Lecture 23 Review

FFT fun.

`octave` introduction

Linear Algebra Highlights

- Physics often requires solution of simultaneous linear equations.
  e.g., coupled oscillators, electrical circuits, …

  Set of equations of the form: $Ax = b$ Solve for x, A & b given.

- Physics often requires solution of eiegnevectors & eigenvalues.
  e.g., normal modes, eigenfrequencies, bound energy states, ……

  Equations of the form: $Ax = \lambda\, x$ Solve for x, λ & A given.

  - These are 2 different classes of problems to solve.
  - Techniques are sophisticated. We will use canned software.

Solution of Linear Simultaneous Equations

Gaussian elimination. Easiest to understand.

$$\begin{array}{rcrrcr} 2u & + & v & +w & = & 1 \\ 4u & + & v & & = & -2 \\ -2u & + & 2v & +w & = & 7 \end{array}$$

$$\begin{array}{rcrrcr} 2u & + & v & +w & = & 1 \\ & - & 1v & -2w & = & -4 \\ & & 3v & +2w & = & 8 \end{array}$$

pivots

$$\begin{array}{rcrrcr} 2u & + & v & +w & = & 1 \\ & - & 1v & -2w & = & -4 \\ & & & -4w & = & -4 \end{array}$$

Count number of operations

- Forward elimination.
- Back substitution.

Where might this technique break down?

LU Decomposition

unique

Write matrix A = LU i.e., factorize A, always OK if A has non-zero pivots

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ \alpha_{10} & 1 & 0 & 0 \\ \alpha_{20} & \alpha_{21} & 1 & 0 \\ \alpha_{30} & \alpha_{31} & \alpha_{32} & 1 \end{bmatrix} \begin{bmatrix} \beta_{00} & \beta_{01} & \beta_{02} & \beta_{03} \\ 0 & \beta_{11} & \beta_{12} & \beta_{13} \\ 0 & 0 & \beta_{22} & \beta_{23} \\ 0 & 0 & 0 & \beta_{33} \end{bmatrix} = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{10} & a_{11} & a_{12} & a_{13} \\ a_{20} & a_{21} & a_{22} & a_{23} \\ a_{30} & a_{31} & a_{32} & a_{33} \end{bmatrix}$$

pivots

Ax = b =(LU)x = L(Ux) = b
Ly = b
<u>Ux</u> = y

a way to proceed.

$$y_0 = \frac{b_0}{\alpha_{00}}$$

$$y_i = \frac{1}{\alpha_{ii}}\left[b_i - \sum_{j=0}^{i-1} \alpha_{ij} y_j\right] \quad i = 1, 2, \ldots, N-1$$

$$x_{N-1} = \frac{y_{N-1}}{\beta_{N-1,N-1}}$$

$$x_i = \frac{1}{\beta_{ii}}\left[y_i - \sum_{j=I+1}^{N-1} \beta_{ij} x_j\right] \quad i = N-2, N-3, \ldots, 0$$

L & U computed <u>once</u> per A

N^3 steps.

LU Decomposition (2)

What to do if A has zero pivots?

If A has an inverse (i.e., is “non-singular”),

reorder rows of A beforehand to prevent zero pivots $A \rightarrow PA$

$PA = LU$

P = “permutation matrix” (reorders rows of A)

$$P_{24} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

e.g., swaps row 2 & 4 of A

$PAx = Pb$ has same solution x as $Ax = b$.

Exercise (from chemistry !):

$$\alpha\, O_2 + \beta\, C_4H_9NH_2 \rightarrow \gamma\, CO_2 + \delta\, H_20 + N_2$$

Find correct stoichiometry (use `octave` to find α, β, γ, δ).

Octave notes

$Ax = b$

Define A in usual way.

`octave:3> a = [1,3,5; 1, 5, 6; 3, 7, 9]` for example.

`octave:4> b = [2, 5,9]'` for example.

`octave:4> x = a\b`

a\ is octave speak for a $^{-1}$.

octave does NOT compute the inverse of a to solve for x.

Many variants to LU decomposition.
These depend on structure of A: degree of symmetry, sparseness, …

Summary

Gaussian elimination.

LU decomposition

Don't suffer in silence. Scream for help!!!