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 $x_{\text{min}}$ & $f(x_{\text{min}})$
  - 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 $g_0 = h_0$
  – Calculate scalars $\lambda_i$, $\gamma_i$
  – 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!

\[
\lambda_i = \frac{g_i \cdot g_i}{h_i \cdot A \cdot h_i} = \frac{g_i \cdot h_i}{h_i \cdot A \cdot h_i}
\]

\[
\gamma_i = \frac{(g_{i+1} - g_i) \cdot g_{i+1}}{g_i \cdot g_i}
\]

\[
g_{i+1} = g_i - \lambda_i A \cdot h_i
\]

\[
h_{i+1} = g_{i+1} + \gamma_i h_i
\]

\[
g_i \cdot g_j = 0
\]

\[
h_i \cdot A \cdot h_j = 0
\]

\[
g_i \cdot h_j = 0
\]
Multiple Level Single Linkage

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

Eigenproblems

- Regular eigenproblem: \( Ax = \lambda x \)
- Generalized eigenproblem: \( Ax = \lambda Bx \)
- Common examples in research
  - Schrödinger’s equation: \(-\frac{\hbar^2}{2m} \hat{\nabla}^2 \Psi + \hat{\nabla} \Psi = E\Psi\)
  - EM master eqn: \( \nabla \times [\varepsilon^{-1}(\nabla \times H)] = \left(\frac{\omega}{c}\right)^2 H \)
- 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: $A^T A = 1$
• Unitary: $A^\dagger A = 1$
• 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.