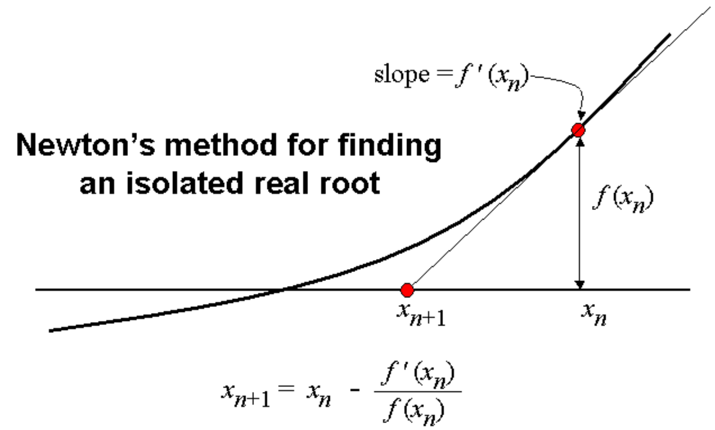
Crout's algorithm



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

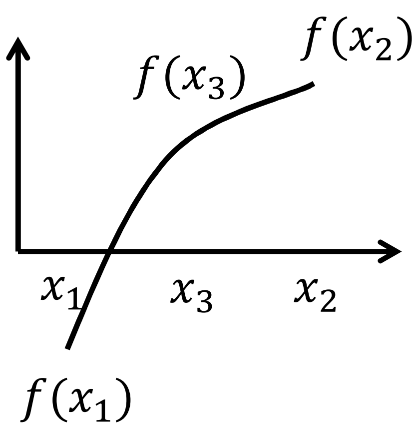


Importance of Bracketing

- 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

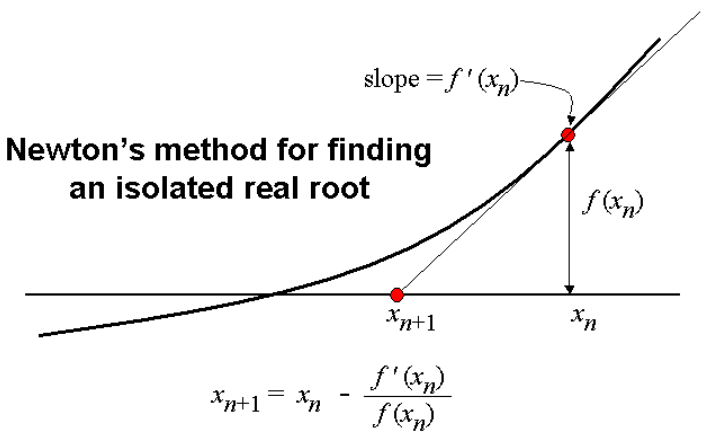
Bisection

- 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



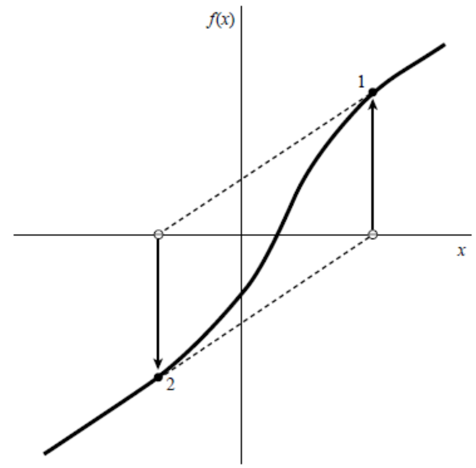
Newton-Raphson Method

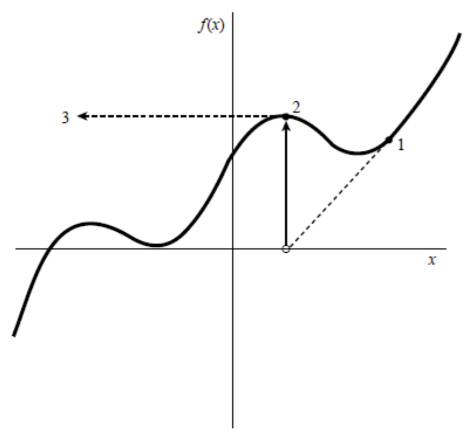
- Key assumption: system is nearly linear in region between starting point and root
- When sufficiently close, converge quadratically on correct value (from Taylor expansion)



