Eigenvalue Problems

Lecture 2

Dr. Amr Bayoumi

Fall 2016

Arab Academy for Science and Technology - Cairo

Outline

- Definition
- Basic Procedure
- Example Systems
- Finite Difference Representation

Definitions

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

A: n x n Matrix

x : n x 1 vector

λ_i : scalar factor called "Eigenvalue"

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda_i \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

Problem:

Find possible values of $\lambda : i \leq$ n *independent* values

Procedure for Finding Eigenvalues

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda_i \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$a_{11}\, x_1 + a_{12} x_2 = \lambda_i\, x_1$$

$$a_{21}\, x_1 + a_{22}\, x_2 = \lambda_i\, x_2$$

$$[A \quad -\lambda I]\boldsymbol{x} = 0$$

Condition for Solution Existence:

Det (A – λ I) = $|A \quad -\lambda I|$ **= 0**

$$(a_{11} - \lambda_i) x_1 + a_{12}\, x_2 = 0$$

$$a_{21}\, x_1 + (a_{22} - \lambda_i) x_2 = 0$$

In this example:

$$(a_{11} - \lambda_i)\,(a_{22} - \lambda_i) - a_{12} a_{21} = 0$$

$$\lambda_i^{\,2} - (a_{11} + a_{22})\lambda_i - a_{12} a_{21} + a_1 + a_{22} = 0$$

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \lambda_i \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

Find roots of equation:

$$\lambda_{1,2} = [-b \pm \sqrt{b^2 - 4ac}\ ] / 2a$$

Example for Finding Eigenvalues

$$\begin{bmatrix} 2 & 1 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \lambda_i \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$2\,x_1 + x_2 = \lambda_i\, x_1$$
$$2\,x_1 + 3\,x_2 = \lambda_i\, x_2$$

$$(2 - \lambda_i)x_1 + x_2 = 0$$
$$2\,x_1 + (3 - \lambda_i)x_2 = 0$$

$$\begin{bmatrix} 2 & 1 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \lambda_i \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

Condition for Solution Existence:

$$\text{Det}\,(\mathbf{A} - \lambda\,\mathbf{I}) = |\boldsymbol{A} \quad - \lambda \boldsymbol{I}| = 0$$

In this example:

$$(2 - \lambda_i)\,(3 - \lambda_i) - (2)(1) = 0$$
$$\lambda_i^{\,2} - 5\,\lambda_i + 4 = 0$$

Eigenvalues: Find roots of equation:

$$\lambda_1 = 2.5 + 1.5 = 4$$
$$\lambda_2 = 2.5 - 1.5 = 1$$

To Find Eigenvectors: *Solve for* **x** *Vector*

For Eigenvalue $\lambda_1=4$

$$(2-4)x_1 + x_2 = 0$$
$$2x_1 + (3-4)x_2 = 0$$

$$-2x_1 + x_2 = 0$$
$$2x_1 - x_2 = 0$$
$$x_2 = 2x_1$$

Assume $x_1 = 1$ ➔ $x_2 = 2$

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

For Eigenvalue $\lambda_2=1$

$$(2-1)x_1 + x_2 = 0$$
$$2x_1 + (3-1)x_2 = 0$$

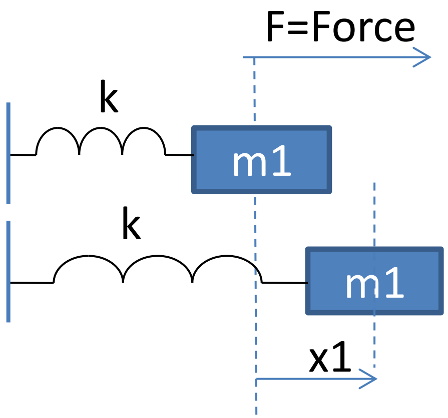
$$x_1 + x_2 = 0$$
$$2x_1 + 2x_2 = 0$$
$$x_2 = -x_1$$

Assume $x_1 = 1$ ➔ $x_2 = -1$

$$\mathbf{x}_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Example Applications for Eigenvalue Problem: Dual Mass Spring System

