The Chemistry Maths Book

Erich Steiner

University of Exeter

Second Edition 2008

Solutions

Chapter 19 The matrix eigenvalue problem

Section 19.1

Find the inverse of the matrix of the coefficients, and use it to solve the equations:

1. $2x - 3y = 8$

$4x + \ \ y = 2$

Let $\quad \mathbf{Ax} = \mathbf{b}$ where $\mathbf{A} = \begin{pmatrix} 2 & -3 \\ 4 & 1 \end{pmatrix}$, $\mathbf{x} = \begin{pmatrix} x \\ y \end{pmatrix}$, $\mathbf{b} = \begin{pmatrix} 8 \\ 2 \end{pmatrix}$

Then $\quad \det \mathbf{A} = 14$, $\widehat{\mathbf{A}} = \begin{pmatrix} 1 & 3 \\ -4 & 2 \end{pmatrix} \rightarrow \mathbf{A}^{-1} = \frac{1}{14}\begin{pmatrix} 1 & 3 \\ -4 & 2 \end{pmatrix}$ (Exercise 47 of Chapter 18)

Therefore, by equation (19.4),

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \rightarrow \begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{14}\begin{pmatrix} 1 & 3 \\ -4 & 2 \end{pmatrix}\begin{pmatrix} 8 \\ 2 \end{pmatrix} = \frac{1}{14}\begin{pmatrix} 14 \\ -28 \end{pmatrix} = \begin{pmatrix} 1 \\ -2 \end{pmatrix}$$

2. $$\left.\begin{aligned} x + \ \ y + \ \ z &= 6 \\ x + 2y + 3z &= 14 \\ x + 4y + 9z &= 36 \end{aligned}\right\} \rightarrow \mathbf{A} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \\ 1 & 4 & 9 \end{pmatrix}, \ \mathbf{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \ \mathbf{b} = \begin{pmatrix} 6 \\ 14 \\ 36 \end{pmatrix}$$

Then $\quad \det \mathbf{A} = 2$, $\widehat{\mathbf{A}} = \begin{pmatrix} 6 & -5 & 1 \\ -6 & 8 & -2 \\ 2 & -3 & 1 \end{pmatrix} \rightarrow \mathbf{A}^{-1} = \frac{1}{2}\begin{pmatrix} 6 & -5 & 1 \\ -6 & 8 & -2 \\ 2 & -3 & 1 \end{pmatrix}$

and $\quad \mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \rightarrow \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 6 & -5 & 1 \\ -6 & 8 & -2 \\ 2 & -3 & 1 \end{pmatrix}\begin{pmatrix} 6 \\ 14 \\ 36 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2 \\ 4 \\ 6 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$

3. $$\left.\begin{aligned} w + x \qquad + z &= 2 \\ x + y + z &= 6 \\ w \qquad + y + z &= 3 \\ w + x + y \qquad &= 4 \end{aligned}\right\} \rightarrow \mathbf{A} = \begin{pmatrix} 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}, \ \mathbf{x} = \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix}, \ \mathbf{b} = \begin{pmatrix} 2 \\ 6 \\ 3 \\ 4 \end{pmatrix}$$

Then $\quad \det \mathbf{A} = -3$, $\widehat{\mathbf{A}} = \begin{pmatrix} 1 & -2 & 1 & 1 \\ 1 & 1 & -2 & 1 \\ -2 & 1 & 1 & 1 \\ 1 & 1 & 1 & -2 \end{pmatrix} \rightarrow \mathbf{A}^{-1} = -\frac{1}{3}\begin{pmatrix} 1 & -2 & 1 & 1 \\ 1 & 1 & -2 & 1 \\ -2 & 1 & 1 & 1 \\ 1 & 1 & 1 & -2 \end{pmatrix}$

and $\quad \mathbf{x} = \mathbf{A}^{-1}\mathbf{b} \rightarrow \begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = -\frac{1}{3}\begin{pmatrix} 1 & -2 & 1 & 1 \\ 1 & 1 & -2 & 1 \\ -2 & 1 & 1 & 1 \\ 1 & 1 & 1 & -2 \end{pmatrix}\begin{pmatrix} 2 \\ 6 \\ 3 \\ 4 \end{pmatrix} = \begin{pmatrix} -1 \\ 2 \\ 3 \\ 1 \end{pmatrix}$

Section 19.2

Find the eigenvalues and eigenvectors of the following matrices:

4. $\mathbf{A} = \begin{pmatrix} 2 & 2 \\ 1 & 3 \end{pmatrix}$

The secular equations are

$$\begin{aligned} (2-\lambda)x \quad + \quad 2y \quad &= 0 \\ x \quad + \quad (3-\lambda)y &= 0 \end{aligned}$$

The characteristic equation of **A** is

$$\det(\mathbf{A}-\lambda\mathbf{I}) = 0 \quad \to \quad \begin{vmatrix} 2-\lambda & 2 \\ 1 & 3-\lambda \end{vmatrix} = (2-\lambda)(3-\lambda) - 2 = \lambda^2 - 5\lambda + 4$$

$$= (\lambda-1)(\lambda-4) = 0 \text{ when } \lambda = 1, \lambda = 4$$

The eigenvalues of **A** are therefore $\lambda_1 = 1, \lambda_2 = 4$. The corresponding eigenvectors are obtained by solving the secular equations for each value of λ. Thus, using the first of the equations,

$$\lambda = \lambda_1 = 1: \quad (2-\lambda_1)x + 2y = x + 2y = 0 \quad \to \quad x = -2y \quad \to \quad \mathbf{x}_1 = y\begin{pmatrix} -2 \\ 1 \end{pmatrix}$$

$$\lambda = \lambda_2 = 4: \quad (2-\lambda_2)x + 2y = -2x + 2y = 0 \quad \to \quad x = y \quad \to \quad \mathbf{x}_2 = y\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

5. $\mathbf{A} = \begin{pmatrix} 2 & 0 \\ 0 & -3 \end{pmatrix}$

The characteristic equation of **A** is

$$\begin{vmatrix} 2-\lambda & 0 \\ 0 & -3-\lambda \end{vmatrix} = -(2-\lambda)(3+\lambda) = 0 \text{ when } \lambda = 2, \lambda = -3$$

The secular equations are

$$(2-\lambda)x = 0$$

$$(-3-\lambda)y = 0$$

Then $\quad \lambda = \lambda_1 = 2: \quad y = 0 \quad \to \quad \mathbf{x}_1 = x\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$\lambda = \lambda_2 = -3: \quad x = 0 \quad \to \quad \mathbf{x}_2 = y\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

6. $\begin{pmatrix} 3 & 1 \\ -1 & 3 \end{pmatrix}$

The secular equations are

$$\begin{aligned} (3-\lambda)x &+ y &= 0 \\ -x &+ (3-\lambda)y &= 0 \end{aligned}$$

The characteristic equation is

$$\begin{vmatrix} 3-\lambda & 1 \\ -1 & 3-\lambda \end{vmatrix} = (3-\lambda)^2 + 1 = \lambda^2 - 6\lambda + 10$$

$$= 0 \text{ when } \lambda = \frac{6 \pm \sqrt{36-40}}{2} = 3 \pm i$$

Then $\lambda = \lambda_1 = 3 - i: \quad ix + y = 0 \rightarrow y = -ix \rightarrow \mathbf{x}_1 = x\begin{pmatrix} 1 \\ -i \end{pmatrix}$

