Large Scale Eigenvalue Problems: Iterative Methods

Lecture 4

Dr. Amr Bayoumi

Fall 2014

Arab Academy for Science and Technology - Cairo

Outline

- Iterative Solutions:
  - Highest Eigenvalue: Power Method
  - Lowest Eigenvalue: Inverse Power Method
  - Other Eigenvalues: Eigenvalue Substitution

Power Method: Dominant Eigenvalue

Target: $\mathbf{y} = A\mathbf{x} = \lambda\mathbf{x}$

Start with all 1's **x** vector: $\mathbf{x_0}=[1\ 1\ \ldots\ 1]^T$

$\mathbf{y}_1 = A\mathbf{x}_0 = \lambda^{(1)}\mathbf{x_1}$ (*Iteration number = 1*)

$\lambda^{(1)}$= element in $\mathbf{y}_1$ with highest absolute value

$$\mathbf{x}_1 = \frac{1}{\lambda^{(1)}}\mathbf{y}_1 = \frac{1}{\lambda^{(1)}}A\mathbf{x}_0$$

$\mathbf{y}_2 = A\mathbf{x}_1$ (*Iteration number = 2*)

$\lambda^{(2)}$= element in $\mathbf{y}_2$ with highest absolute value

$$\mathbf{x}_2 = \frac{1}{\lambda^{(2)}}\mathbf{y}_2 \text{ , ...}$$

$$\mathbf{y}_k = A\mathbf{x}_{k-1} = \lambda^{(k)}\mathbf{x}_k$$

$$\mathbf{x}_k = \frac{1}{\lambda^{(k)}}\mathbf{y}_k$$

Power Method: Dominant Eigenvalue Proof

Assume $\mathbf{x} = d_1\mathbf{v_1} + d_2\mathbf{v_2} + \ldots\ldots + d_n\mathbf{v_n}$

Where $\mathbf{v_n}$ are linearly independent eigenvectors

$$\mathrm{A}\mathbf{x} = \lambda\mathbf{x}$$

$$\mathrm{A}\mathbf{x} = \lambda_1 d_1\mathbf{v}_1 + \lambda_2 d_2\mathbf{v}_2 + \ldots\ldots + \lambda_n d_n\mathbf{v}_n$$

$$\mathrm{A}^2\mathbf{x} = \lambda_1{}^2 d_1\mathbf{v}_1 + \lambda_2{}^2 d_2\mathbf{v}_2 + \ldots\ldots + \lambda_n{}^2 d_n\mathbf{v}_n$$

After k iterations:

$$\mathrm{A}^k\mathbf{x} = \lambda_1{}^k d_1\mathbf{v}_1 + \lambda_2{}^k d_2\mathbf{v}_2 + \ldots\ldots + \lambda_n{}^k d_n\mathbf{v}_n$$

$$\frac{1}{\lambda_1{}^k}\mathrm{A}^k\mathbf{x} = d_1\mathbf{v}_1 + (\lambda_2/\lambda_1)^k d_2\mathbf{v}_2 \ldots + (\lambda_n/\lambda_1)^k d_n\mathbf{v}_n$$

If λ_1 is considerably higher than λ_2 , …, λ_n: $\frac{1}{\lambda_1{}^k}\mathrm{A}^k\mathbf{x} \to d_1\mathbf{v}_1$

Power Method: Dominant Eigenvalue

Target: $\mathbf{y} = A\mathbf{x} = \lambda\mathbf{x}$

Start with all 1's **x** vector: $\mathbf{x_0}=[1\ 1\ \ldots\ 1]^T$

$\mathbf{y}_1 = A\mathbf{x}_0 = \lambda^{(1)}\mathbf{x_1}$ (*Iteration number = 1*)

$\lambda^{(1)}$= element in $\mathbf{y}_1$ with highest absolute value

$$\mathbf{x}_1 = \frac{1}{\lambda^{(1)}}\mathbf{y}_1 = \frac{1}{\lambda^{(1)}}A\mathbf{x}_0$$

$\mathbf{y}_2 = A\mathbf{x}_1$ (*Iteration number = 2*)

$\lambda^{(2)}$= element in $\mathbf{y}_2$ with highest absolute value

$$\mathbf{x}_2 = \frac{1}{\lambda^{(2)}}\mathbf{y}_2 = \frac{1}{\lambda_2\lambda_1}A^2\mathbf{x}_0 \text{ -->} \approx \frac{1}{\lambda^2}A^2\mathbf{x}_0$$

$$\mathbf{x}_k = \frac{1}{\lambda_k}\mathbf{y}_\mathrm{k} \text{ -->} \approx \frac{1}{\lambda^k}A^k\mathbf{x}_0$$