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 $a \to 0$

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

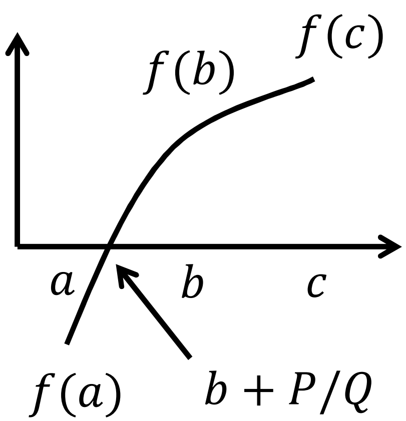
$$G = \frac{d \ln|P_n(x)|}{dx}$$

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

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

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 $f(b) \to 0$



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

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

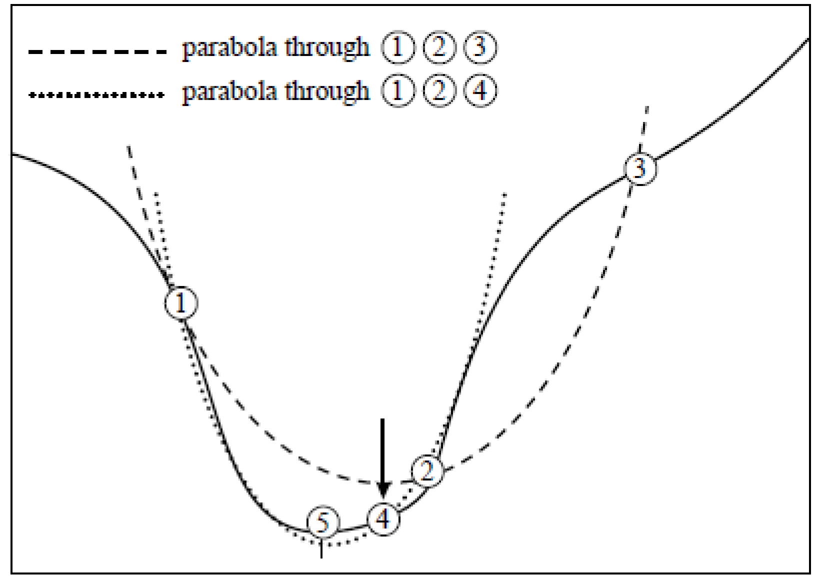
$$T = \frac{f(a)}{f(c)}$$

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

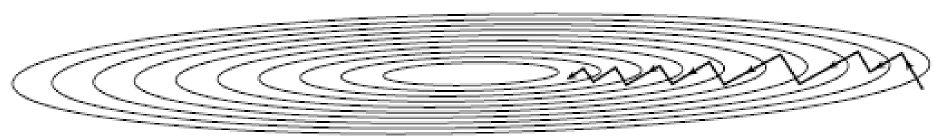
$$Q = (T-1)(R-1)(S-1)$$

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)

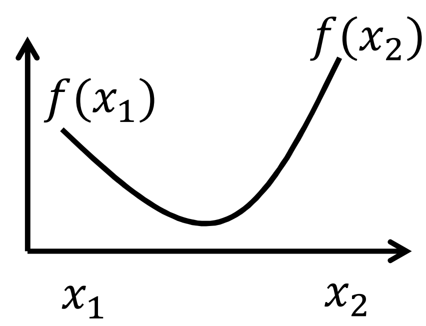


These and further images from "Numerical Recipes," by WH Press *et al*.



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)