$\lambda = \lambda_2 = 3 + i: \quad -ix + y = 0 \rightarrow y = ix \rightarrow \mathbf{x}_2 = x\begin{pmatrix} 1 \\ i \end{pmatrix}$

7. $\begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}$

The secular equations are

$$\begin{aligned} (3-\lambda)x &+ y &= 0 \\ x &+ (3-\lambda)y &= 0 \end{aligned}$$

The characteristic equation is

$$\begin{vmatrix} 3-\lambda & 1 \\ 1 & 3-\lambda \end{vmatrix} = (3-\lambda)^2 - 1 = (\lambda-2)(\lambda-4)$$

$$= 0 \text{ when } \lambda = 2, \lambda = 4$$

Then $\lambda = \lambda_1 = 2: \quad x + y = 0 \rightarrow y = -x \rightarrow \mathbf{x}_1 = x\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$\lambda = \lambda_2 = 4: \quad -x + y = 0 \rightarrow y = x \rightarrow \mathbf{x}_2 = x\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

8. $\begin{pmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 2 & 1 \end{pmatrix}$

The secular equations are

$$\begin{array}{llcccl} (1) & (1-\lambda)x & + & 2y & & =0 \\ (2) & 2x & + & (1-\lambda)y & & =0 \\ (3) & & & 2y & + \ (1-\lambda)z & =0 \end{array}$$

The characteristic equation of is

$$\begin{vmatrix} 1-\lambda & 2 & 0 \\ 2 & 1-\lambda & 0 \\ 0 & 2 & 1-\lambda \end{vmatrix} = (1-\lambda)\left[(1-\lambda)^2-4\right] = (1-\lambda)(\lambda+1)(\lambda-3)$$

$$= 0 \text{ when } \lambda = -1, +1, +3$$

Then $\lambda = \lambda_1 = -1$: $\left.\begin{array}{l} (1)\ \ 2x+2y=0 \ \rightarrow \ y=-x \\ (3)\ \ 2y+2z=0 \ \rightarrow \ z=-y=x \end{array}\right\} \rightarrow \ \mathbf{x}_1 = x\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$

$\lambda = \lambda_2 = +1$: $\left.\begin{array}{l} (1)\ \ 2y=0 \ \rightarrow \ y=0 \\ (2)\ \ 2x=0 \ \rightarrow \ x=0 \end{array}\right\} \rightarrow \ \mathbf{x}_2 = z\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$\lambda = \lambda_3 = +3$: $\left.\begin{array}{l} (1)\ -2x+2y=0 \ \rightarrow \ y=x \\ (3)\ \ \ 2y-2z=0 \ \rightarrow \ z=y=x \end{array}\right\} \rightarrow \ \mathbf{x}_3 = x\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$

9. $\begin{pmatrix} 0 & 3 & 0 \\ 3 & 0 & 3 \\ 0 & 3 & 0 \end{pmatrix}$

The secular equations are

$$\begin{array}{llcccl} (1) & -\lambda x & + & 3y & & =0 \\ (2) & 3x & + & -\lambda y & + \ \ 3z & =0 \\ (3) & & & 3y & + \ -\lambda z & =0 \end{array}$$

The characteristic equation is

$$\begin{vmatrix} -\lambda & 3 & 0 \\ 3 & -\lambda & 3 \\ 0 & 3 & -\lambda \end{vmatrix} = -\lambda(\lambda^2-18) = 0 \text{ when } \lambda = 0, \pm 3\sqrt{2}$$

$\lambda = \lambda_1 = 0$: $\left.\begin{array}{l} (1)\ \ 3y=0 \ \rightarrow \ y=0 \\ (2)\ \ 3x+3z=0 \ \rightarrow \ z=-x \end{array}\right\} \rightarrow \ \mathbf{x}_1 = x\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$

$\lambda = \lambda_2 = +3\sqrt{2}$: $\left.\begin{array}{l} (1)\ \ -3\sqrt{2}x+3y=0 \ \rightarrow \ y=\sqrt{2}x \\ (3)\ \ \ 3y-3\sqrt{2}z=0 \ \rightarrow \ z=y/\sqrt{2}=x \end{array}\right\} \rightarrow \ \mathbf{x}_2 = x\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$

$\lambda = \lambda_3 = -3\sqrt{2}$: $\left.\begin{array}{l} (1)\ \ \ 3\sqrt{2}x+3y=0 \ \rightarrow \ y=-\sqrt{2}x \\ (3)\ \ \ 3y+3\sqrt{2}z=0 \ \rightarrow \ z=-y/\sqrt{2}=x \end{array}\right\} \rightarrow \ \mathbf{x}_3 = x\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$

10. $\mathbf{A} = \begin{pmatrix} 3 & 4 \\ -4 & -5 \end{pmatrix}$

The secular equations are

$$\begin{aligned} (3-\lambda)x &+ 4y &= 0 \\ -4x &+ (-5-\lambda)y &= 0 \end{aligned}$$

The characteristic equation is

$$\begin{vmatrix} 3-\lambda & 4 \\ -4 & -5-\lambda \end{vmatrix} = \lambda^2 + 2\lambda + 1 = (\lambda+1)^2 = 0 \text{ when } \lambda = -1 \text{ (double)}$$

Then $\lambda = -1$: $(3-\lambda)x + 4y = 4x + 4y = 0 \rightarrow y = -x \rightarrow \mathbf{x} = x\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

and the matrix has only one eigenvector corresponding to the doubly-degenerate eigenvalue.

11. $\begin{pmatrix} 4 & 0 & 2 \\ -6 & 1 & -4 \\ -6 & 0 & -3 \end{pmatrix}$

The secular equations are

$$\begin{aligned} &(1) \quad (4-\lambda)x & & + 2z &= 0 \\ &(2) \quad -6x &+ (1-\lambda)y & - 4z &= 0 \\ &(3) \quad -6x & & + (-3-\lambda)z &= 0 \end{aligned}$$

The characteristic equation is

$$\begin{vmatrix} 4-\lambda & 0 & 2 \\ -6 & 1-\lambda & -4 \\ -6 & 0 & -3-\lambda \end{vmatrix} = \lambda(1-\lambda)^2 = 0 \text{ when } \lambda = 0, \lambda = 1 \text{ (double)}$$

Then $\lambda = \lambda_1 = 0$: $\left.\begin{aligned} &(1) \quad 4x + 2z = 0 \rightarrow z = -2x \\ &(2) \; -6x + y - 4z \rightarrow y = 6x + 4z = -2x \end{aligned}\right\} \rightarrow \mathbf{x}_1 = x\begin{pmatrix} 1 \\ -2 \\ -2 \end{pmatrix}$

but $\lambda = 1$: $3x + 2z = 0 \rightarrow z = -3x/2$

from all three equations, so that y is not determined for the degenerate eigenvalue. If $y = ax$ then

$$\mathbf{x}_1 = x\begin{pmatrix} 1 \\ a \\ -3/2 \end{pmatrix}, \quad \text{all } a \text{ (and } x\text{).}$$

Section 19.3

Normalize the eigenvectors obtained in

12. Exercise 5

$$\mathbf{x}_1 = x\begin{pmatrix}1\\0\end{pmatrix}:\quad \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_1 = x^2\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = x^2 = 1 \text{ when } x = 1 \quad\rightarrow\quad \mathbf{x}_1 = \begin{pmatrix}1\\0\end{pmatrix}$$

$$\mathbf{x}_2 = y\begin{pmatrix}0\\1\end{pmatrix}:\quad \mathbf{x}_2^{\mathsf{T}}\mathbf{x}_2 = y^2\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = y^2 = 1 \text{ when } y = 1 \quad\rightarrow\quad \mathbf{x}_2 = \begin{pmatrix}0\\1\end{pmatrix}$$

