Report #4
Introduction to Frontiers of Computational Science

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1 Problem 1

Solve the following equations.

$$\begin{aligned}
\frac{d}{dt}x_1(t) &= \mu\left(-x_1(t) + x_2(t)\right) \\
\frac{d}{dt}x_2(t) &= \mu\left(x_1(t) - 2x_2(t) + x_3(t)\right) \\
\frac{d}{dt}x_3(t) &= \mu\left(x_2(t) - x_3(t)\right) \qquad (1)
\end{aligned}$$

where $x_i(0) = x_i^0$, $(i = 1, 2, 3)$

1.1 Answer

Using denotation

$$\dot{x}_i(t) = \frac{d}{dt}x_i(t) \quad (i = 1, 2, 3)$$

we can rearrange those equation (1);

$$\begin{aligned}
\dot{x}_1(t) &= \mu\,(-x_1(t) \quad + x_2(t) \qquad\qquad) \\
\dot{x}_2(t) &= \mu\,(x_1(t) \quad - 2x_2(t) \quad + x_3(t)) \\
\dot{x}_3(t) &= \mu\,(\qquad\qquad x_2(t) \quad - x_3(t)) \qquad (2)
\end{aligned}$$

Using the homogeneous system of linear differential equations;

$$\dot{x} = Ax \qquad (x(t) = x_1(t), \cdots, x_m(t)) \qquad (3)$$

A is matrix which have size $m \times m$, for instance, we take α is the eigenvalue of this matrix and W is eigen vector for this eigenvalues.

$$AW = \alpha W$$

then we set

$$x(t) = e^{\alpha t}W \qquad (4)$$

as solution for the equation (3). And we rewrite equation as follows

$$A = \begin{pmatrix} -\mu & \mu & 0 \\ \mu & -2\mu & \mu \\ 0 & \mu & -\mu \end{pmatrix}$$

And then to find the eigenvalues;

$$A - \alpha I = \begin{pmatrix} -\mu - \alpha & \mu & 0 \\ \mu & -2\mu - \alpha & \mu \\ 0 & \mu & -\mu - \alpha \end{pmatrix} \tag{5}$$

For solve this equation, we take $\det(A - \alpha I) = 0$. So,

$$\begin{aligned} \det(A - \alpha I) &= (-\mu - \alpha) \begin{vmatrix} -2\mu - \alpha & \mu \\ \mu & -\mu - \alpha \end{vmatrix} - \mu \begin{vmatrix} \mu & \mu \\ 0 & -\mu - \alpha \end{vmatrix} \\ &= (-\mu - \alpha)\left(\mu^2 + 3\alpha + \alpha^2\right) - \mu\left(-\mu^2 - \alpha\mu\right) \\ &= -3\alpha\mu^2 - 4\alpha^2\mu - \alpha^3 \\ &= \alpha(\alpha + \mu)(\alpha + 3\mu) = 0 \end{aligned}$$

So, the eigenvalues are

$$\alpha = 0, \qquad \alpha = -\mu \qquad \alpha = -3\mu$$

For case $\alpha_1 = 0$,

$$A - 0 = \begin{pmatrix} -\mu & \mu & 0 \\ \mu & -2\mu & \mu \\ 0 & \mu & -\mu \end{pmatrix}$$

We construct the augmented matrix $\left(A - \alpha I \vdots 0\right)$ and convert it to row echelon form

$$\begin{pmatrix} -\mu & \mu & 0 & 0 \\ \mu & -2\mu & \mu & 0 \\ 0 & \mu & -\mu & 0 \end{pmatrix} \longrightarrow \begin{pmatrix} -\mu & \mu & 0 & 0 \\ 0 & -\mu & \mu & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{6}$$

Rewriting this augmented matrix as a linear system gives

$$\begin{aligned} -\mu x_1 + \mu x_2 &= 0 \\ -\mu x_2 + \mu x_3 &= 0 \end{aligned}$$

So, the eigenvector $\mathbf{e}_1$ is given by:

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \tag{7}$$

For case $\alpha_2 = -\mu$;

$$A - (-\mu)I = \begin{pmatrix} 0 & \mu & 0 \\ -\mu & -\mu & \mu \\ 0 & \mu & 0 \end{pmatrix}$$

then

$$A - (-\mu)I = \begin{pmatrix} 0 & \mu & 0 & 0 \\ -\mu & -\mu & \mu & 0 \\ 0 & \mu & 0 & 0 \end{pmatrix} \longrightarrow \begin{pmatrix} \mu & -\mu & \mu & 0 \\ 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{8}$$

Rewriting this augmented matrix as a linear system gives

$$\begin{aligned} \mu x_1 - \mu x_2 + \mu x_3 &= 0 \\ \mu x_2 &= 0 \end{aligned}$$

So, the eigenvector $\mathbf{e}_2$ is given by:

$$\mathbf{e}_2 = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \tag{9}$$

For case $\alpha_3 = -3\mu$;

$$A - (-3\mu)I = \begin{pmatrix} 2\mu & \mu & 0 \\ \mu & \mu & \mu \\ 0 & \mu & 2\mu \end{pmatrix}$$

then

$$A - (-3\mu)I = \begin{pmatrix} 2\mu & \mu & 0 & 0 \\ \mu & \mu & \mu & 0 \\ 0 & \mu & 2\mu & 0 \end{pmatrix} \longrightarrow \begin{pmatrix} 2\mu & \mu & 0 & 0 \\ 0 & \frac{1}{2}\mu & \mu & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{10}$$

