ECE 595, Section 10 Numerical Simulations Lecture 7: Optimization and Eigenvalues

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Outline

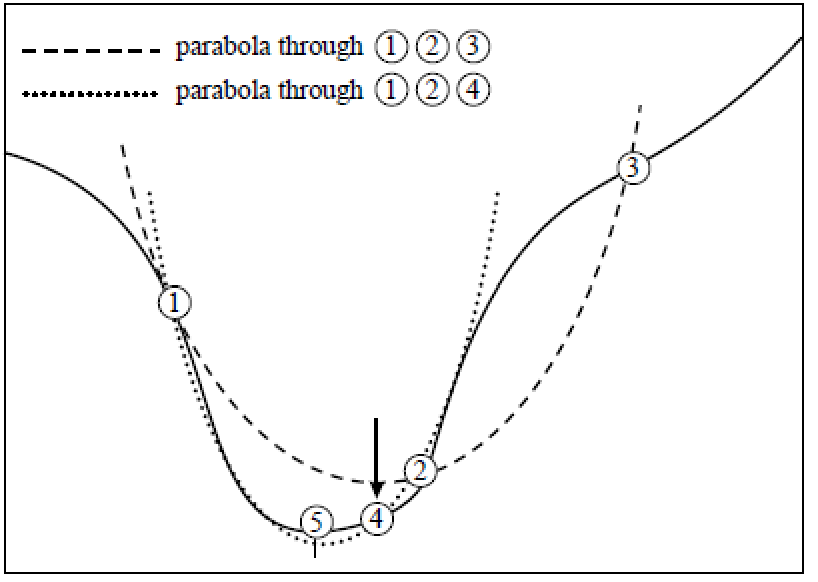
- Recap from Friday
- Optimization Methods
  - Brent's Method
  - Golden Section Search
  - Downhill Simplex
  - Conjugate gradient methods
  - Multiple level, single linkage (MLSL)
- Eigenproblems
  - Power Method
  - Factorization Methods

Recap from Friday

- Methods for finding zeros:
  - Bisection – bracket + continuously halve intervals
  - Newton-Raphson method – uses tangent
  - Laguerre’s method – for polynomials
  - Brent’s method –inverse quadratic interpolation
- Optimization – key distinctions
  - Convexity – refers to problem difficulty
  - Locality – how widely to search
  - Gradient-based – accelerates search

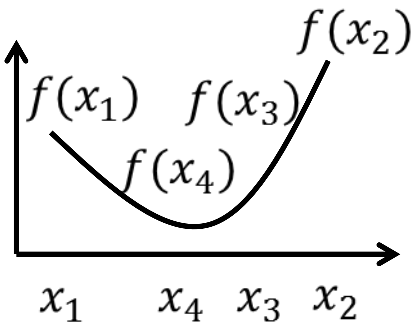
Brent’s Method: Finding Optima

- 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



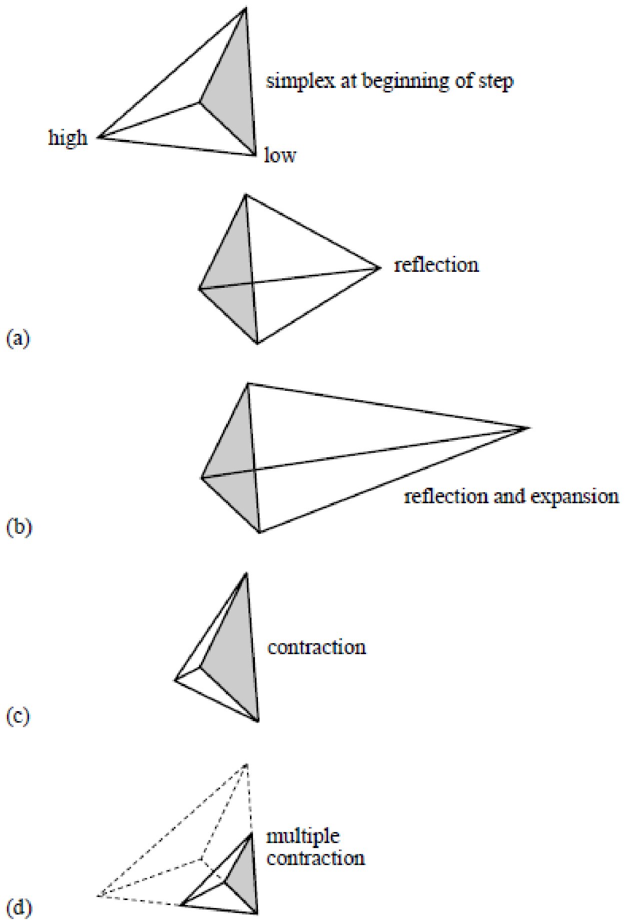
Golden Section Search

- 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!

