ECE 595, Section 10
Numerical Simulations
Lecture 2: Problems in Numerical Computing

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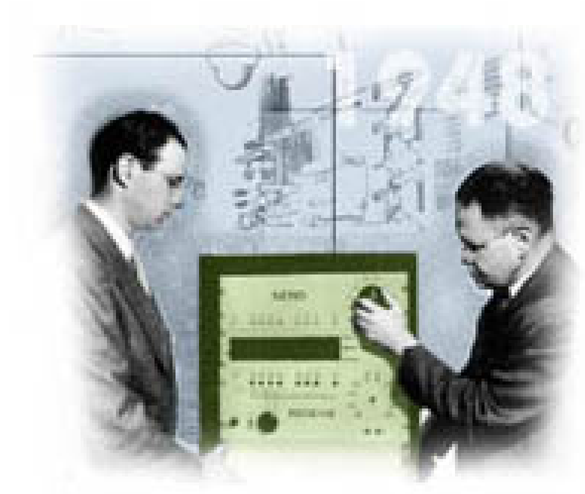
Outline

- Overall Goals
- Finding Special Values
- Fourier Transforms
- Eigenproblems
- Ordinary Differential Equations
- Partial Differential Equations

Recap: Goals for This Class

- Learn/review key mathematics
- **Learn widely-used numerical techniques**
- Become a capable user of this software
- Appreciate strengths and weaknesses of competing algorithms
- Convey your research results to an audience of colleagues



RW Hamming (left), developing error-correcting codes (AT&T)

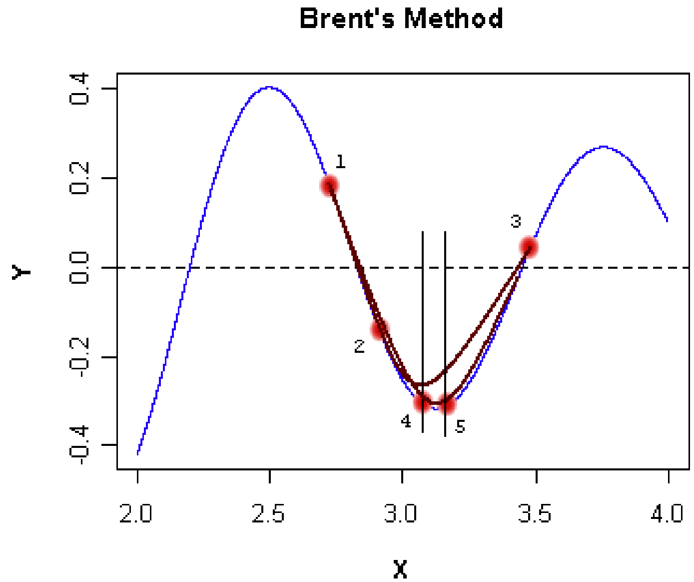
Finding Special Values

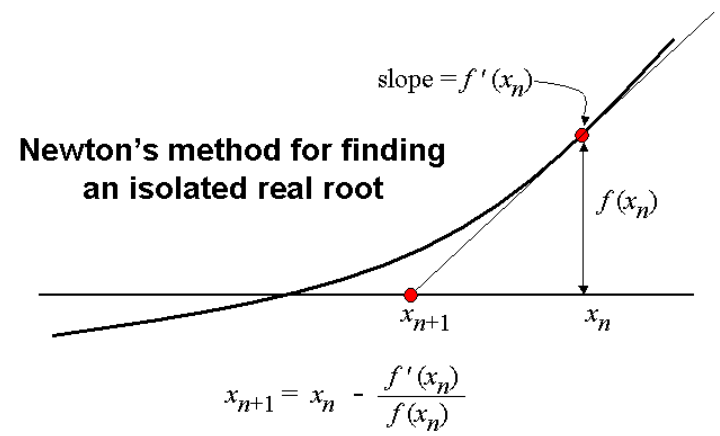
- Finding zeros
  - 1D versus multidimensional
  - Speed versus certainty
- Finding minima and maxima (optimization)
  - Convex vs. non-convex problems
  - Global vs. local search
  - Derivative vs. non-derivative search

Finding Zeros

- Key concept: bracketing
- Bisection – continuously halve intervals
- Brent's method – adds inverse quadratic interpolation
- Newton-Raphson method – uses tangent
- Laguerre's method – assume spacing of roots at a and b:

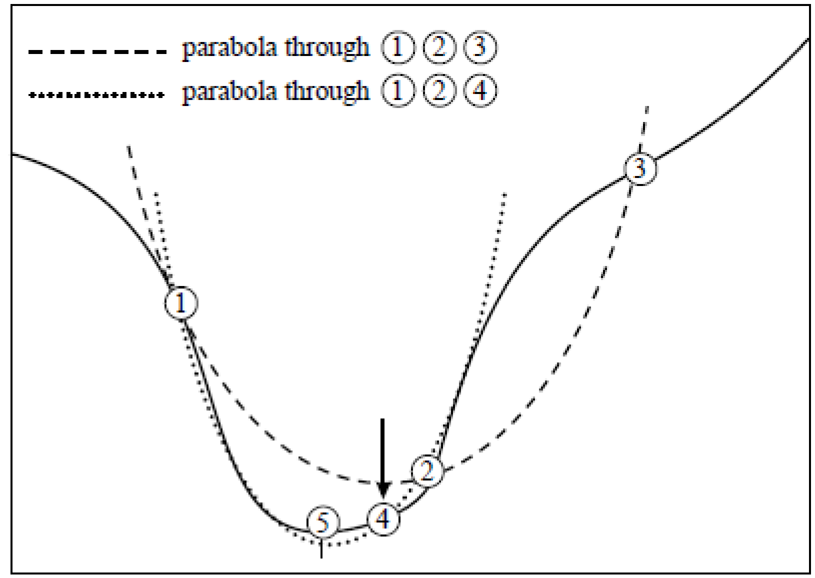
$$a = \frac{n}{G \pm \sqrt{(n-1)(nH - G^2)}}$$





Finding Minima (or Maxima)

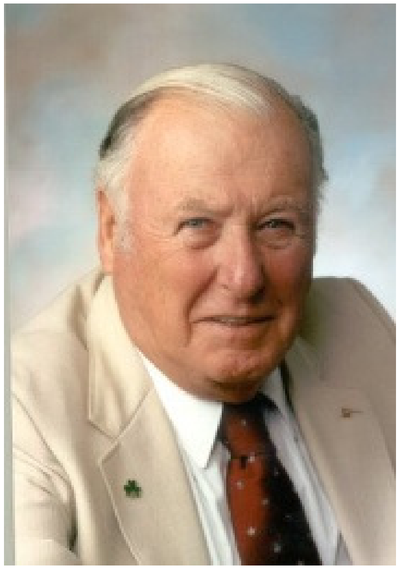
- Golden Section Search
- Brent's Method
- Downhill Simplex
- Conjugate gradient methods
- Multiple level, single linkage (MLSL)