Single Mass, Single Spring, Fixed Boundaries



$$F = m_1 \ddot{x}_1 = -k\, x_1$$

$$\ddot{x}_1 + \frac{k}{m1} x_1 = 0$$

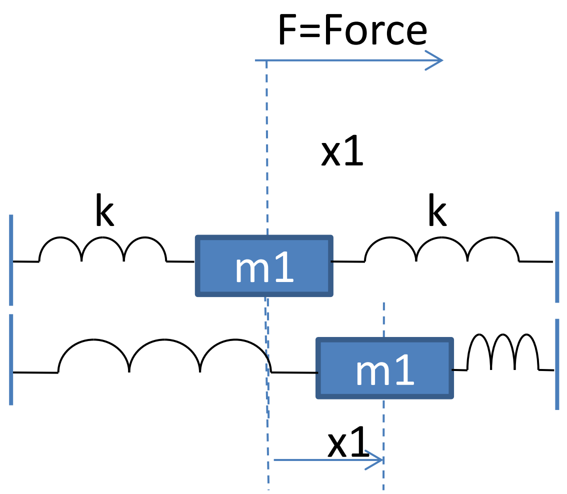
Solution:

$$x_1 = C_1 \sin \omega t$$

$$\ddot{x}_1 = -C_1 \omega^2 \sin \omega t$$

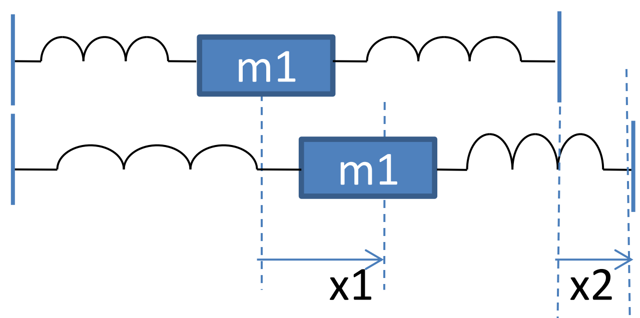
After: S. Capra and R. Canale, Numerical Methods for Engineers, 5th Ed. McGraw Hill

Example Applications for Eigenvalue Problem: Dual Mass Spring System



Single Mass, Dual Spring, Fixed Boundaries

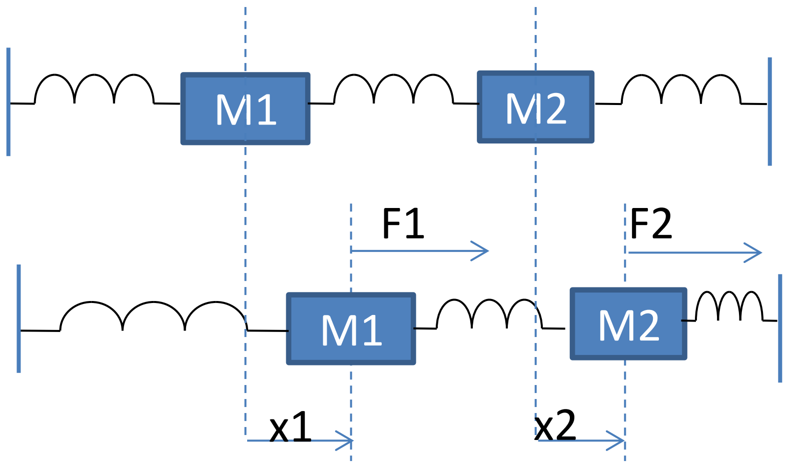
$$F = m_1\, \ddot{x}_1 = -2k\, x_1$$



Single Mass, Dual Spring, Moving Boundaries

$$F = m_1\, \ddot{x}_1 = -k\, x_1 - k(x_1 - x_2)$$

Example Applications for Eigenvalue Problem: Dual Mass Spring System



Dual Mass, Dual Spring, Fixed Boundaries

$$F_1 = m_1\ddot{x}_1 = -k(x_1) - k(x_1 - x_2)$$
$$F_2 = m_2\ddot{x}_2 = -k(x_2) - k(x_2 - x_1)$$

$$\ddot{x}_1 = -\frac{2k}{m_1}(x_1) + \frac{k}{m_1}(x_2)$$
$$\ddot{x}_2 = \frac{k}{m_2}(x_1) - \frac{2k}{m_2}(x_2)$$

Using $x_i = C_i \sin \omega t$, we get the Eigenvalue problem:

$$\left(\frac{2k}{m_1} - \omega^2\right) C_1 - \frac{k}{m_2} C_2 = 0$$

$$-\frac{k}{m_2} C_1 + \left(\frac{2k}{m_2} - \omega^2\right) C_2 = 0$$

$\Longleftrightarrow$

$$\begin{bmatrix} a_{11} - \lambda & a_{21} \\ a_{21} & a_{22} - \lambda \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Required Eigenvalue: $\lambda = \omega^2$

Example Applications for Eigenvalue Problem: Dual Mass Spring System

Dual Mass, Dual Spring, Fixed Boundaries

Example:

- $m_1 = m_2 = 40$ Kg, $k = 200$N/m
- Eigenvalues: $\lambda_1 = \omega^2_1 = 15$ sec $^{-2}$, $\lambda_2 = \omega^2_2 = 5$ sec $^{-2}$
- Eigenvectors:

$$\begin{bmatrix} 1 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

After: S. Capra and R. Canale, Numerical Methods for Engineers, 5th Ed. McGraw Hill

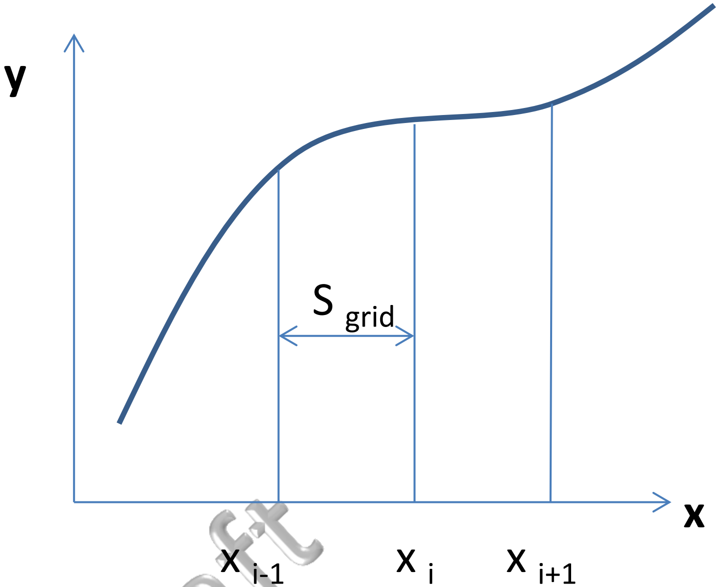
Eigenvalue using Finite Difference Implementation

Finite Difference Representation of Derivatives

- **Using most basic *Centered* difference equation:**

$$\frac{dy_i}{dx} = \frac{y_{i+1} - y_{i-1}}{2\,S_{grid}}$$

$$\frac{d^2y_i}{dx^2} = \frac{y_{i+1} - 2y_i + y_{i-1}}{S^2_{grid}}$$



Example: 2-Node D.E. with Boundary Conditions

$$y''_1 = a_{11}(y_1) + a_{12}(y_2)$$
$$y''_2 = a_{21}\,(y_1) + a_{22}(y_2)$$

Using Finite Difference (FD):

$$\frac{y_2 - 2y_1 + y_0}{S^2_{grid}} = a_{11}(y_1) + a_{12}(y_2)$$

$$\frac{y_3 - 2y_2 + y_1}{S^2_{grid}} = a_{21}(y_1) + a_{22}(y_2)$$

y_0 and y_3 are given as Boundary Conditions, no need to solve for.

Examples Applications for Eigenvalue + Finite Difference: Schrodinger's Equation

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$$

$$k^2 = 2m(E-U)/\hbar^2$$

$$\frac{d^2\varphi}{dx^2} = \frac{\Psi_{i+1} - 2\Psi_i + \Psi_{i-1}}{s^2_{grid}}$$

Second Order Differential Equation using Finite Difference (FD)

2-Node D.E.

$$y'' = -k^2 y$$

$$y'' + k^2 y = 0$$

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{S^2_{grid}} + k^2 y_i = 0$$

