PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF in Olin 103

Discussion for Lecture 15 – Chap. 4 (F & W)

Analysis of motion near equilibrium

1. Small oscillations about equilibrium
2. Normal modes of vibration

Your questions –

From Can -- If we know the eigenvector and eigenvalue, can we find the original matrix? What exactly are their relationships?

Short answer – If we know all of the eigenvalues and eigenvectors, we can reconstruct the matrix.

From Wells -- Do normal modes correspond to resonance frequencies of the system?

Short answer – Yes. If a harmonic force at a natural frequency is applied, resonance occurs.

From Owen -- The molecule on slide six looks like H2O. How do the results of numerical integration (molecular dynamics) compare to the analytical results from the eigenvalue problem? (Comparing the "experimental" vs theoretical omega values for different vibrational modes)

Short answer – The example is a linear molecule like CO_2 – depending on the spring constant k, the agreement can be reasonable…

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/23/2021	Chap. 1	Introduction	#1	8/27/2021
2	Wed, 8/25/2021	Chap. 1	Scattering theory	#2	8/30/2021
3	Fri, 8/27/2021	Chap. 1	Scattering theory		
4	Mon, 8/30/2021	Chap. 1	Scattering theory	#3	9/01/2021
5	Wed, 9/01/2021	Chap. 1	Summary of scattering theory	#4	9/03/2021
6	Fri, 9/03/2021	Chap. 2	Non-inertial coordinate systems	#5	9/06/2021
7	Mon, 9/06/2021	Chap. 3	Calculus of Variation	#6	9/10/2021
8	Wed, 9/08/2021	Chap. 3	Calculus of Variation		
9	Fri, 9/10/2021	Chap. 3 & 6	Lagrangian Mechanics	#7	9/13/2021
10	Mon, 9/13/2021	Chap. 3 & 6	Lagrangian Mechanics	#8	9/17/2021
11	Wed, 9/15/2021	Chap. 3 & 6	Constants of the motion		
12	Fri, 9/17/2021	Chap. 3 & 6	Hamiltonian equations of motion	#9	9/20/2021
13	Mon, 9/20/2021	Chap. 3 & 6	Liouville theorm	#10	9/22/2021
14	Wed, 9/22/2021	Chap. 3 & 6	Canonical transformations		
15	Fri, 9/24/2021	Chap. 4	Small oscillations about equilibrium	#11	9/27/2021
16	Mon, 9/27/2021	Chap. 4	Normal modes of vibration		