Rewriting this augmented matrix as a linear system gives

$$\begin{aligned} 2\mu x_1 + \mu x_2 &= 0 \\ \frac{1}{2}\mu x_2 + \mu x_3 &= 0 \end{aligned}$$

So, the eigenvector $\mathbf{e}_3$ is given by:

$$\mathbf{e}_3 = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \tag{11}$$

The general solution is

$$\mathbf{x}(t) = C_1 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + e^{-\mu t} C_2 \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} + C_3 e^{-3\mu t} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \tag{12}$$

With substitute the initial condition for C_1, C_2, C_3 we get

$$\begin{aligned} C_1 - C_2 + C_3 &= x_1^0 \\ C_1 - 2C_3 &= x_2^0 \\ C_1 + C_2 + C_3 &= x_3^0 \end{aligned}$$

we get

$$\mathbf{x}(t) = \frac{x_1^0 + x_2^0 + x_3^0}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + \frac{-x_1^0 + x_3^0}{2} e^{-\mu t} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} + \frac{x_1^0 + x_2^0 + x_3^0}{6} e^{-3\mu t} \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix} \tag{13}$$

2 Problem 2

Check $\begin{pmatrix}1\\1\\1\end{pmatrix}$, $\begin{pmatrix}-1\\0\\1\end{pmatrix}$, and $\begin{pmatrix}1\\-2\\1\end{pmatrix}$ are perpendicular each others. Normalized and check the unitary condition.

2.1 Answer

For the perpendicular relation, we can use that

$$\mathbf{e}_m^* \cdot \mathbf{e}_n = 0 \text{ for m} \neq n$$

Now, $\mathbf{e}_1 \cdot \mathbf{e}_2$

$$\begin{pmatrix}1 & 1 & 1\end{pmatrix} \cdot \begin{pmatrix}-1\\0\\1\end{pmatrix} = 1 + 0 - 1 = 0$$

then, $\mathbf{e}_1 \cdot \mathbf{e}_3$

$$\begin{pmatrix}1 & 1 & 1\end{pmatrix} \cdot \begin{pmatrix}1\\-2\\1\end{pmatrix} = 1 - 2 + 1 = 0$$

and, $\mathbf{e}_2 \cdot \mathbf{e}_3$

$$\begin{pmatrix}-1 & 0 & 1\end{pmatrix} \cdot \begin{pmatrix}1\\-2\\1\end{pmatrix} = -1 + 0 + 1 = 0$$

The normalized given;

$$\mathbf{e}_1 = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}$$

$$\mathbf{e}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\0\\1\end{pmatrix}$$

$$\mathbf{e}_3 = \frac{1}{\sqrt{6}}\begin{pmatrix}1\\-2\\1\end{pmatrix}$$

For the unitary relation, take $Q = \begin{pmatrix}\mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3\end{pmatrix}$.

$$Q = \begin{pmatrix}\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}}\\ \frac{1}{\sqrt{3}} & 0 & -\frac{2}{\sqrt{6}}\\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}}\end{pmatrix}$$

So the invers of Q, Q^{-1} is like these processes.

$$\det Q = \frac{1}{\sqrt{3}}\left(0 + \frac{2}{\sqrt{12}}\right) + \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{18}} + \frac{2}{\sqrt{18}}\right) + \frac{1}{\sqrt{6}}\left(\frac{1}{\sqrt{6}} - 0\right) = \frac{1}{3} + \frac{1}{2} + \frac{1}{6} = 1$$

$$Q^T = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix}$$

then

$$Q_{11} = \begin{vmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{vmatrix} = \frac{1}{\sqrt{3}} \qquad Q_{12} = \begin{vmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{vmatrix} = -\frac{1}{\sqrt{3}} \qquad Q_{13} = \begin{vmatrix} -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} \end{vmatrix} = \frac{1}{\sqrt{3}}$$

$$Q_{21} = \begin{vmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{vmatrix} = \frac{1}{\sqrt{2}} \qquad Q_{22} = \begin{vmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{vmatrix} = 0 \qquad Q_{23} = \begin{vmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} \end{vmatrix} = -\frac{1}{\sqrt{2}}$$

$$Q_{31} = \begin{vmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{1}{\sqrt{2}} \end{vmatrix} = \frac{1}{\sqrt{6}} \qquad Q_{32} = \begin{vmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{vmatrix} = \frac{2}{\sqrt{6}} \qquad Q_{33} = \begin{vmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & 0 \end{vmatrix} = \frac{1}{\sqrt{6}}$$

then

$$\mathrm{adj}(Q) = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix}$$

and the invers of Q is

$$\begin{aligned} Q^{-1} &= \frac{1}{\det(Q)} \left(\mathrm{adj}(Q)\right) \\ Q^{-1} &= \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix} \\ Q^{-1} &= Q^T \qquad \text{unitary relation proven.} \end{aligned}$$