13. Exercise 7

$$\mathbf{x}_1 = x\begin{pmatrix}1\\-1\end{pmatrix}:\quad \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_1 = x^2\begin{pmatrix}1 & -1\end{pmatrix}\begin{pmatrix}1\\-1\end{pmatrix} = 2x^2 = 1 \text{ when } x = 1/\sqrt{2} \quad\rightarrow\quad \mathbf{x}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

$$\mathbf{x}_2 = x\begin{pmatrix}1\\1\end{pmatrix}:\quad \mathbf{x}_2^{\mathsf{T}}\mathbf{x}_2 = x^2\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = 2x^2 = 1 \text{ when } x = 1/\sqrt{2} \quad\rightarrow\quad \mathbf{x}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

14. Exercise 8

$$\mathbf{x}_1 = x\begin{pmatrix}1\\-1\\1\end{pmatrix}:\quad \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_1 = x^2\begin{pmatrix}1 & -1 & 1\end{pmatrix}\begin{pmatrix}1\\-1\\1\end{pmatrix} = 3x^2 = 1 \text{ when } x = 1/\sqrt{3} \quad\rightarrow\quad \mathbf{x}_1 = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\-1\\1\end{pmatrix}$$

$$\mathbf{x}_2 = z\begin{pmatrix}0\\0\\1\end{pmatrix}:\quad \mathbf{x}_2^{\mathsf{T}}\mathbf{x}_2 = z^2\begin{pmatrix}0 & 0 & 1\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix} = z^2 = 1 \text{ when } z = 1 \quad\rightarrow\quad \mathbf{x}_2 = \begin{pmatrix}0\\0\\1\end{pmatrix}$$

$$\mathbf{x}_3 = x\begin{pmatrix}1\\1\\1\end{pmatrix}:\quad \mathbf{x}_3^{\mathsf{T}}\mathbf{x}_3 = x^2\begin{pmatrix}1 & 1 & 1\end{pmatrix}\begin{pmatrix}1\\1\\1\end{pmatrix} = 3x^2 = 1 \text{ when } x = 1/\sqrt{3} \quad\rightarrow\quad \mathbf{x}_3 = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}$$

15. Exercise 9

$$\mathbf{x}_1 = x\begin{pmatrix}1\\0\\-1\end{pmatrix}:\quad \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_1 = x^2\begin{pmatrix}1 & 0 & -1\end{pmatrix}\begin{pmatrix}1\\0\\-1\end{pmatrix} = 2x^2 = 1 \text{ when } x = 1/\sqrt{2} \quad\rightarrow\quad \mathbf{x}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix}$$

$$\mathbf{x}_2 = x\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix}:\quad \mathbf{x}_2^{\mathsf{T}}\mathbf{x}_2 = x^2\begin{pmatrix}1 & \sqrt{2} & 1\end{pmatrix}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix} = 4x^2 = 1 \text{ when } x = 1/2 \quad\rightarrow\quad \mathbf{x}_2 = \frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix}$$

$$\mathbf{x}_3 = x\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}:\quad \mathbf{x}_3^{\mathsf{T}}\mathbf{x}_3 = x^2\begin{pmatrix}1 & -\sqrt{2} & 1\end{pmatrix}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix} = 4x^2 = 1 \text{ when } x = 1/2 \quad\rightarrow\quad \mathbf{x}_3 = \frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}$$

Show that the sets of eigenvectors of the symmetric matrices are orthogonal in

16. Exercise 5 (and 12)

$$\mathbf{x}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix},\ \mathbf{x}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ \to\ \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_2 = \begin{pmatrix} 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 + 0 = 0$$

17. Exercise 7 (and 13)

$$\mathbf{x}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix},\ \mathbf{x}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \ \to\ \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_2 = \frac{1}{2}\begin{pmatrix} 1 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{2}(1-1) = 0$$

18. Exercise 9 (and 15)

$$\mathbf{x}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},\ \mathbf{x}_2 = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix},\ \ \mathbf{x}_3 = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

$$\to\ \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_2 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2\sqrt{2}}(1+0-1) = 0$$

$$\to\ \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_3 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 1 & 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2\sqrt{2}}(1+0-1) = 0$$

$$\to\ \mathbf{x}_2^{\mathsf{T}}\mathbf{x}_3 = \frac{1}{4}\begin{pmatrix} 1 & \sqrt{2} & 1 \end{pmatrix}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{4}(1-2+1) = 0$$

19. Given the three vectors

$$\mathbf{x}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix},\ \mathbf{x}_2 = \begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix},\ \mathbf{x}_3 = \begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix},$$

use Schmidt orthogonalization to **(i)** find new vectors $\mathbf{x}_2'$ and $\mathbf{x}_3'$ that are orthogonal to $\mathbf{x}_1$,

(ii) find the new vector $\mathbf{x}_3''$ that is orthogonal to both $\mathbf{x}_1$ and $\mathbf{x}_2'$.

(i) We have

$$\left.\begin{aligned} \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_1 &= \begin{pmatrix} 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = 3 \\ \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_2 &= \begin{pmatrix} 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix} = 6 \\ \mathbf{x}_1^{\mathsf{T}}\mathbf{x}_3 &= \begin{pmatrix} 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix} = 6 \end{aligned}\right\} \ \to\ \frac{\mathbf{x}_1^{\mathsf{T}}\mathbf{x}_2}{\mathbf{x}_1^{\mathsf{T}}\mathbf{x}_1} = 2,\ \ \frac{\mathbf{x}_1^{\mathsf{T}}\mathbf{x}_3}{\mathbf{x}_1^{\mathsf{T}}\mathbf{x}_1} = 2$$

Therefore $\mathbf{x}_2' = \mathbf{x}_2 - \dfrac{\mathbf{x}_1^{\mathsf{T}}\mathbf{x}_2}{\mathbf{x}_1^{\mathsf{T}}\mathbf{x}_1}\mathbf{x}_1 = \begin{pmatrix}3\\1\\2\end{pmatrix} - 2\begin{pmatrix}1\\1\\1\end{pmatrix} = \begin{pmatrix}1\\-1\\0\end{pmatrix}$

and $\mathbf{x}_3' = \mathbf{x}_3 - \dfrac{\mathbf{x}_1^{\mathsf{T}}\mathbf{x}_3}{\mathbf{x}_1^{\mathsf{T}}\mathbf{x}_1}\mathbf{x}_1 = \begin{pmatrix}3\\2\\1\end{pmatrix} - 2\begin{pmatrix}1\\1\\1\end{pmatrix} = \begin{pmatrix}1\\0\\-1\end{pmatrix}$

are orthogonal to $\mathbf{x}_1$.

