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

\[ x_{n+1} = x_n - \frac{f'(x_n)}{f(x_n)} \]
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 $b \rightarrow b + P/Q$
  - Repeat as $f(b) \rightarrow 0$

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

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

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

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

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