PHY 711 – Assignment #11

September 24, 2021

1. Find the eigenvalues and eigenvectors of the 2×2 matrix

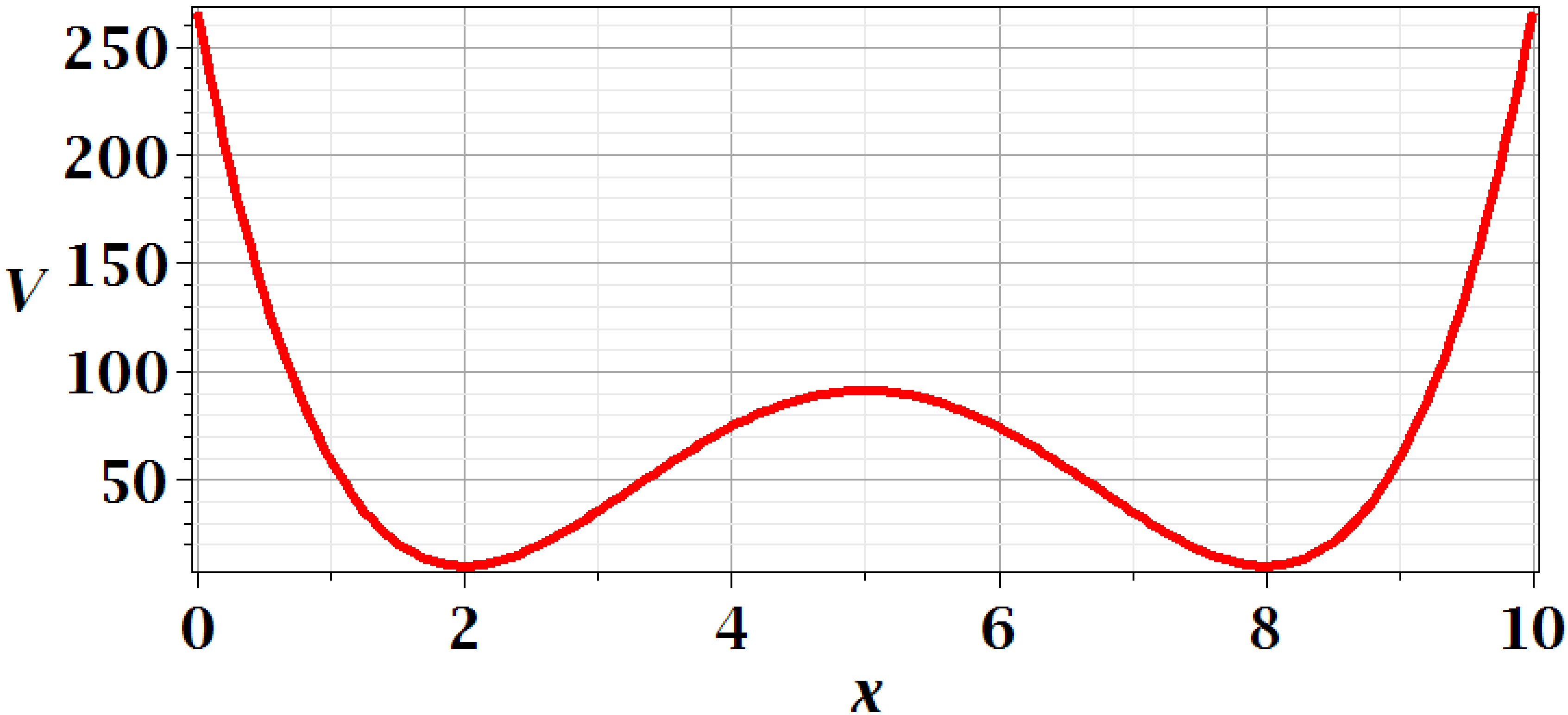
$$M = \begin{pmatrix} 7 & -1 \\ -1 & 7 \end{pmatrix}.$$

2. Find the eigenvalues and eigenvectors of the 3×3 matrix

$$M = \begin{pmatrix} 7 & -1 & 0 \\ -1 & 7 & -1 \\ 0 & -1 & 7 \end{pmatrix}.$$

Motivation for studying small oscillations – many interacting systems have stable and meta-stable configurations which are well approximated by:

$$V(x) \approx V(x_{eq}) + \tfrac{1}{2}\left(x - x_{eq}\right)^2 \left.\frac{d^2V}{dx^2}\right|_{x_{eq}} = V(x_{eq}) + \tfrac{1}{2}k\left(x - x_{eq}\right)^2$$



Equations of motion for a single oscillator:

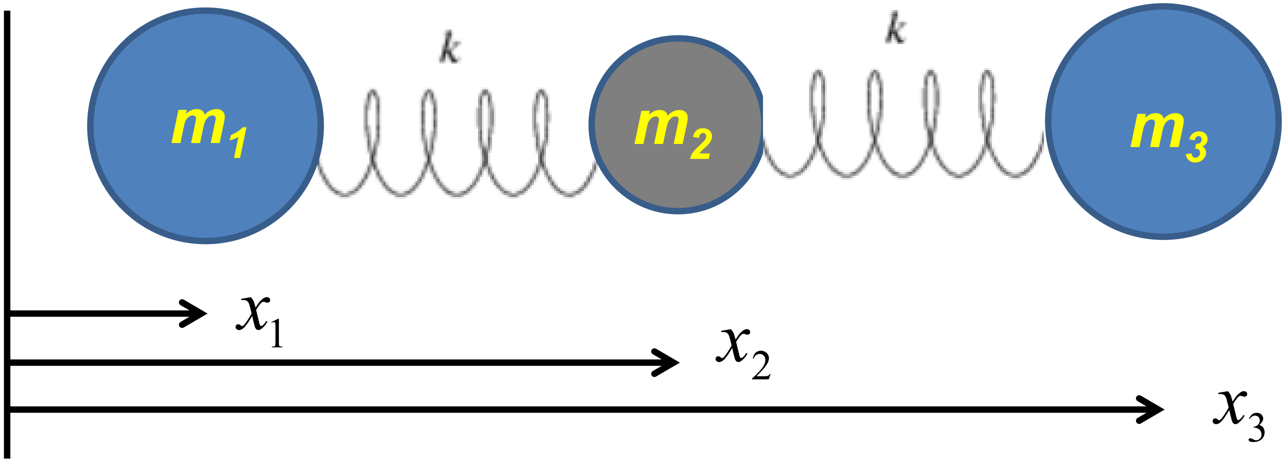
Let $k \equiv m\omega^2$

$$L(x,\dot{x},t) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x} \qquad \Rightarrow m\ddot{x} = -m\omega^2 x$$

$$x(t) = A\sin(\omega t + \varphi)$$

Example – linear molecule



$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 - \frac{1}{2}k\left(x_2 - x_1 - \ell_{12}\right)^2 - \frac{1}{2}k\left(x_3 - x_2 - \ell_{23}\right)^2$$

$$L=\frac{1}{2}m_1\dot{x}_1^2+\frac{1}{2}m_2\dot{x}_2^2+\frac{1}{2}m_3\dot{x}_3^2$$

$$-\frac{1}{2}k\left(x_2-x_1-\ell_{12}\right)^2-\frac{1}{2}k\left(x_3-x_2-\ell_{23}\right)^2$$

Let: $\quad x_1\rightarrow x_1-x_1^0 \qquad x_2\rightarrow x_2-x_1^0-\ell_{12} \qquad x_3\rightarrow x_3-x_1^0-\ell_{12}-\ell_{23}$

$$L=\frac{1}{2}m_1\dot{x}_1^2+\frac{1}{2}m_2\dot{x}_2^2+\frac{1}{2}m_3\dot{x}_3^2-\frac{1}{2}k\left(x_2-x_1\right)^2-\frac{1}{2}k\left(x_3-x_2\right)^2$$

Coupled equations of motion:

$$m_1\ddot{x}_1=k\left(x_2-x_1\right)$$

$$m_2\ddot{x}_2=-k\left(x_2-x_1\right)+k\left(x_3-x_2\right)=k\left(x_1-2x_2+x_3\right)$$

$$m_3\ddot{x}_3=-k\left(x_3-x_2\right)$$

Coupled equations of motion :

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

$$m_2\ddot{x}_2 = -k(x_2 - x_1) + k(x_3 - x_2) = k(x_1 - 2x_2 + x_3)$$

$$m_3\ddot{x}_3 = -k(x_3 - x_2)$$

Let $x_i(t) = X_i^\alpha e^{-i\omega_\alpha t}$ where X_i^α and ω_α are to be determined

$$-\omega_\alpha^2 m_1 X_1^\alpha = k\left(X_2^\alpha - X_1^\alpha\right)$$

$$-\omega_\alpha^2 m_2 X_2^\alpha = k\left(X_1^\alpha - 2X_2^\alpha + X_3^\alpha\right)$$

$$-\omega_\alpha^2 m_3 X_3^\alpha = -k\left(X_3^\alpha - X_2^\alpha\right)$$

Coupled linear equations:

$$-\omega_\alpha^2 m_1 X_1^\alpha = k\left(X_2^\alpha - X_1^\alpha\right)$$

$$-\omega_\alpha^2 m_2 X_2^\alpha = k\left(X_1^\alpha - 2X_2^\alpha + X_3^\alpha\right)$$

$$-\omega_\alpha^2 m_3 X_3^\alpha = -k\left(X_3^\alpha - X_2^\alpha\right)$$

Matrix form:

$$\begin{pmatrix} k-\omega_\alpha^2 m_1 & -k & 0 \\ -k & 2k-\omega_\alpha^2 m_2 & -k \\ 0 & -k & k-\omega_\alpha^2 m_3 \end{pmatrix}\begin{pmatrix} X_1^\alpha \\ X_2^\alpha \\ X_3^\alpha \end{pmatrix} = 0$$

Matrix form:

$$\begin{pmatrix} k-\omega_\alpha^2 m_1 & -k & 0 \\ -k & 2k-\omega_\alpha^2 m_2 & -k \\ 0 & -k & k-\omega_\alpha^2 m_3 \end{pmatrix} \begin{pmatrix} X_1^\alpha \\ X_2^\alpha \\ X_3^\alpha \end{pmatrix} = 0$$

More convenient form:

Let $Y_i \equiv \sqrt{m_i} X_i$ Equations for Y_i take the form:

$$\begin{pmatrix} \kappa_{11}-\omega_\alpha^2 & -\kappa_{12} & 0 \\ -\kappa_{12} & 2\kappa_{22}-\omega_\alpha^2 & -\kappa_{23} \\ 0 & -\kappa_{23} & \kappa_{33}-\omega_\alpha^2 \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = 0$$

where $\kappa_{ij} = \kappa_{ji} \equiv \dfrac{k}{\sqrt{m_i m_j}}$

Digression:

Eigenvalue properties of matrices $\mathbf{M}\mathbf{y}_{\alpha} = \lambda_{\alpha}\mathbf{y}_{\alpha}$

Hermitian matrix: $H_{ij} = H^{*}{}_{ji}$

Theorem for Hermitian matrices:

$$\lambda_{\alpha} \text{ have real values and } \mathbf{y}_{\alpha}^{H} \cdot \mathbf{y}_{\beta} = \delta_{\alpha\beta}$$

Unitary matrix: $\mathbf{U}\mathbf{U}^{H} = \mathbf{I}$

$$\left|\lambda_{\alpha}\right| = 1 \text{ and } \mathbf{y}_{\alpha}^{H} \cdot \mathbf{y}_{\beta} = \delta_{\alpha\beta}$$

Digression on matrices -- continued

Eigenvalues of a matrix are "invariant" under a similarity transformation

Eigenvalue properties of matrix: $\mathbf{M}\mathbf{y}_\alpha = \lambda_\alpha \mathbf{y}_\alpha$

Transformed matrix: $\mathbf{M}'\mathbf{y}'_\alpha = \lambda'_\alpha \mathbf{y}'_\alpha$

If $\mathbf{M}' = \mathbf{S}\mathbf{M}\mathbf{S}^{-1}$ then $\lambda'_\alpha = \lambda_\alpha$ and $\mathbf{S}^{-1}\mathbf{y}'_\alpha = \mathbf{y}_\alpha$

Proof $\mathbf{S}\mathbf{M}\mathbf{S}^{-1}\mathbf{y}'_\alpha = \lambda'_\alpha \mathbf{y}'_\alpha$

$$\mathbf{M}\left(\mathbf{S}^{-1}\mathbf{y}'_\alpha\right) = \lambda'_\alpha \left(\mathbf{S}^{-1}\mathbf{y}'_\alpha\right)$$

Example of transformation:

