Week 3 - Monday

Monday, February 8, 2021 2:08 PM

Linear Equations $A\vec{x} = \vec{b}$

Examples of linear Systems

Optimization Problems

* Quantum Mechanics (Hamiltonian Systems) $\rightarrow \hat{H}\psi = E\psi$

(Coupled) spring systems

* Classical Mechanics Systems (first-order) $\rightarrow \nabla^2 \psi = \rho$

$\vec{F} = m\vec{a}$

ρ_m gravity

ρ_e charge

Stochastic Processes $\underline{A}^{P}\psi$

Solution Methods
① Gauss-Jordan Elimination
② LU decomposition
③ Matrix Inversion
④ SVD - Friday

① G.J. Elimination $A\vec{x} = \vec{b}$

$$\vec{A} = \begin{pmatrix} 10 & -7 & 1 \\ -3 & 2 & 6 \\ 5 & -1 & 5 \end{pmatrix} \quad \vec{b} = \begin{pmatrix} 8 \\ 4 \\ 6 \end{pmatrix}$$

① $(A|b)$ look at Augmented Matrix

② take linear combinations of rows to get upper-triangular form

③ back-substituting to solve.

$$\left(\begin{array}{ccc|c} 10 & -7 & 1 & 8 \\ -3 & 2 & 6 & 4 \\ 5 & -1 & 5 & 6 \end{array}\right) \longrightarrow \begin{array}{l} R_1 \\ R_2 \rightarrow \left(R_2 + \frac{3}{10}R_1\right)10 \\ R_3 \rightarrow \left(R_3 - \frac{5}{10}R_1\right)2 \end{array} \left(\begin{array}{ccc|c} 10 & -7 & 1 & 8 \\ 0 & -1 & 63 & 64 \\ 0 & 5 & 9 & 4 \end{array}\right)$$

R_1
R_2
$R_3 \to \frac{1}{384}(R_3 + 5R_2)$
$$\left(\begin{array}{ccc|c} 10 & -7 & 1 & 8 \\ 0 & -1 & 63 & 64 \\ 0 & 0 & 1 & 1 \end{array}\right)$$

★ Maintain Precision:
Keep rows w/ large coeffs ↓
large ↓
$\# X = \#$

$R_2 \to -(R_2 - 63R_3)$
$$\left(\begin{array}{ccc|c} 10 & -7 & 1 & 8 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & 1 \end{array}\right)$$

$R_1 \to \frac{1}{10}(R_1 + 7R_2 - R_3)$
$$\left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & 1 \end{array}\right)$$

$$\Downarrow$$
$$X = \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}$$

② L-U decomposition

$$A = L \cdot U$$

$$\begin{pmatrix} 10 & -7 & 1 \\ -3 & 2 & 6 \\ 5 & -1 & 5 \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}$$

↳ diagonal components of $L = 1$
are a free choice (under-determined system)

$$= \begin{pmatrix} 1 & 0 & 0 \\ -\frac{3}{10} & 1 & 0 \\ \frac{5}{10} & l_{32} & 1 \end{pmatrix} \begin{pmatrix} 10 & -7 & 1 \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}$$

→ Numerical Recipes 2.3.1 has explicit sum

$l_{32} \to 25/36$

$u_{22} = (2 - 21/10)$
$u_{23} = (6 + 3/10)$
$u_{33} = 2$

★ $\det(A) = \det(L \cdot U) = \det(L)\det(U) \overset{1}{=} \det(U) = \underline{\underline{\prod_i u_{ii}}}$

$\underline{\vec{y} \equiv U \cdot \vec{x}}$

$A\vec{x} = \vec{b}$
$= L \cdot U\vec{x} = b$
$L\vec{y} = \vec{b}$ → use forward sub. to find $\vec{y}$

$= L \cdot U \vec{x} = b$

$\underline{L \vec{y} = \vec{b}}$ → use forward sub. to find $\vec{y}$

$U \vec{x} = \vec{y}$ → Use back-sub. to find $\vec{x}$

Inversion Similar to Gauss-Jordan Elimination

① $(A | I)$

② Perform row interchanges, linear combinations to get $A \to I$, $I \to A^{-1}$

Null spaces $\vec{A} \vec{x} = 0$

- Vectors with no eigenvalue $(=0)$
- A not invertible
- Friday: SVD will help/handle

Eigenvalue finding

- Rayleigh Method
- Iterative Methods
- If diagonalization is known
- look @ polynomial roots

$$A \vec{v}_{\lambda_1} = \lambda_1 \vec{v}_{\lambda_1}$$

Power Iteration

$$\vec{v} = c_1 \vec{v}_{\lambda_1} + c_2 \vec{v}_{\lambda_2} + \cdots$$

$$\lim_{p \to \infty} A^p \vec{v} = c_1 \lambda_1^p \vec{v}_{\lambda_1} + c_2 \lambda_2^p \vec{v}_{\lambda_2} + \cdots$$

isolate largest λ

Converge linearly

$$\lim_{p \to \infty} (A - \mu I)^{-p} \vec{v} = c_1 (\lambda_1 - \mu)^{-p} \vec{v}_{\lambda_1} + \cdots$$

$\frac{1}{(\lambda_1 - \mu)^p}$ v.s. $\frac{1}{(\lambda_2 - \mu)^p}$

isolates smallest $\lambda - \mu$, eigenvalue closest to μ

Refinement: each time we multiply by $(A-\mu I)^{-1}$,

$$\rightarrow \mu \rightarrow \frac{\vec{v}^T A \vec{v}}{|\vec{v}|^2} \rightarrow \lambda$$

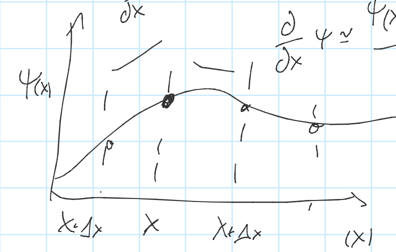
Converge "Cubically"

QM:

$$\left.\begin{aligned} H\psi &= E\psi \\ \nabla^2 \psi &= \rho \end{aligned}\right\} \quad \nabla^2 \psi \rightarrow \frac{\partial^2}{\partial x^2}\psi(x)$$

$H \rightarrow \nabla^2$

$$\frac{\partial}{\partial x}\psi \approx \frac{\psi(x) - \psi(x-\Delta x)}{\Delta x} \qquad \frac{\partial}{\partial x}\psi \approx \frac{\psi(x+\Delta x) - \psi(x)}{\Delta x}$$



$$\frac{1}{\Delta x^2}\begin{pmatrix} & & \ddots & & & \\ \cdots & 1 & -2 & 1 & \cdots & \\ 0 & 0 & 1 & -2 & 1 & \cdots \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & \cdots \\ & & \cdots & & 1 & -2 & 1 & \cdots \\ & & & & & \ddots \end{pmatrix}\begin{pmatrix} \vdots \\ \psi(x-\Delta x) \\ \psi(x) \\ \psi(x+\Delta x) \\ \vdots \end{pmatrix} = V(x)$$

$$\frac{\partial^2}{\partial x^2}\psi = \frac{\psi(x+\Delta x) - 2\psi(x) + \psi(x-\Delta x)}{\Delta x^2}$$