$$y_{i+1} - (2 - S^2_{grid} k^2)\, y_i + y_{i-1} = 0$$

$$-y_{i+1} + (2 - \lambda)\, y_i - y_{i-1} = 0$$

Analytical Solution for Schrodinger's Eqn.
Infinite Well

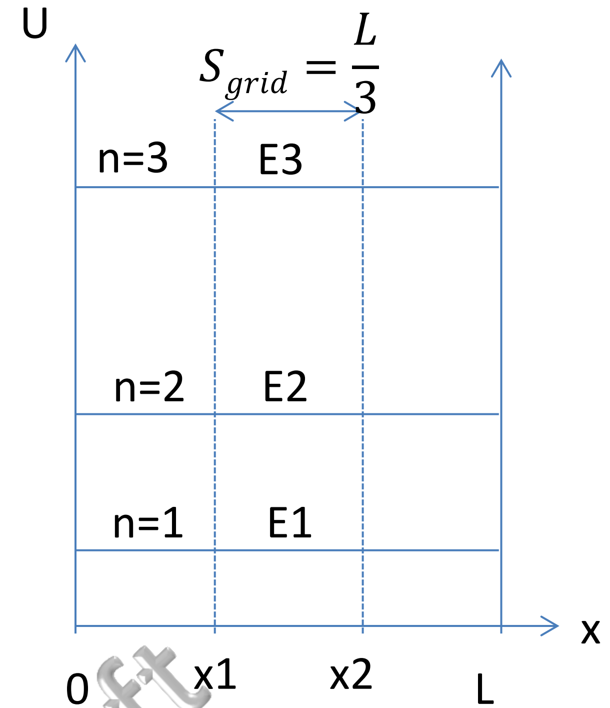
Solution: **U=0 for 0<x<L**

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

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

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

Thus: $\varphi_0^{(n)}$=0, $\varphi_3^{(n)}$ = 0 (nodes 0 and 3 are present, but removed from equations since they are known. We now have 2 instead of 4 eqns.)



E_n = 0.6024x10^{-19} n^2 *Joules* = 0.3765 n^2 *eV*

E_1= 0.3765 eV, E_2= 1.506 eV, E_3= 3.388 eV

Eigenvalue FD 2-Node Schrodinger Eq.

Polynomial Method

$$\begin{bmatrix} 2-\lambda & -1 \\ -1 & 2-\lambda \end{bmatrix} \begin{bmatrix} \varphi_1 \\ \varphi_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Det ()= $(2-\lambda)^2 - 1 = 0$

$2 - \lambda = \pm\sqrt{1}$

$\lambda_1 = 1, \; \lambda_2 = 3$

$$\lambda_n = S^2{}_{grid}\, k_n{}^2 , \; k_n = \frac{\sqrt{\lambda_n}}{S_{grid}} = \frac{\sqrt{\lambda_n}}{L/3}$$

Draft

k_1 (FD)= $3.0\text{x}10^9$, k_1 (*Analytical*) = $3.14\text{x}10^9$

k_2 (FD)= $5.196\text{x}10^9$, k_2 (*Analytical*) = $6.28\text{x}10^9$

Eigenvalue FD 2-Node Schrodinger Eq.

Find ψ_i

$$\begin{bmatrix} 2-\lambda & -1 \\ -1 & 2-\lambda \end{bmatrix}\begin{bmatrix} \varphi_1 \\ \varphi_2 \end{bmatrix}=\begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$\lambda_1 = 1,\ \lambda_2 = 3$

λ_1: $\varphi_1 = 1$, $\varphi_2 = 1$

λ_2: $\varphi_1 = 1$, $\varphi_2 = -1$

Analytical: (A_1 & A_2 are normalization coefficients)

λ_1: $\varphi_1^{(1)} = A_1 \sin(\frac{1\pi}{L}\frac{L}{3}) = 0.866025\, A_1,$

$\varphi_2^{(1)} = A_1 \sin(\frac{1\pi}{L}\frac{2L}{3}) = 0.866025 A_1$

λ_2: $\varphi_1^{(2)} = A_2 \sin(\frac{2\pi}{L}\frac{L}{3}) = 0.866025\, A_2,$

$\varphi_2^{(2)} = A_2 \sin\left(\frac{2\pi}{L}\frac{2L}{3}\right) = -\,0.866025 A_2$

Refinement: Use Three Internal Nodes

$$\begin{bmatrix} 2-\lambda & -1 & 0 \\ -1 & 2-\lambda & -1 \\ 0 & -1 & 2-\lambda \end{bmatrix} \begin{bmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Det ()= $(2-\lambda)\,[(2-\lambda)^2 - 1] - (-1)\,[(-1)(2-\lambda) - 0\,] + 0 = 0$

$(2-\lambda)[(2-\lambda)^2 - 1 - 1] = 0$

$(2-\lambda) = 0, \quad \textit{and} \quad (2-\lambda) = \pm\sqrt{2}$

$\lambda_1 = 0.5857, \quad \lambda_2 = 2, \quad \lambda_3 = 3.4142, \quad S_{grid} = \frac{L}{4}$

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

k_1 (FD)= $3.061\text{x}10^9$, k_1 (*Analytical*) = $3.14\text{x}10^9$ ***(improvement over 2 nodes)***

k_2 (FD)= $5.656\text{x}10^9$, k_2 (*Analytical*) = $6.28\text{x}10^9$ ***(improvement over 2 nodes)***

k_3 (FD)= $7.391\text{x}10^9$, k_3 (*Analytical*) = $9.42\text{x}10^9$ *(First time to appear)*

Exercise:

Find φ_1, .., φ_3 and compare with exact solution