Original problem written in eigenvalue form:

$$\begin{pmatrix} k/m_1 & -k/m_1 & 0 \\ -k/m_2 & 2k/m_2 & -k/m_2 \\ 0 & -k/m_3 & k/m_3 \end{pmatrix}\begin{pmatrix} X_1^\alpha \\ X_2^\alpha \\ X_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} X_1^\alpha \\ X_2^\alpha \\ X_3^\alpha \end{pmatrix}$$

Let $\mathbf{S} = \begin{pmatrix} \sqrt{m_1} & 0 & 0 \\ 0 & \sqrt{m_2} & 0 \\ 0 & 0 & \sqrt{m_3} \end{pmatrix}$; $\mathbf{SMS}^{-1} = \begin{pmatrix} \kappa_{11} & -\kappa_{12} & 0 \\ -\kappa_{12} & 2\kappa_{22} & -\kappa_{23} \\ 0 & -\kappa_{23} & \kappa_{33} \end{pmatrix}$

Let $\mathbf{Y} \equiv \mathbf{SX}$

$$\begin{pmatrix} \kappa_{11} & -\kappa_{12} & 0 \\ -\kappa_{12} & 2\kappa_{22} & -\kappa_{23} \\ 0 & -\kappa_{23} & \kappa_{33} \end{pmatrix}\begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

where $\kappa_{ij} = \kappa_{ji} \equiv \dfrac{k}{\sqrt{m_i m_j}}$

In our case:

$$\begin{pmatrix} \kappa_{11} & -\kappa_{12} & 0 \\ -\kappa_{12} & 2\kappa_{22} & -\kappa_{23} \\ 0 & -\kappa_{23} & \kappa_{33} \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

for $m_1 = m_3 \equiv m_O$ and $m_2 \equiv m_C$ (CO_2)

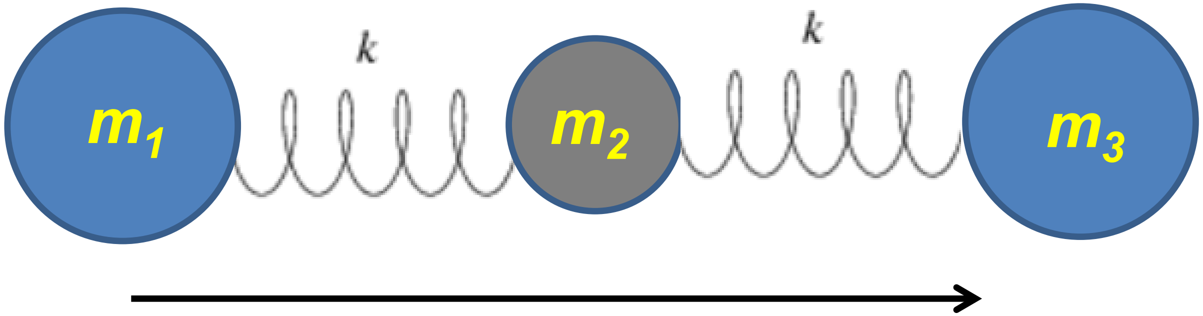
$$\begin{pmatrix} \kappa_{OO} & -\kappa_{OC} & 0 \\ -\kappa_{OC} & 2\kappa_{CC} & -\kappa_{OC} \\ 0 & -\kappa_{OC} & \kappa_{OO} \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

Eigenvalues and eigenvectors :