Inverse Power Method: Smallest Absolute Eigenvalue

Target: $\mathbf{y} = A^{-1}\mathbf{x} = \lambda^{-1}\mathbf{x} = \propto \mathbf{x}$

$$B\mathbf{x} = \propto \mathbf{x}$$

At iteration k: $\frac{B^k}{\alpha_1{}^k}\mathbf{x}$ ---> $d_1\,\mathbf{v}_1$

Dominant $\propto$ is equivalent to smallest absolute λ

Use LU factorization to solve for y:

$$A\mathbf{y}^{(k)} = \mathbf{x}^{(k-1)}$$

Find dominant element in y(k) as $\propto$

Keep on, then least $\lambda = \propto^{-1}$

Power Method: Rest of Eigenvalues

- Find one eigenvalue using power or inverse power method, λ_1
- Use it to shift a new set of l, such that

  $\lambda' = \lambda - \lambda_1$

- Solve for the next eigenvalue in:

$\mathbf{y} = \mathrm{C}\mathbf{x} = [\mathbf{A} - \lambda_1 \mathbf{I}]\mathbf{x}$ **(Power Method: Most Dominant)**

Or :

$\mathbf{y} = \mathrm{D}\mathbf{x} = [\mathbf{B} - \alpha_1 \mathbf{I}]\mathbf{x}$ **(Inverse Power Method: Least Dominant)**

One eigenvalue is 0 (previously found, shifted)

$\lambda_2 = \lambda'_1 + \lambda_1$ **or** $\alpha_2 = \alpha'_1 + \alpha_1$

Analytical Solution for Schrodinger's Eqn. Infinite Well (3 Internal Nodes)

Solution: **U=0 for 0<x<L**

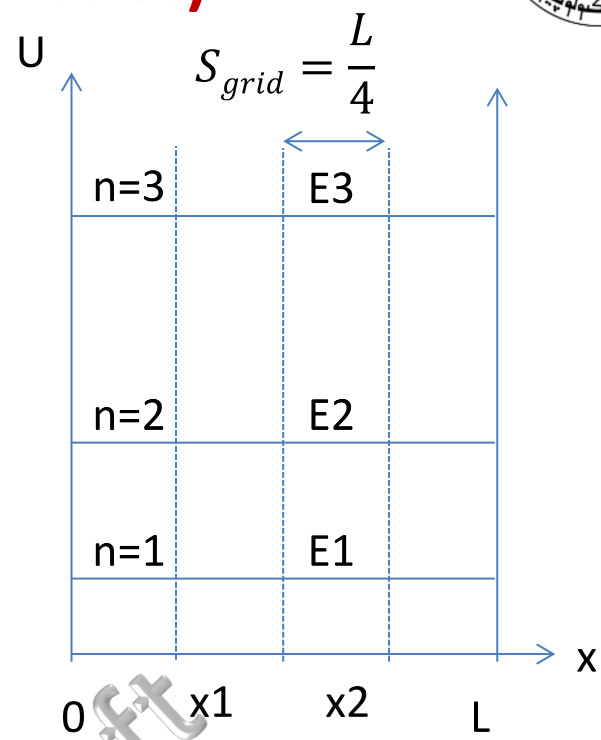
$$k_n = \frac{n\pi}{L};\ En = \frac{\hbar^2 k^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$\varphi_i^{(n)} = An\sin(\frac{n\pi}{L}\ \mathrm{x})$$

Boundary Conditions : $\varphi^{(n)}(0)=0$, $\varphi^{(n)}(L)=0$

Thus: $\varphi_0^{(n)}=0$, $\varphi_4^{(n)} = 0$

For L = 1nm, m=9.1x10^{-31}Kg, $\hbar$=1.054x10^{-34}J.s



FD 3-Node Schrodinger Eqn:

Refinement: Use Three Internal Nodes

$$\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y1 \\ y2 \\ y3 \end{bmatrix}$$

$$S_{grid} = \frac{L}{4}, \ \lambda_n = S^2_{grid} k_n^2, \ k_n = \frac{\sqrt{\lambda_n}}{S_{grid}} = \frac{\sqrt{\lambda_n}}{L/4}$$

k_1 (Power)= 3.061×10^9, k_1 (*Analytical*) = 3.14×10^9

k_2 (Power)= 5.656×10^9, k_2 (*Analytical*) = 6.28×10^9

k_3 (Power)= 7.391×10^9, k_3 (*Analytical*) = 9.42×10^9