(ii) We have

$$\left.\begin{aligned}(\mathbf{x}_2')^{\mathsf{T}}\mathbf{x}_2' &= (1\quad -1\quad 0)\begin{pmatrix}1\\-1\\0\end{pmatrix} = 2\\ (\mathbf{x}_2')^{\mathsf{T}}\mathbf{x}_3' &= (1\quad -1\quad 0)\begin{pmatrix}1\\0\\-1\end{pmatrix} = 1\end{aligned}\right\} \to \frac{(\mathbf{x}_2')^{\mathsf{T}}\mathbf{x}_3'}{(\mathbf{x}_2')^{\mathsf{T}}\mathbf{x}_2'} = \frac{1}{2}$$

Therefore $\mathbf{x}_3'' = \mathbf{x}_3' - \dfrac{\mathbf{x}_2'^{\mathsf{T}}\mathbf{x}_3'}{\mathbf{x}_2'^{\mathsf{T}}\mathbf{x}_2'} = \mathbf{x}_3' - \dfrac{1}{2}\mathbf{x}_2' = \begin{pmatrix}1\\0\\-1\end{pmatrix} - \dfrac{1}{2}\begin{pmatrix}1\\-1\\0\end{pmatrix} = \begin{pmatrix}1/2\\1/2\\-1\end{pmatrix}$

is orthogonal to $\mathbf{x}_1$ and $\mathbf{x}_2'$.

20. The Hückel Hamiltonian matrix of butadiene is

$$\mathbf{H} = \begin{pmatrix}\alpha & \beta & 0 & 0\\ \beta & \alpha & \beta & 0\\ 0 & \beta & \alpha & \beta\\ 0 & 0 & \beta & \alpha\end{pmatrix}$$

Find **(i)** the eigenvalues (in terms of α and β), **(ii)** the orthonormal eigenvectors. You may find the following relations useful: $\phi = (\sqrt{5}+1)/2$ (the 'golden section', see Section 7.2), $\phi^2 = (\sqrt{5}+3)/2$, $\phi - 1 = (\sqrt{5}-1)/2 = 1/\phi$, $\phi^2 - 1 = \phi$, $\phi^2 - \phi = 1$.

(i) The characteristic determinant

$$\begin{vmatrix}\alpha - E & \beta & 0 & 0\\ \beta & \alpha - E & \beta & 0\\ 0 & \beta & \alpha - E & \beta\\ 0 & 0 & \beta & \alpha - E\end{vmatrix} = (\alpha - E)^4 - 3\beta^2(\alpha - E)^2 + \beta^4$$

is a quadratic in $(\alpha - E)^2$ and is zero when E is an eigenvalue of the matrix $\mathbf{H}$. Then

$$(\alpha - E)^4 - 3(\alpha - E)^2\beta^2 + \beta^4 = 0 \text{ when } (\alpha - E)^2 = \frac{3\beta^2 \pm \sqrt{9\beta^4 - 4\beta^4}}{2} = \left(\frac{3 \pm \sqrt{5}}{2}\right)\beta^2$$

$$\to E = \alpha \pm \left(\frac{3 \pm \sqrt{5}}{2}\right)^{1/2}\beta = \alpha \pm \left(\frac{1 \pm \sqrt{5}}{2}\right)\beta$$

The eigenvalues are then, in order of increasing value (given that $\beta < 0$),

$$E_1 = \alpha + \left(\frac{1+\sqrt{5}}{2}\right)\beta = \alpha + \phi\beta$$

$$E_2 = \alpha + \left(\frac{1-\sqrt{5}}{2}\right)\beta = \alpha + (\phi - 1)\beta$$

$$E_3 = \alpha - \left(\frac{1-\sqrt{5}}{2}\right)\beta = \alpha - (\phi - 1)\beta$$

$$E_4 = \alpha - \left(\frac{1+\sqrt{5}}{2}\right)\beta = \alpha - \phi\beta$$

(ii) The secular equations are

$$\begin{array}{llllllll}
(1) & (\alpha - E)c_1 & + & \beta c_2 & & & & = 0 \\
(2) & \beta c_1 & + & (\alpha - E)c_2 & + & \beta c_3 & & = 0 \\
(3) & & & \beta c_2 & + & (\alpha - E)c_3 & + \quad \beta c_4 & = 0 \\
(4) & & & & & \beta c_3 & + \quad (\alpha - E)c_4 & = 0
\end{array}$$

For $E = E_1 = \alpha + \phi\beta \quad \rightarrow \quad \dfrac{\alpha - E}{\beta} = -\phi$, and dividing the equations by β ,

$$\begin{array}{lll}
(1) & -\phi c_1 + c_2 = 0 & \rightarrow \quad c_2 = \phi c_1 \\
(2) & c_1 - \phi c_2 + c_3 = 0 & \rightarrow \quad c_3 = -c_1 + \phi c_2 = (\phi^2 - 1)c_1 = \phi c_1 \\
(3) & c_3 - \phi c_4 = 0 & \rightarrow \quad c_4 = c_3 / \phi = c_1
\end{array}$$

The eigenvector corresponding to eigenvalue $E_1 = \alpha + \phi\beta$ is therefore

$$\mathbf{x}_1 = c_1 \begin{pmatrix} 1 \\ \phi \\ \phi \\ 1 \end{pmatrix}$$

For normalization, $\mathbf{x}_1{}^{\mathsf{T}}\mathbf{x}_1 = c_1{}^2(1 + \phi^2 + \phi^2 + 1) = 1$ when $c_1 = 1\big/\sqrt{2(1+\phi^2)} = 1\big/\sqrt{2(\phi + 2)}$.

Therefore, putting $C = 1\big/\sqrt{2(\phi+2)}$, the normalized eigenvector is

$$\mathbf{x}_1 = C \begin{pmatrix} 1 \\ \phi \\ \phi \\ 1 \end{pmatrix}$$

Similarly for the other eigenvalues,

$$\mathbf{x}_2 = C \begin{pmatrix} \phi \\ 1 \\ -1 \\ -\phi \end{pmatrix}, \quad \mathbf{x}_3 = C \begin{pmatrix} \phi \\ -1 \\ -1 \\ \phi \end{pmatrix}, \quad \mathbf{x}_4 = C \begin{pmatrix} 1 \\ -\phi \\ \phi \\ -1 \end{pmatrix},$$

21. The Hückel Hamiltonian matrix of cyclopropene is

$$\mathbf{H} = \begin{pmatrix} \alpha & \beta & \beta \\ \beta & \alpha & \beta \\ \beta & \beta & \alpha \end{pmatrix}$$

(i) Show that the eigenvalues are $E_1 = \alpha + 2\beta$, $E_2 = E_3 = \alpha - \beta$. **(ii)** Find the normalized eigenvector belonging to eigenvalue E_1. **(iii)** Show that an eigenvector belonging to the doubly-degenerate eigenvalue $\alpha - \beta$ has components x_1, x_2, x_3 that satisfy $x_1 + x_2 + x_3 = 0$. **(iv)** Find two orthonormal eigenvectors corresponding to eigenvalue $\alpha - \beta$ (you may find the results of Examples 19.4(ii) and 19.8 useful).

(i) The characteristic equation is

$$\begin{vmatrix} \alpha - E & \beta & \beta \\ \beta & \alpha - E & \beta \\ \beta & \beta & \alpha - E \end{vmatrix} = (\alpha - E)^3 - 3\beta^2(\alpha - E) + 2\beta^3$$

$$= 0 \text{ when } E \text{ is an eigenvalue of } \mathbf{H}.$$

The characteristic equation is a cubic in *E*. If the eigenvalues (the roots of the cubic) are $E_1 = \alpha + 2\beta$, $E_2 = E_3 = \alpha - \beta$, the equation can be written as

$$(E_1 - E)(E_2 - E)(E_3 - E) = 0$$

Therefore

$$(\alpha + 2\beta - E)(\alpha - \beta - E)^2 = (\alpha - E)^3 - 3\beta^2(\alpha - E) + 2\beta^3 = 0$$

as required.