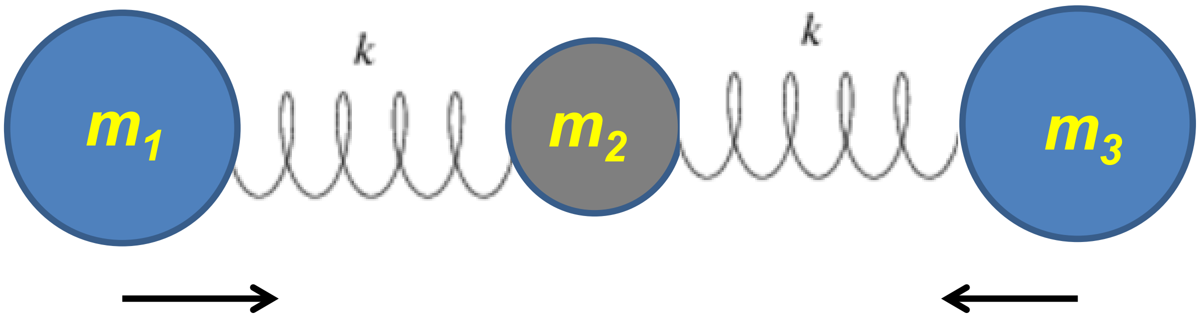
$$\omega_1^2 = 0 \qquad \begin{pmatrix} Y_1^1 \\ Y_2^1 \\ Y_3^1 \end{pmatrix} = N_1 \begin{pmatrix} \sqrt{\frac{m_O}{m_C}} \\ 1 \\ \sqrt{\frac{m_O}{m_C}} \end{pmatrix}, \quad \begin{pmatrix} X_1^1 \\ X_2^1 \\ X_3^1 \end{pmatrix} = N'_1 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\omega_2^2 = \frac{k}{m_O} \qquad \begin{pmatrix} Y_1^2 \\ Y_2^2 \\ Y_3^2 \end{pmatrix} = N_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad \begin{pmatrix} X_1^2 \\ X_2^2 \\ X_3^2 \end{pmatrix} = N'_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

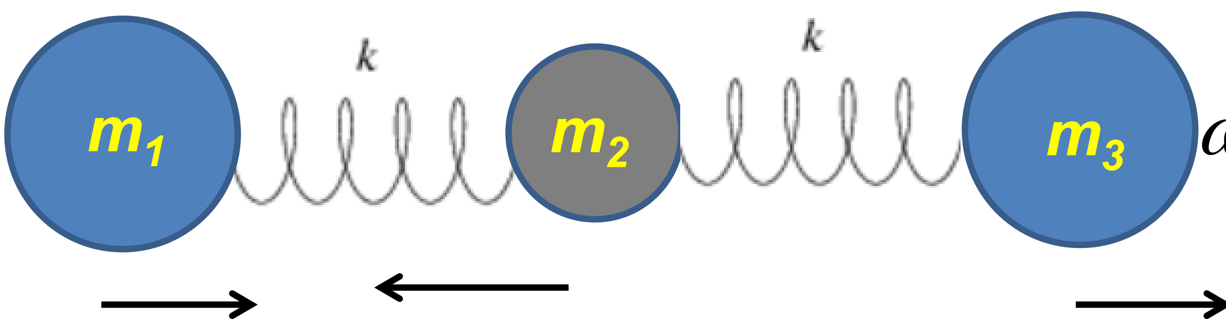
$$\omega_3^2 = \frac{k}{m_O} + \frac{2k}{m_C} \qquad \begin{pmatrix} Y_1^3 \\ Y_2^3 \\ Y_3^3 \end{pmatrix} = N_3 \begin{pmatrix} 1 \\ -2\sqrt{\frac{m_O}{m_C}} \\ 1 \end{pmatrix}, \quad \begin{pmatrix} X_1^3 \\ X_2^3 \\ X_3^3 \end{pmatrix} = N'_3 \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$



$$\omega_1 = 0$$



$$\omega_2 = \sqrt{\frac{k}{m_O}}$$



$$\omega_3 = \sqrt{\frac{k}{m_O} + \frac{2k}{m_C}}$$

General solution :

$$x_i(t) = \Re\left(\sum_\alpha C^\alpha X_i^\alpha e^{-i\omega_\alpha t} \right)$$

For example, normal mode amplitudes

C^α can be determined from initial conditions

Comment on solving for eigenvalues and eigenvectors – while it is reasonable to find these analytically for 2x2 or 3x3 matrices, it is prudent to use Maple or Mathematica for larger systems.

