Question

In question 3 of exercise sheet 7 you found the eigenvalues and eigenvectors for the matrices associated to Allyl radical, Cyclopropenyl, and Trimethlene methane. Use your results to diagonalise these matrices.

Answer

(i) Allyl radical $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ Eigenvalues:0, $\sqrt{2}$, $-\sqrt{2}$

Corresponding eigenvalues $\begin{pmatrix} \alpha \\ 0 \\ -\alpha \end{pmatrix}$, $\begin{pmatrix} \beta \\ \sqrt{2}\beta \\ \beta \end{pmatrix}$ and $\begin{pmatrix} \gamma \\ -\sqrt{2}\gamma \\ \gamma \end{pmatrix}$ which normalise to $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}$, $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix}$ and $\begin{pmatrix} \frac{1}{2} \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix}$ $\left[\text{Note} : \frac{\sqrt{2}}{2} = \frac{\sqrt{2}}{\sqrt{2}\sqrt{2}} = \frac{1}{\sqrt{2}}\right]$

Take the orthogonal matrix $R = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$

The original matrix diagonalises to $R^T AR = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 \\ 0 & 0 & -\sqrt{2} \end{pmatrix}$

(ii) Cyclopropenyl $\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$ Eigenvalues:2, -1, -1

Corresponding eigenvalues $\begin{pmatrix} \alpha \\ \alpha \\ \alpha \end{pmatrix}$, $\begin{pmatrix} \beta \\ -(\beta+\gamma) \\ \gamma \end{pmatrix}$. Using this last eigenvector we can choose two orthognal eigenvectors. For example if $\beta = \gamma = 1$ then we have $\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$ and if $\beta = 1, \gamma = -1$ we have $\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$ so the eigenvalues 2, -1, -1 yield three mutually orthogonal, normalised eigenvectors: $\begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{pmatrix}$, $\begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{-2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix}$ and $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{-1}{\sqrt{2}} \end{pmatrix}$ respectively.

Take the orthogonal matrix $R = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{-2}{\sqrt{6}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$

The original matrix diagonalises to $R^T AR = \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

(iii) Trimethylene methane $\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$ Eigenvalues:0, 0, $\sqrt{3}$, $-\sqrt{3}$.

Four mutually orthogonal eigenvectors $\begin{pmatrix} 2 \\ -1 \\ -1 \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$, $\begin{pmatrix} 1 \\ 1 \\ 1 \\ \sqrt{3} \end{pmatrix}$, $\begin{pmatrix} 1 \\ 1 \\ 1 \\ -\sqrt{3} \end{pmatrix}$ which normalise to $\begin{pmatrix} \frac{2}{\sqrt{6}} \\ \frac{-1}{\sqrt{6}} \\ \frac{-1}{\sqrt{6}} \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \\ 0 \end{pmatrix}$, $\begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$ and $\begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}$ respectively .

Take the orthogonal matrix $R = \begin{pmatrix} \frac{2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{-1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{-1}{\sqrt{6}} & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$

The original matrix diagonalises to $R^T AR = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \\ 0 & 0 & 0 & -\sqrt{3} \end{pmatrix}$