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

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

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

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

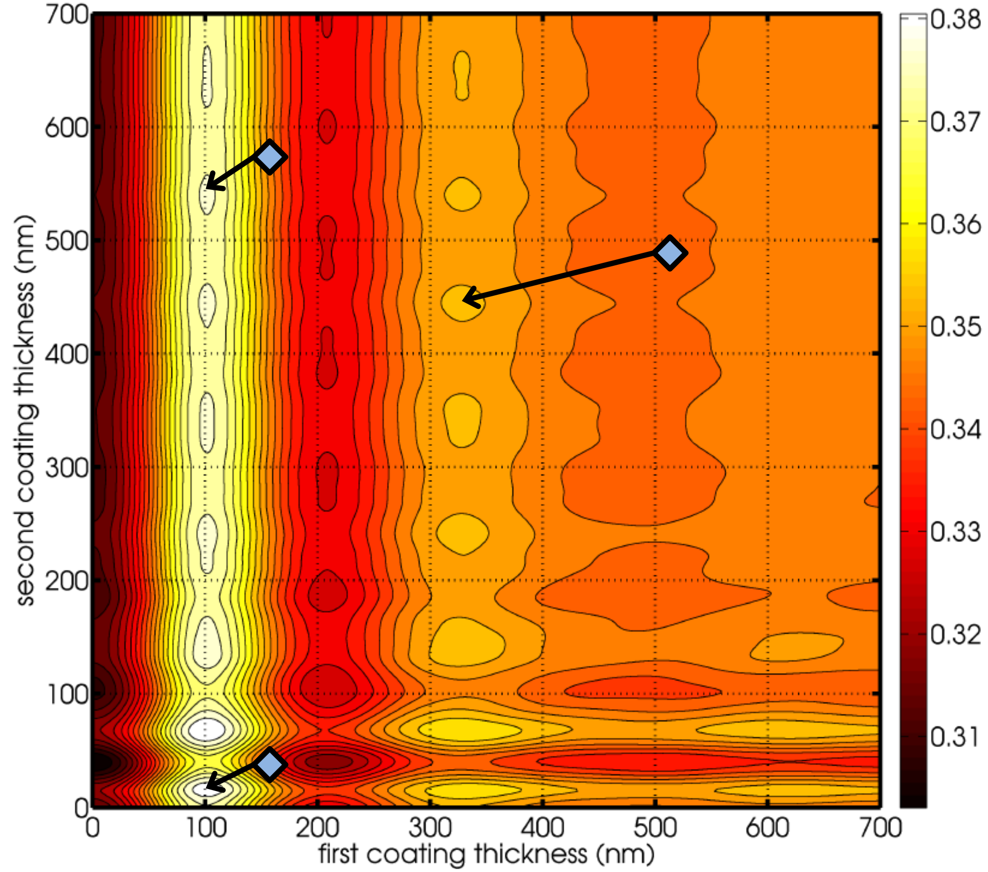
$$\mathbf{g}_i \cdot \mathbf{g}_j = 0$$

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

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

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)

Eigenproblems

- Regular eigenproblem: $Ax = \lambda x$
- Generalized eigenproblem: $Ax = \lambda Bx$
- Common examples in research
  - Schrödinger's equation: $-\frac{\hbar^2}{2m}\hat{\nabla}^2\Psi + \hat{V}\Psi = E\Psi$
  - EM master eqn: $\nabla \times [\epsilon^{-1}(\nabla \times H)] = \left(\frac{\omega}{c}\right)^2 H$
- Direct method – solve: $\det(A - \lambda 1) = 0$

Eigenproblems: Key Terminology

- Symmetric: $A = A^T$
- Hermitian (self-adjoint): $A = A^\dagger -$ implies all real eigenvalues
- Orthogonal: $A^T A = \mathbf{1}$
- Unitary: $A^\dagger A = \mathbf{1}$
- Normal: $AA^\dagger = A^\dagger A$
- Right eigenvectors: $x \cdot A = \lambda x$

Next Class

- Is on Friday, Jan. 23
- Continue discussion of eigenproblems
- Again, refer Chapter 11 of "Numerical Recipes" by W.H. Press *et al*.