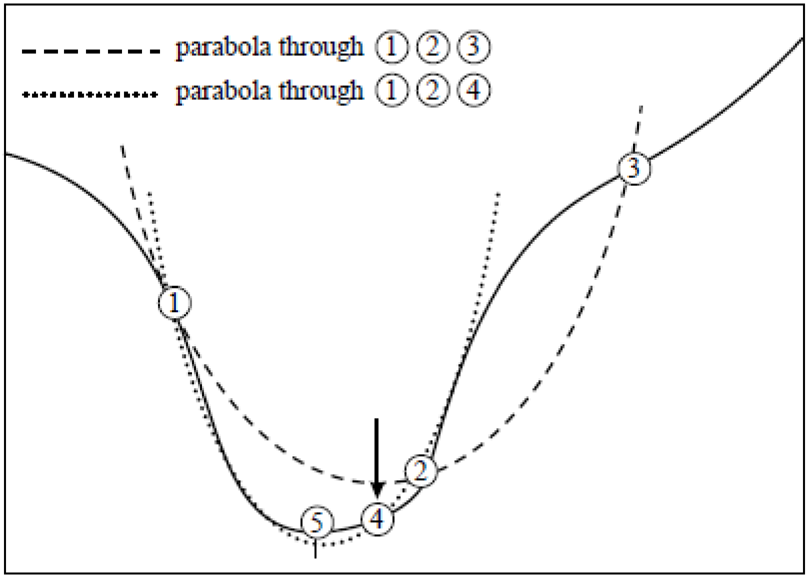


Search Types

- 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

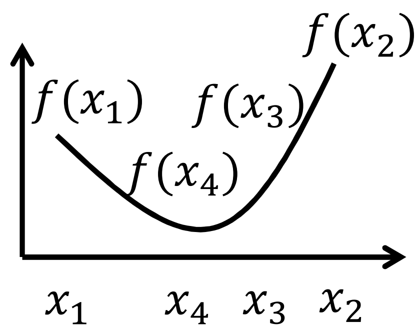
Brent's Method: Finding Optima

- 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



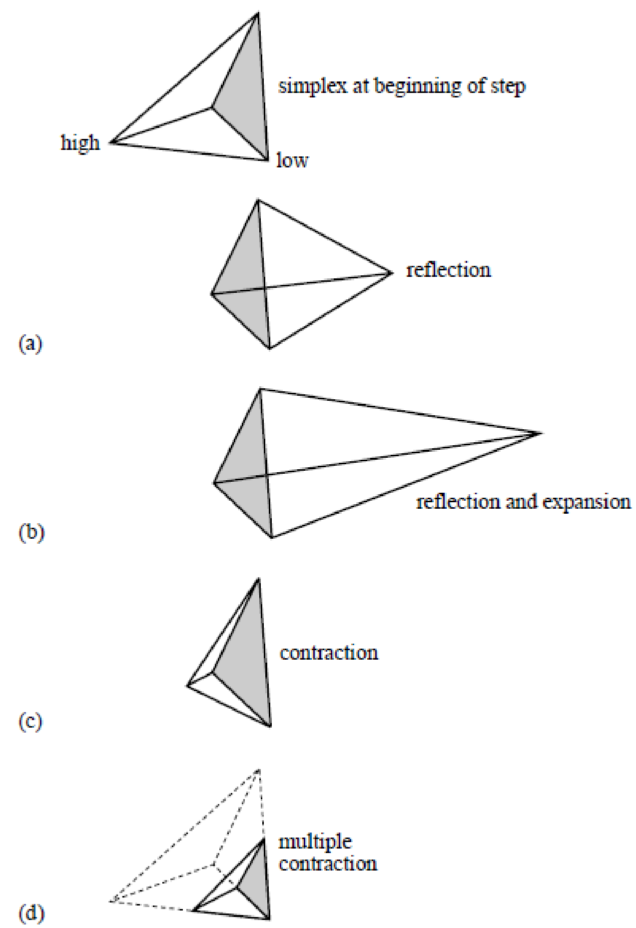
Golden Section Search

- Closely related to bisection approach to finding roots
- Algorithm
  - Taking a downhill step
  - Bracket lowest point with higher values on each side
  - Keep repeating until interval is around $\sqrt{\varepsilon}$



Downhill Simplex Search

- Simplex is a triangle (2D), tetrahedron (3D), etc.
- Algorithm:
  - Create an N-dimensional simplex: $P_i = P_o + \lambda_i \hat{e}_i$
  - Perform one of 4 steps shown on right
  - Repeat until tolerances reached (e.g., for change in simplex end-points, or function values)



Conjugate Gradient Method

- Assumes convex multidimensional function
- Uses derivative information
- Algorithm:
  - Start with initial $g_o = h_o$
  - Calculate scalars λ_i, γ_i
  - Construct new vectors g_{i+1} and h_{i+1}, satisfying orthogonality & conjugacy conditions
  - Repeat until tolerance reached
- Note that no *a priori* knowledge of Hessian matrix *A* is required!

