0.6 pts

Given the following covariance matrix Σ:

$C = $

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

Find the **eigenvalues** (λ) and the corresponding **normalized eigenvectors** (v) for this matrix.

$$\underbrace{(C-\lambda I)}_{\text{eigenvalues}} . \underbrace{V}_{\text{eigenvectors}} = 0 \rightarrow \det(C-\lambda I) = 0$$

$$\det(C-\lambda I) = (2-\lambda)\left[(2-\lambda)^2 - 1\right] - \text{[redacted]}2-\lambda) = 0$$

$$= (2-\lambda)^2 - 2 = 0 \rightarrow \lambda^2 - 4\lambda + 4 - 2 = 0 \rightarrow \lambda^2 - 4\lambda + 2 = 0$$

$\lambda_1 = 2$ $\quad \lambda_2 = 2-\sqrt{2}$ $\quad \lambda_3 = 2+\sqrt{2}$

$$\lambda_1 = 2 : (C-\lambda I)V = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$-y = 0 \rightarrow y = 0$

$-x - z = 0$

$x = -z$

$$V_1 = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix} \rightarrow \hat{V}_1 = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ -1/\sqrt{2} \end{bmatrix}$$

$$\lambda_2 = 2+\sqrt{2} : (C-\lambda I).V_2 = \begin{bmatrix} -\sqrt{2} & -1 & 0 \\ -1 & -\sqrt{2} & -1 \\ 0 & -1 & -\sqrt{2} \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$-\sqrt{2}x - y = 0$

$-x - \sqrt{2}y - z = 0 \rightarrow -1 - \sqrt{2}y - 1 = 0 \rightarrow -\sqrt{2}y = 2$, $y = -\sqrt{2}$

$(-y - \sqrt{2}z = 0)$

$-\sqrt{2}x + \sqrt{2}z = 0$

$\sqrt{2}x = \sqrt{2}z$

$$V_2 = \begin{bmatrix} 1 \\ -\sqrt{2} \\ 1 \end{bmatrix} \rightarrow \hat{V}_2 = \begin{bmatrix} 1/2 \\ -\sqrt{2}/2 \\ 1/2 \end{bmatrix}$$

$$\lambda_3 = 2-\sqrt{2} : (C-\lambda I).V_3 = \begin{bmatrix} \sqrt{2} & -1 & 0 \\ -1 & \sqrt{2} & -1 \\ 0 & -1 & \sqrt{2} \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$\sqrt{2}x - y = 0$

$-x + \sqrt{2}y - z = 0$

$(-y + \sqrt{2}z = 0)$

$$V_3 = \begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix} \rightarrow \hat{V}_3 = \begin{bmatrix} 1/2 \\ \sqrt{2}/2 \\ 1/2 \end{bmatrix}$$

0.4 pts

Atom 1: (2, 3, 1)
Atom 2: (0, 1, 2)
Atom 3: (4, -1, 0)
Atom 4: (1, 0, -2)
Atom 5: (3, 2, 4)

$\lambda_2 > \lambda_1 > \lambda_3$

$$X = \begin{bmatrix} 1/2 & 1/\sqrt{2} & 1/2 \\ -\sqrt{2}/2 & 0 & \sqrt{2}/2 \\ 1/2 & -1/\sqrt{2} & 1/2 \end{bmatrix}$$

a) What are the coordinates of the **centroid** (geometric center) of this system?

b) What is the **translation vector** required to move the centroid of this system to the origin (0, 0, 0)?

$$C_x = \frac{2+0+4+1+3}{5} = \frac{10}{5} = 2$$

$$C_y = \frac{3+1-1+0+2}{5} = \frac{5}{5} = 1$$

$$C_z = \frac{1+2+0-2+4}{5} = \frac{5}{5} = 1$$

$(2,1,1) \rightarrow T(-2,-1,-1)$