(ii) The secular equations are

$$\begin{aligned} &(1) \quad (\alpha - E)x_1 + \beta x_2 + \beta x_3 = 0 \\ &(2) \quad \beta x_1 + (\alpha - E)x_2 + \beta x_3 = 0 \\ &(3) \quad \beta x_1 + \beta x_2 + (\alpha - E)x_3 = 0 \end{aligned}$$

For $E = E_1 = \alpha + 2\beta$

$$\begin{aligned} &(1) \quad -2\beta x_1 + \beta x_2 + \beta x_3 = 0 \\ &(2) \quad \beta x_1 - 2\beta x_2 + \beta x_3 = 0 \\ &(3) \quad \beta x_1 + \beta x_2 - 2\beta x_3 = 0 \end{aligned}$$

Subtract equation (1) from (2) and (1) from (3):

$$\left.\begin{aligned} &(2)-(1) \quad 3\beta x_1 - 3\beta x_2 = 0 \ \rightarrow\ x_2 = x_1 \\ &(3)-(1) \quad 3\beta x_1 - 3\beta x_3 = 0 \ \rightarrow\ x_3 = x_1 \end{aligned}\right\} \rightarrow \mathbf{x}_1 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

(iii) For $E = \alpha - \beta$ all three secular equations reduce to

$$\beta x_1 + \beta x_2 + \beta x_3 = 0$$

Therefore, as for the degenerate eigenvalue in Example 19.4(ii), every independent pair of vectors that satisfies the condition $x_1 + x_2 + x_3 = 0$ is a solution for the degenerate eigenvalue.

Following the procedure described in Examples 19.4(ii), 19.6 and 19.8, a pair of orthonormal eigenvectors belonging to eigenvalue $E = \alpha - \beta$ is

$$\mathbf{x}_2 = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}, \quad \mathbf{x}_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

22. (i) Show that a square matrix **A** and its transpose $\mathbf{A}^\mathsf{T}$ have the same set of eigenvalues. **(ii)** Show that the following two equations are equivalent:

$$\mathbf{A}^\mathsf{T}\mathbf{y} = \lambda\mathbf{y}, \qquad \mathbf{y}^\mathsf{T}\mathbf{A} = \lambda\mathbf{y}^\mathsf{T}$$

The eigenvectors of $\mathbf{A}^\mathsf{T}$ are in general different from those of **A** (unless **A** is a symmetric). The vector **y** is sometimes called a **left-eigenvector** of **A**, and an 'ordinary' eigenvector **x** of **A** is then called a **right-eigenvector**.

(iii) Find the eigenvalues and corresponding normalized right- and left-eigenvectors of

$$\mathbf{A} = \begin{pmatrix} 3 & 2 \\ 0 & 2 \end{pmatrix}.$$

(i) By equation (18.19), the secular determinants of **A** and its transpose $\mathbf{A}^\mathsf{T}$ are the same. The eigenvalues of **A** and $\mathbf{A}^\mathsf{T}$ are therefore the same.

(ii) By equation (18.41)

$$\mathbf{A}^\mathsf{T}\mathbf{y} = \lambda\mathbf{y} \xrightarrow{\text{transpose}} (\mathbf{A}^\mathsf{T}\mathbf{y})^\mathsf{T} = (\lambda\mathbf{y})^\mathsf{T} \;\to\; \mathbf{y}^\mathsf{T}\mathbf{A} = \lambda\mathbf{y}^\mathsf{T}$$

(iii) The characteristic equation is

$$\begin{vmatrix} 3-\lambda & 2 \\ 0 & 2-\lambda \end{vmatrix} = (3-\lambda)(2-\lambda) = 0 \text{ when } \lambda = 2, 3$$

For the **right-eigenvectors**,

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x} \;\to\; \begin{pmatrix} 3-\lambda & 2 \\ 0 & 2-\lambda \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = 0 \;\to\; \begin{matrix} (3-\lambda)x & + & 2y & = 0 \\ & & (2-\lambda)y & = 0 \end{matrix}$$

Then $\lambda = \lambda_1 = 2: \; x + 2y = 0 \;\to\; x = -2y \;\to\; \mathbf{x}_1 = \frac{1}{\sqrt{5}}\begin{pmatrix} -2 \\ 1 \end{pmatrix}$ (normalized)

$\lambda = \lambda_2 = 3: \; y = 0 \;\to\; \mathbf{x}_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

For the **left-eigenvectors**,

$$\mathbf{y}^{\mathsf{T}}\mathbf{A} = \lambda\mathbf{y}^{\mathsf{T}} \quad \to \quad \begin{pmatrix} x & y \end{pmatrix}\begin{pmatrix} 3-\lambda & 2 \\ 0 & 2-\lambda \end{pmatrix} = 0 \quad \to \quad \begin{aligned} (3-\lambda)x \qquad\qquad\qquad &= 0 \\ 2x \quad + \quad (2-\lambda)y &= 0 \end{aligned}$$

Then $\lambda = \lambda_1 = 2: \quad x = 0 \qquad\qquad \to \quad \mathbf{y}_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$\lambda = \lambda_2 = 3: \quad 2x - y = 0 \quad \to \quad y = 2x \quad \to \quad \mathbf{y}_2 = \dfrac{1}{\sqrt{5}}\begin{pmatrix} 1 \\ 2 \end{pmatrix}$

Section 19.4

23. For the matrix

$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 2 & 1 \end{pmatrix}$$

of Exercise 8, construct **(i)** the matrix **X** of the eigenvectors and **(ii)** the diagonal matrix **D** of the $\lambda = \lambda_2 = +1$ eigenvalues**. (iii)** Show that $\mathbf{AX} = \mathbf{DX}$.

By Exercise 8, the eigenvalues and (unnormalized) eigenvectors of matrix **A** are

$$\lambda_1 = -1, \quad \mathbf{x}_1 = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}; \qquad \lambda_2 = 1, \quad \mathbf{x}_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}; \qquad \lambda_3 = 3, \quad \mathbf{x}_3 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Then **(i)** $\mathbf{X} = \begin{pmatrix} 1 & 0 & 1 \\ -1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix}$ **(ii)** $\mathbf{D} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix}$

(iii) $\mathbf{AX} = \begin{pmatrix} 1 & 2 & 0 \\ 2 & 1 & 0 \\ 0 & 2 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 \\ -1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 3 \\ 1 & 0 & 3 \\ -1 & 1 & 3 \end{pmatrix}$

$\mathbf{XD} = \begin{pmatrix} 1 & 0 & 1 \\ -1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 3 \\ 1 & 0 & 3 \\ -1 & 1 & 3 \end{pmatrix}$

and $\mathbf{AX} = \mathbf{DX}$

24. Repeat Exercise 23 for the matrix $\begin{pmatrix} 0 & 3 & 0 \\ 3 & 0 & 3 \\ 0 & 3 & 0 \end{pmatrix}$ of Exercise 9.

By Exercise 9, the eigenvalues and (unnormalized) eigenvectors of matrix **A** are

$$\lambda_1 = 0, \ \mathbf{x}_1 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}; \qquad \lambda_2 = 3\sqrt{2}, \ \mathbf{x}_2 = \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}; \qquad \lambda_3 = -3\sqrt{2}, \ \mathbf{x}_3 = \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

Then **(i)** $\mathbf{X} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & \sqrt{2} & -\sqrt{2} \\ -1 & 1 & 1 \end{pmatrix}$ **(ii)** $\mathbf{D} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 3\sqrt{2} & 0 \\ 0 & 0 & -3\sqrt{2} \end{pmatrix}$

(iii) $$\mathbf{AX} = \begin{pmatrix} 0 & 3 & 0 \\ 3 & 0 & 3 \\ 0 & 3 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & 1 \\ 0 & \sqrt{2} & -\sqrt{2} \\ -1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 3\sqrt{2} & -3\sqrt{2} \\ 0 & 6 & 6 \\ 0 & 3\sqrt{2} & -3\sqrt{2} \end{pmatrix}$$

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

and $\mathbf{AX} = \mathbf{DX}$

25. (i) For the matrix $\mathbf{A} = \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}$ of Exercise 7, construct the matrix **X** of the eigenfunctions of **A**, and find its inverse, $\mathbf{X}^{-1}$.