$$\lambda_i = \frac{\mathbf{g}_i \cdot \mathbf{g}_i}{\mathbf{h}_i \cdot \mathbf{A} \cdot \mathbf{h}_i} = \frac{\mathbf{g}_i \cdot \mathbf{h}_i}{\mathbf{h}_i \cdot \mathbf{A} \cdot \mathbf{h}_i}$$

$$\gamma_i = \frac{(\mathbf{g}_{i+1} - \mathbf{g}_i) \cdot \mathbf{g}_{i+1}}{\mathbf{g}_i \cdot \mathbf{g}_i}$$

$$\mathbf{g}_{i+1} = \mathbf{g}_i - \lambda_i \mathbf{A} \cdot \mathbf{h}_i$$

$$\mathbf{h}_{i+1} = \mathbf{g}_{i+1} + \gamma_i \mathbf{h}_i$$

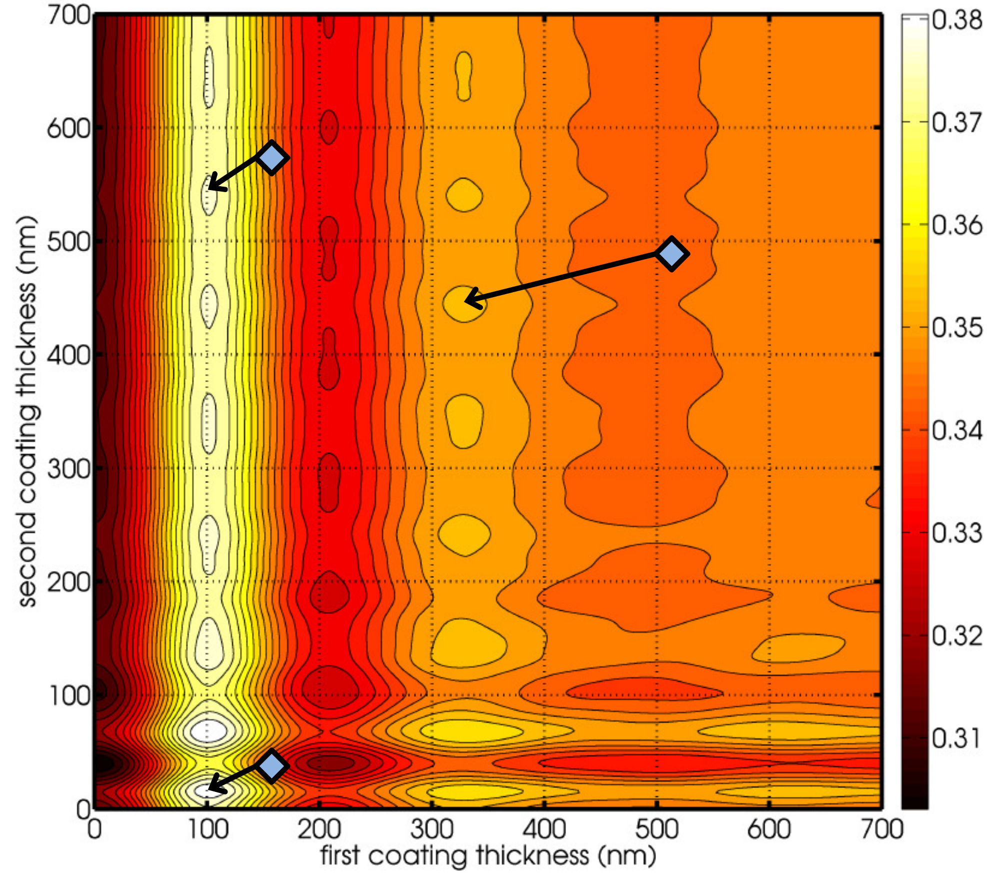
$$\mathbf{g}_i \cdot \mathbf{g}_j = 0$$

$$\mathbf{h}_i \cdot \mathbf{A} \cdot \mathbf{h}_j = 0$$

$$\mathbf{g}_i \cdot \mathbf{h}_j = 0$$

Multiple Level Single Linkage

- Global search
- Algorithm:
  - Quasi-random sequence of starting points
  - Local optimization (e.g., conjugate gradient)
  - Heuristic tracks basins of convergence



M. Ghebrebrhan, P. Bermel, *et al.*, *Opt. Express* **17**, 7505 (2009)

Next Class

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