Maple example

Mathematica example

Additional digression on matrix properties

Singular value decomposition

It is possible to factor any real matrix **A** into unitary matrices **V** and **U** together with positive diagonal matrix **Σ**:

$$\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathbf{H}}$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma_N \end{pmatrix}$$

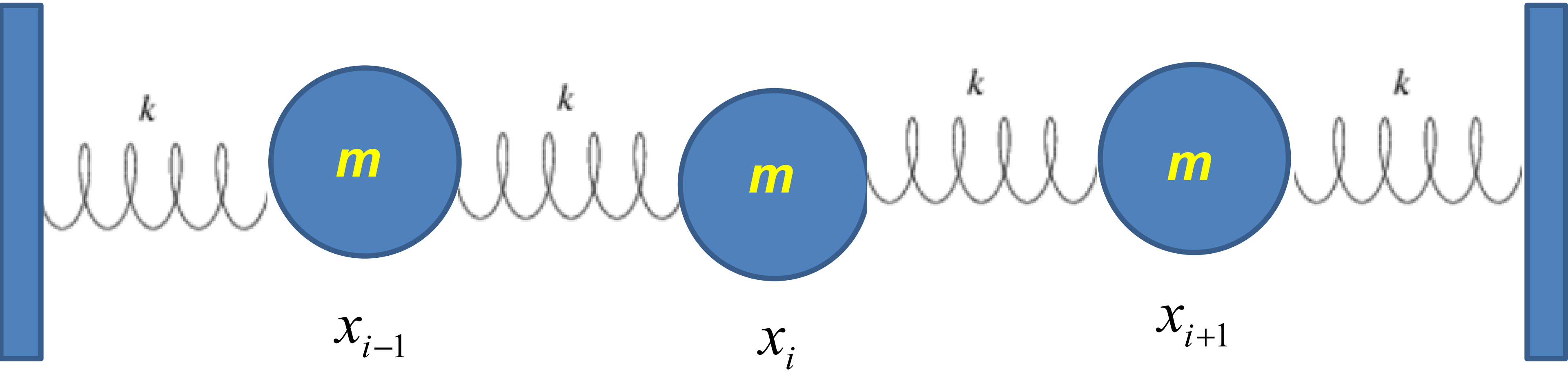
Singular value decomposition -- continued

Consider using SVD to solve a singular linear algebra problem $\quad \mathbf{AX} = \mathbf{B}$

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^H$$

$$\mathbf{X} = \sum_{i \text{ for } \sigma_i > \varepsilon} \mathbf{v}_i \frac{\langle \mathbf{u}_i^H \mid \mathbf{B} \rangle}{\sigma_i}$$

Consider an extended system of masses and springs:



Note: each mass coordinate is measured relative to its equilibrium position x_i^0

$$L = T - V = \frac{1}{2} m \sum_{i=1}^{N} \dot{x}_i^2 - \frac{1}{2} k \sum_{i=0}^{N} \left(x_{i+1} - x_i \right)^2$$

Note: In fact, we have N masses; x_0 and x_{N+1} will be treated using boundary conditions.

$$L = T - V = \frac{1}{2} m \sum_{i=1}^{N} \dot{x}_i^2 - \frac{1}{2} k \sum_{i=0}^{N} \left(x_{i+1} - x_i \right)^2$$

$$x_0 \equiv 0 \text{ and } x_{N+1} \equiv 0$$

From Euler - Lagrange equations :

$$m\ddot{x}_1 = k\left(x_2 - 2x_1\right)$$

$$m\ddot{x}_2 = k\left(x_3 - 2x_2 + x_1\right)$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$m\ddot{x}_i = k\left(x_{i+1} - 2x_i + x_{i-1}\right)$$