(ii) Calculate $\mathbf{D} = \mathbf{X}^{-1}\mathbf{AX}$ and confirm that **D** is the diagonal matrix of the eigenvalues of **A**.

By Exercise 7, the eigenvalues and normalized eigenvectors of **A** are

$$\lambda_1 = 2, \quad \mathbf{x}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}; \qquad \lambda_2 = 4, \quad \mathbf{x}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix};$$

Then **(i)** $\mathbf{X} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$ $\mathbf{X}^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$ (by equation (18.43))

(ii) $$\mathbf{X}^{-1}\mathbf{AX} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 2 & 4 \\ -2 & 4 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 4 & 0 \\ 0 & 8 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 4 \end{pmatrix}$$

$$= \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} = \mathbf{D}$$

Repeat Exercise 25 for:

26. $\mathbf{A}=\begin{pmatrix}2 & 2\\ 1 & 3\end{pmatrix}$ of Exercise 4

By Exercise 4, the eigenvalues and eigenvectors of $\mathbf{A}$ are

$$\lambda_1=1,\quad \mathbf{x}_1=\frac{1}{\sqrt{5}}\begin{pmatrix}2\\ -1\end{pmatrix};\qquad \lambda_2=4,\quad \mathbf{x}_2=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix};$$

Then **(i)** $\mathbf{X}=\begin{pmatrix}2/\sqrt{5} & 1/\sqrt{2}\\ -1/\sqrt{5} & 1/\sqrt{2}\end{pmatrix}\qquad \mathbf{X}^{-1}=\frac{1}{3}\begin{pmatrix}\sqrt{5} & -\sqrt{5}\\ \sqrt{2} & 2\sqrt{2}\end{pmatrix}$

(ii) $$\mathbf{X}^{-1}\mathbf{A}\mathbf{X}=\frac{1}{3}\begin{pmatrix}\sqrt{5} & -\sqrt{5}\\ \sqrt{2} & 2\sqrt{2}\end{pmatrix}\begin{pmatrix}2 & 2\\ 1 & 3\end{pmatrix}\begin{pmatrix}2/\sqrt{5} & 1/\sqrt{2}\\ -1/\sqrt{5} & 1/\sqrt{2}\end{pmatrix}$$

$$=\frac{1}{3}\begin{pmatrix}\sqrt{5} & -\sqrt{5}\\ \sqrt{2} & 2\sqrt{2}\end{pmatrix}\begin{pmatrix}2/\sqrt{5} & 1/\sqrt{2}\\ -1/\sqrt{5} & 1/\sqrt{2}\end{pmatrix}=\frac{1}{3}\begin{pmatrix}3 & 0\\ 0 & 12\end{pmatrix}=\begin{pmatrix}1 & 0\\ 0 & 4\end{pmatrix}$$

$$=\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}=\mathbf{D}$$

27. $\mathbf{A}=\begin{pmatrix}1 & 2 & 0\\ 2 & 1 & 0\\ 0 & 2 & 1\end{pmatrix}$ of Exercise 8

By Exercise 8, the eigenvalues and (unnormalized) eigenvectors of $\mathbf{A}$ are

$$\lambda_1=-1,\quad \mathbf{x}_1=\begin{pmatrix}1\\ -1\\ 1\end{pmatrix};\quad \lambda_2=1,\quad \mathbf{x}_2=\begin{pmatrix}0\\ 0\\ 1\end{pmatrix};\qquad \lambda_2=3,\quad \mathbf{x}_3=\begin{pmatrix}1\\ 1\\ 1\end{pmatrix}$$

Then **(i)** $\mathbf{X}=\begin{pmatrix}1 & 0 & 1\\ -1 & 0 & 1\\ 1 & 1 & 1\end{pmatrix}\qquad \mathbf{X}^{-1}=\frac{1}{2}\begin{pmatrix}1 & -1 & 0\\ -2 & 0 & 2\\ 1 & 1 & 0\end{pmatrix}$

(ii) $$\mathbf{X}^{-1}\mathbf{A}\mathbf{X}=\frac{1}{2}\begin{pmatrix}1 & -1 & 0\\ -2 & 0 & 2\\ 1 & 1 & 0\end{pmatrix}\begin{pmatrix}1 & 2 & 0\\ 2 & 1 & 0\\ 0 & 2 & 1\end{pmatrix}\begin{pmatrix}1 & 0 & 1\\ -1 & 0 & 1\\ 1 & 1 & 1\end{pmatrix}$$

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

$$=\begin{pmatrix}\lambda_1 & 0 & 0\\ 0 & \lambda_2 & 0\\ 0 & 0 & \lambda_3\end{pmatrix}=\mathbf{D}$$

28. $\mathbf{A}=\begin{pmatrix}0&3&0\\3&0&3\\0&3&0\end{pmatrix}$ of Exercise 9

By Exercise 9, the eigenvalues and eigenvectors of $\mathbf{A}$ are

$$\lambda_1=0,\ \mathbf{x}_1=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix};\quad \lambda_2=3\sqrt{2},\ \mathbf{x}_2=\frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix};\quad \lambda_2=-3\sqrt{2},\ \mathbf{x}_3=\frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}$$

Then **(i)** $\mathbf{X}=\begin{pmatrix}1/\sqrt{2}&1/2&1/2\\0&1/\sqrt{2}&-1/\sqrt{2}\\-1/\sqrt{2}&1/2&1/2\end{pmatrix}$ $\qquad\mathbf{X}^{-1}=\begin{pmatrix}1/\sqrt{2}&0&-1/\sqrt{2}\\1/2&1/\sqrt{2}&1/2\\1/2&-1/\sqrt{2}&1/2\end{pmatrix}$

(ii) $$\mathbf{X}^{-1}\mathbf{A}\mathbf{X}=\begin{pmatrix}1/\sqrt{2}&0&-1/\sqrt{2}\\1/2&1/\sqrt{2}&1/2\\1/2&-1/\sqrt{2}&1/2\end{pmatrix}\begin{pmatrix}0&3&0\\3&0&3\\0&3&0\end{pmatrix}\begin{pmatrix}1/\sqrt{2}&1/2&1/2\\0&1/\sqrt{2}&-1/\sqrt{2}\\-1/\sqrt{2}&1/2&1/2\end{pmatrix}$$

$$=\begin{pmatrix}1/\sqrt{2}&0&-1/\sqrt{2}\\1/2&1/\sqrt{2}&1/2\\1/2&-1/\sqrt{2}&1/2\end{pmatrix}\begin{pmatrix}0&3/\sqrt{2}&-3/\sqrt{2}\\0&3&3\\0&3/\sqrt{2}&-3/\sqrt{2}\end{pmatrix}=\begin{pmatrix}0&0&0\\0&3/\sqrt{2}&0\\0&0&-3/\sqrt{2}\end{pmatrix}$$

$$=\begin{pmatrix}\lambda_1&0&0\\0&\lambda_2&0\\0&0&\lambda_3\end{pmatrix}=\mathbf{D}$$