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

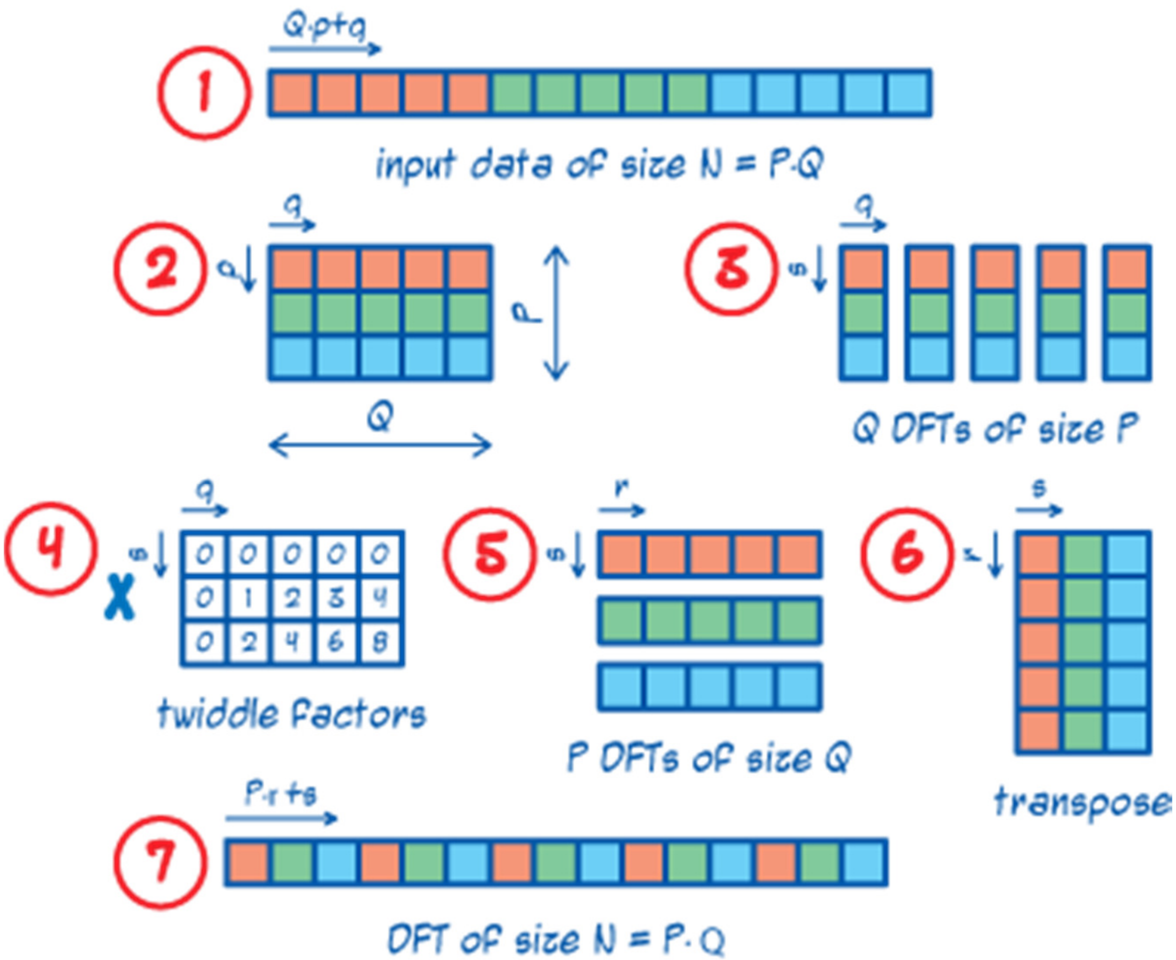
Recap: Fourier Transforms

- DFT defined by:
  $F(n) = \sum_{i=1}^{N} f(x_i) e^{-2\pi j(x_i n / x_N)}$
- Naïve approach treats each frequency individually
- Can combine operations together for significant speed-up (e.g., Cooley-Tukey algorithm)
- Specialized algorithms depending on data type



J.W. Cooley (IEEE Global History Network)

Cooley-Tukey Algorithm



Recap: Eigenproblems

- Generalized eigenproblem: $Ax = \lambda Bx$
- Solution method will depend on properties of *A* and *B*
- Techniques have greatly varying computational complexity
- Sometimes, full solution is unnecessary

Eigenproblems

- Direct method: solve $\det(A-\lambda 1)=0$
- Similarity transformations: $A \rightarrow Z^{-1}AZ$
  - Atomic transformations: construct each Z explicitly
  - Factorization methods: QR and QL methods

Atomic Transformations in Eigenproblems

- Jacobi

$$\mathbf{P}_{pq} = \begin{bmatrix} 1 & & & & & & \\ & \cdots & & & & & \\ & & c & \cdots & s & & \\ & & \vdots & 1 & \vdots & & \\ & & -s & \cdots & c & & \\ & & & & & \cdots & \\ & & & & & & 1 \end{bmatrix} \qquad \mathbf{A}' = \mathbf{P}_{pq}^T \cdot \mathbf{A} \cdot \mathbf{P}_{pq} \qquad S' = S - 2|a_{pq}|^2$$

- Householder

$$\mathbf{P} = \mathbf{1} - 2\mathbf{w} \cdot \mathbf{w}^T \qquad \mathbf{A}' = \mathbf{P} \cdot \mathbf{A} \cdot \mathbf{P} = \left[\begin{array}{c|cccc} a_{11} & k & 0 & \cdots & 0 \\ \hline k & & & & \\ 0 & & & & \\ \vdots & & & \text{irrelevant} & \\ 0 & & & & \end{array}\right]$$

- Keep iterating until off-diagonal elements are small, or use factorization approach