$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

$$m\ddot{x}_N = k\left(x_{N-1} - 2x_N\right)$$

Matrix formulation --

Assume $x_i(t) = X_i e^{-i\omega t}$

$$\frac{m}{k}\omega^2 \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_{N-1} \\ X_N \end{pmatrix} = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \cdots & \cdots & -1 & 2 & -1 \\ \cdots & \cdots & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_{N-1} \\ X_N \end{pmatrix}$$

Can solve as an eigenvalue problem --

> with(LinearAlgebra);

=

$$> A := \begin{bmatrix} 5 & -1 & 0 & 0 & 0 \\ -1 & 5 & -1 & 0 & 0 \\ 0 & -1 & 5 & -1 & 0 \\ 0 & 0 & -1 & 5 & -1 \\ 0 & 0 & 0 & -1 & 5 \end{bmatrix};$$

> Eigenvalues(A);

$$\begin{bmatrix} 5 \\ 6 \\ 4 \\ 5-\sqrt{3} \\ 5+\sqrt{3} \end{bmatrix}$$

This example also has an algebraic solution --

From Euler - Lagrange equations :

$$m\ddot{x}_j = k\left(x_{j+1} - 2x_j + x_{j-1}\right) \qquad \text{with } x_0 = 0 = x_{N+1}$$

Try : $\quad x_j(t) = Ae^{-i\omega t + iqaj}$

$$-\omega^2 Ae^{-i\omega t+iqaj} = \frac{k}{m}\left(e^{iqa} - 2 + e^{-iqa}\right)Ae^{-i\omega t+iqaj}$$

$$-\omega^2 = \frac{k}{m}\left(2\cos\left(qa\right) - 2\right)$$

$$\Rightarrow \omega^2 = \frac{4k}{m}\sin^2\left(\frac{qa}{2}\right)$$

From Euler-Lagrange equations -- continued:

$$m\ddot{x}_j = k\left(x_{j+1} - 2x_j + x_{j-1}\right) \qquad \text{with } x_0 = 0 = x_{N+1}$$

Try: $x_j(t) = Ae^{-i\omega t + iqaj}$ $\Rightarrow \omega^2 = \frac{4k}{m}\sin^2\left(\frac{qa}{2}\right)$

Note that: $x_j(t) = Be^{-i\omega t - iqaj}$ $\Rightarrow \omega^2 = \frac{4k}{m}\sin^2\left(\frac{qa}{2}\right)$

General solution:

$$x_j(t) = \Re\left(Ae^{-i\omega t + iqaj} + Be^{-i\omega t - iqaj}\right)$$

Impose boundary conditions:

$$x_0(t) = \Re\left(Ae^{-i\omega t} + Be^{-i\omega t}\right) = 0$$

$$x_{N+1}(t) = \Re\left(Ae^{-i\omega t + iqa(N+1)} + Be^{-i\omega t - iqa(N+1)}\right) = 0$$

Impose boundary conditions -- continued:

$$x_0(t) = \Re\left(Ae^{-i\omega t} + Be^{-i\omega t} \right) = 0$$

$$x_{N+1}(t) = \Re\left(Ae^{-i\omega t + iqa(N+1)} + Be^{-i\omega t - iqa(N+1)} \right) = 0$$

$$\Rightarrow B = -A$$

$$x_{N+1}(t) = \Re\left(Ae^{-i\omega t}\left(e^{iqa(N+1)} - e^{-iqa(N+1)} \right)\right) = 0$$

$$\Rightarrow \sin\left(qa(N+1) \right) = 0$$

$$\Rightarrow \quad qa(N+1) = \nu\pi \quad \text{where } \nu = 0,1,2\cdots$$

$$qa = \frac{\nu\pi}{N+1}$$

Summary of results:

$$\Rightarrow \omega_\nu^2 = \frac{4k}{m}\sin^2\left(\frac{\nu\pi}{2(N+1)}\right) \qquad x_n = \Re\left(2iA\sin\left(\frac{\nu\pi n}{N+1}\right)\right)$$

$$\nu = 0,1,\ldots N \qquad n = 1,2,\ldots\ldots N$$