Section 19.5

Express in matrix form:

By equations (19.35) and (19.36)

29. $5x^2-2xy-3y^2=(x\ \ y)\begin{pmatrix}5&-1\\-1&-3\end{pmatrix}\begin{pmatrix}x\\y\end{pmatrix}$

30. $4xy=(x\ \ y)\begin{pmatrix}0&2\\2&0\end{pmatrix}\begin{pmatrix}x\\y\end{pmatrix}$

By equations (19.37) to (19.39) for $n=3$,

31. $3x^2-4xy+2xz-6yz+y^2-2z^2=\begin{pmatrix}x&y&z\end{pmatrix}\begin{pmatrix}3&-2&1\\-2&1&-3\\1&-3&-2\end{pmatrix}\begin{pmatrix}x\\y\\z\end{pmatrix}$

Transform the following quadratic forms into canonical form:

32. $7x_1^2 + 6\sqrt{3}x_1x_2 + 13x_2^2$

We have $\quad Q = 7x_1^2 + 6\sqrt{3}x_1x_2 + 13x_2^2$

$$= (x_1 \;\; x_2)\begin{pmatrix} 7 & 3\sqrt{3} \\ 3\sqrt{3} & 13 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \mathbf{x}^{\mathsf{T}}\mathbf{A}\mathbf{x}$$

(a) For the eigenvalues of matrix **A,**

$$\begin{vmatrix} 7-\lambda & 3\sqrt{3} \\ 3\sqrt{3} & 13-\lambda \end{vmatrix} = (\lambda-4)(\lambda-16) = 0 \text{ when } \lambda = 4, 16 \quad \to \quad \lambda_1 = 4,\ \lambda_2 = 16$$

and $\quad \mathbf{D} = \begin{pmatrix} 4 & 0 \\ 0 & 16 \end{pmatrix}$

is the diagonal matrix of the eigenvalues of **A**

(b) For the eigenvectors, the secular equations are

$$\begin{aligned} (7-\lambda)x_1 \quad &+ \quad 3\sqrt{3}x_2 &= 0 \\ 3\sqrt{3}x_1 \quad &+ \quad +(13-\lambda)x_2 &= 0 \end{aligned}$$

Then $\quad \lambda = \lambda_1 = 4: \quad 3x_1 + 3\sqrt{3}x_2 = 0 \;\to\; x_1 = -\sqrt{3}x_2 \;\to\; \mathbf{x}_1 = \frac{1}{2}\begin{pmatrix} \sqrt{3} \\ -1 \end{pmatrix}$ (normalized)

$$\lambda = \lambda_2 = 16: \; -9x_1 + 3\sqrt{3}x_2 = 0 \;\to\; x_2 = \sqrt{3}x_1 \;\to\; \mathbf{x}_2 = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}$$

(c) The matrix of the eigenvectors is

$$\mathbf{X} = (\mathbf{x}_1 \;\; \mathbf{x}_2) = \frac{1}{2}\begin{pmatrix} \sqrt{3} & 1 \\ -1 & \sqrt{3} \end{pmatrix} \text{ with transpose } \mathbf{X}^{\mathsf{T}} = \frac{1}{2}\begin{pmatrix} \sqrt{3} & -1 \\ 1 & \sqrt{3} \end{pmatrix}$$

Then

$$Q = \mathbf{y}^{\mathsf{T}}\mathbf{D}\mathbf{y} = \lambda_1 y_1^2 + \lambda_2 y_2^2 = 4y_1^2 + 16y_2^2$$

where

$$\mathbf{y} = \mathbf{X}^{\mathsf{T}}\mathbf{x} \;\to\; \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \sqrt{3} & -1 \\ 1 & \sqrt{3} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \;\to\; \begin{cases} y_1 = \frac{1}{2}(\sqrt{3}x_1 - x_2) \\ y_2 = \frac{1}{2}(x_1 + \sqrt{3}x_2) \end{cases}$$

33. $ax^2 + 2bxy + ay^2$

We have $Q = (x_1 \;\; x_2)\begin{pmatrix} a & b \\ b & a \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \mathbf{x}^{\mathsf{T}}\mathbf{A}\mathbf{x}$

(a) For the eigenvalues of matrix **A,**

$$\begin{vmatrix} a-\lambda & b \\ b & a-\lambda \end{vmatrix} = (a-\lambda)^2 - b^2 \text{ when } a-\lambda = \pm b \;\;\to\;\; \lambda_1 = a+b,\, \lambda_2 = a-b$$

and $\mathbf{D} = \begin{pmatrix} a+b & 0 \\ 0 & a-b \end{pmatrix}$

is the diagonal matrix of the eigenvalues of **A**

(b) For the eigenvectors, the secular equations are

$$\begin{array}{cccc} (a-\lambda)x_1 & + & bx_2 & = 0 \\ bx_1 & + & +(a-\lambda)x_2 & = 0 \end{array}$$

Then $\lambda = \lambda_1 = a+b: \quad -bx_1 + bx_2 = 0 \;\to\; x_1 = x_2 \;\to\; \mathbf{x}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$\lambda = \lambda_2 = a-b: \quad bx_1 + bx_2 = 0 \;\to\; x_1 = -x_2 \;\to\; \mathbf{x}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

(c) The matrix of the eigenvectors is

$$\mathbf{X} = (\mathbf{x}_1 \;\; \mathbf{x}_2) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \mathbf{X}^{\mathsf{T}}$$

Then

$$Q = \mathbf{y}^{\mathsf{T}}\mathbf{D}\mathbf{y} = \lambda_1 y_1^2 + \lambda_2 y_2^2 = (a+b)y_1^2 + (a-b)y_2^2$$

where

$$\mathbf{y} = \mathbf{X}^{\mathsf{T}}\mathbf{x} \;\to\; \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \;\to\; \begin{cases} y_1 = \frac{1}{\sqrt{2}}(x_1 + x_2) \\ y_2 = \frac{1}{\sqrt{2}}(x_1 - x_2) \end{cases}$$

34. $3x_1^{\ 2}+2x_1x_2+2x_1x_4+3x_2^{\ 2}+2x_2x_3+3x_3^{\ 2}+2x_3x_4+3x_4^{\ 2}$

We have $$Q=\begin{pmatrix}x_1 & x_2 & x_3 & x_4\end{pmatrix}\begin{pmatrix}3&1&0&1\\1&3&1&0\\0&1&3&1\\1&0&1&3\end{pmatrix}\begin{pmatrix}x_1\\x_2\\x_3\\x_4\end{pmatrix}=\mathbf{x}^{\mathsf{T}}\mathbf{Ax}$$

As in Example 19.9, with $\alpha=3,\ \beta=1$, the eigenvalues of **A** are

$$\lambda_1=5,\quad \lambda_2=\lambda_3=3,\quad \lambda_4=1$$

and a set of eigenfunctions is

$$\mathbf{x}_1=\frac{1}{2}\begin{pmatrix}1\\1\\1\\1\end{pmatrix},\qquad \mathbf{x}_2=\frac{1}{2}\begin{pmatrix}1\\1\\-1\\-1\end{pmatrix},\qquad \mathbf{x}_3=\frac{1}{2}\begin{pmatrix}1\\-1\\-1\\1\end{pmatrix},\qquad \mathbf{x}_4=\frac{1}{2}\begin{pmatrix}1\\-1\\1\\-1\end{pmatrix}$$