Factorization in Eigenproblems

- Most common approach known as QR method

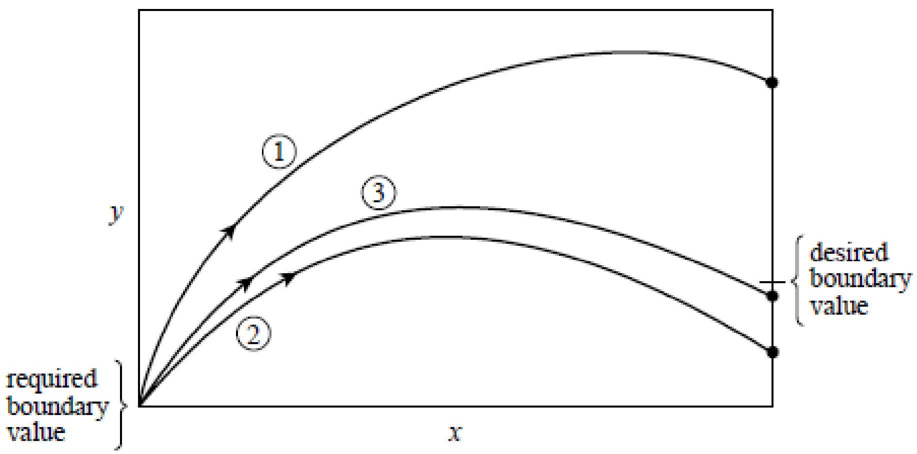
$$\mathbf{A} = \mathbf{Q} \cdot \mathbf{R} \qquad \mathbf{A}' = \mathbf{R} \cdot \mathbf{Q} \qquad \mathbf{A}' = \mathbf{Q}^T \cdot \mathbf{A} \cdot \mathbf{Q}$$

- Can also do the same with $\mathbf{A} = \mathbf{Q} \cdot \mathbf{L}$
- Slow in general, but fast in certain cases:
  - Tridiagonal matrices
  - Hessenberg matrix

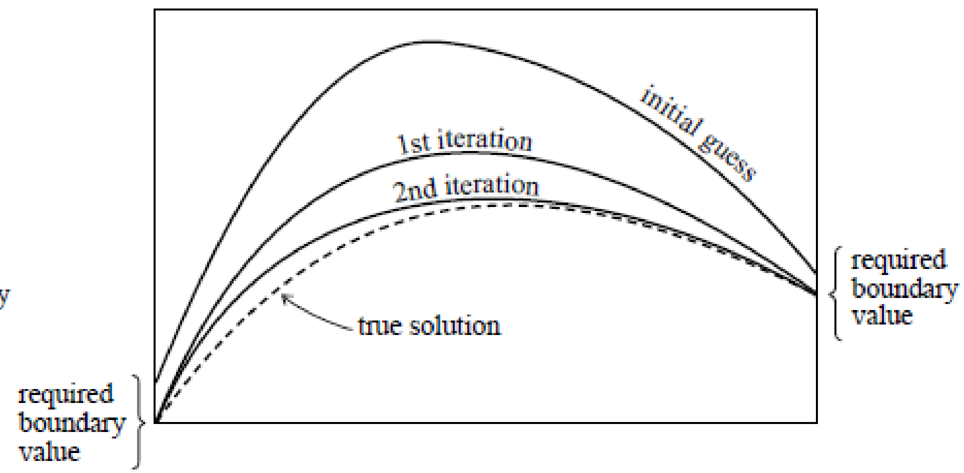
Ordinary Differential Equations

- Euler method – naïve rearrangement of ODE
- Runge-Kutta methods – match multiple Euler steps to a higher-order Taylor expansion
- Richardson extrapolation – extrapolate computed value to 0 step size
- Predictor-corrector methods – store solution to extrapolate next point, and then correct it

ODE Boundary Value Problems



Shooting Method



Boundary Value Method

Partial Differential Equations

- Classes: parabolic, hyperbolic, and elliptic

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right) \qquad \frac{\partial^2 u}{\partial t^2} = v^2\frac{\partial^2 u}{\partial x^2} \qquad \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x,y)$$

- Initial value vs. boundary value problems
- Finite difference
- Finite element methods
- Monte-Carlo
- Spectral
- Variational methods

Next Class

- Introduction to computational complexity
- Please read Chapter 1 of "Computational Complexity: A Modern Approach" by Arora & Barak