The matrix of the eigenvectors is

$$\mathbf{X}=(\mathbf{x}_1\ \ \mathbf{x}_2)=\frac{1}{2}\begin{pmatrix}1&1&1&1\\1&1&-1&-1\\1&-1&-1&1\\1&-1&1&-1\end{pmatrix}=\mathbf{X}^{\mathsf{T}}$$

Then

$$Q=\lambda_1y_1^2+\lambda_2y_2^2+\lambda_3y_3^2+\lambda_4y_4^2=5y_1^2+3y_2^2+3y_3^2+y_4^2$$

where

$$\mathbf{y}=\mathbf{X}^{\mathsf{T}}\mathbf{x}\ \ \rightarrow\ \begin{pmatrix}y_1\\y_2\\y_3\\y_4\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1&1&1&1\\1&1&-1&-1\\1&-1&-1&1\\1&-1&1&-1\end{pmatrix}\begin{pmatrix}x_1\\x_2\\x_3\\x_4\end{pmatrix}\ \rightarrow\ \begin{cases}y_1=\frac{1}{2}(x_1+x_2+x_3+x_4)\\ y_2=\frac{1}{2}(x_1+x_2-x_3-x_4)\\ y_3=\frac{1}{2}(x_1-x_2-x_3+x_4)\\ y_4=\frac{1}{2}(x_1-x_2+x_3-x_4)\end{cases}$$

35. Derive equations (19.44) for the components of the inertia tensor. [Hint: Expand equation (16.60), $\boldsymbol{l} = mr^2\boldsymbol{\omega} - m(\boldsymbol{r}\cdot\boldsymbol{\omega})\boldsymbol{r}$, for the angular momentum in terms of components.]

We express the terms on the right side of equation (16.60) in terms of components:

$$\boldsymbol{\omega} = \omega_x\boldsymbol{i} + \omega_y\boldsymbol{j} + \omega_z\boldsymbol{k} \quad \rightarrow \quad mr^2\boldsymbol{\omega} = mr^2\omega_x\boldsymbol{i} + mr^2\omega_y\boldsymbol{j} + mr^2\omega_z\boldsymbol{k}$$

$$\begin{aligned}\boldsymbol{r}\cdot\boldsymbol{\omega} = x\omega_x + y\omega_y + z\omega_z \quad \rightarrow \quad m(\boldsymbol{r}\cdot\boldsymbol{\omega})\boldsymbol{r} &= (mx\omega_x + my\omega_y + mz\omega_z)(x\boldsymbol{i} + y\boldsymbol{j} + z\boldsymbol{k}) \\ &= \boldsymbol{i}\left[mx^2\omega_x + mxy\omega_y + mxz\omega_z\right] \\ &\quad + \boldsymbol{j}\left[myx\omega_x + my^2\omega_y + myz\omega_z\right] \\ &\quad + \boldsymbol{k}\left[mzx\omega_x + mzy\omega_y + mz^2\omega_z\right]\end{aligned}$$

Therefore, using $r^2 = x^2 + y^2 + z^2$,

$$\begin{aligned}\boldsymbol{l} = mr^2\boldsymbol{\omega} - m(\boldsymbol{r}\cdot\boldsymbol{\omega})\boldsymbol{r} &= mr^2\omega_x\boldsymbol{i} + mr^2\omega_y\boldsymbol{j} + mr^2\omega_z\boldsymbol{k} \\ &\quad - \boldsymbol{i}\left[mx^2\omega_x + mxy\omega_y + mxz\omega_z\right] \\ &\quad - \boldsymbol{j}\left[myx\omega_x + my^2\omega_y + myz\omega_z\right] \\ &\quad - \boldsymbol{k}\left[mzx\omega_x + mzy\omega_y + mz^2\omega_z\right] \\ &= \boldsymbol{i}\left[m(y^2 + z^2)\omega_x - mxy\omega_y - mxz\omega_z\right] \\ &\quad + \boldsymbol{j}\left[-myx\omega_x + m(z^2 + x^2)\omega_y - myz\omega_z\right] \\ &\quad + \boldsymbol{k}\left[-mzx\omega_x - mzy\omega_y + m(x^2 + y^2)\omega_z\right]\end{aligned}$$

In matrix form,

$$\begin{pmatrix} l_x \\ l_y \\ l_z \end{pmatrix} = \begin{pmatrix} m(y^2 + z^2) & -mxy & -mxz \\ -myx & m(z^2 + x^2) & -myz \\ -mzx & -mzy & m(x^2 + y^2) \end{pmatrix} \begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}$$

By equation (19.46), $\boldsymbol{l} = \mathbf{I}\boldsymbol{\omega}$ where the matrix **I** is the moment of inertia tensor. Therefore

$$\begin{pmatrix} l_x \\ l_y \\ l_z \end{pmatrix} = \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix} \begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}$$

$$\rightarrow \quad \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix} = \begin{pmatrix} m(y^2 + z^2) & -mxy & -mxz \\ -myx & m(z^2 + x^2) & -myz \\ -mzx & -mzy & m(x^2 + y^2) \end{pmatrix}$$

Section 19.6

Find the complex conjugate and Hermitian conjugate of the following matrices

36. $\begin{pmatrix} 1+i & 2-i \\ 3+i & -i \end{pmatrix}$

$$\mathbf{A} = \begin{pmatrix} 1+i & 2-i \\ 3+i & -i \end{pmatrix} \to \mathbf{A}^* = \begin{pmatrix} 1-i & 2+i \\ 3-i & i \end{pmatrix} \to \mathbf{A}^\dagger = (\mathbf{A}^*)^\mathsf{T} = \begin{pmatrix} 1-i & 3-i \\ 2+i & i \end{pmatrix}$$

37. $\begin{pmatrix} 2 & i \\ -i & 1 \end{pmatrix}$

$$\mathbf{A} = \begin{pmatrix} 2 & i \\ -i & 1 \end{pmatrix} \to \mathbf{A}^* = \begin{pmatrix} 2 & -i \\ i & 1 \end{pmatrix} \to \mathbf{A}^\dagger = (\mathbf{A}^*)^\mathsf{T} = \begin{pmatrix} 2 & i \\ -i & 1 \end{pmatrix}$$

38. $\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$

$$\mathbf{A} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \to \mathbf{A}^* = \begin{pmatrix} 0 & i & 0 \\ -i & 0 & i \\ 0 & -i & 0 \end{pmatrix} \to \mathbf{A}^\dagger = (\mathbf{A}^*)^\mathsf{T} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

39. If $\mathbf{a} = \begin{pmatrix} i \\ 1 \\ -i \end{pmatrix}$ and $\mathbf{b} = \begin{pmatrix} 2i \\ 0 \\ 3 \end{pmatrix}$, find **(i)** $\mathbf{a}^\dagger\mathbf{a}$ **(ii)** $\mathbf{b}^\dagger\mathbf{b}$ **(iii)** $\mathbf{a}^\dagger\mathbf{b}$ **(iv)** $\mathbf{b}^\dagger\mathbf{a}$

(i) $\mathbf{a}^\dagger\mathbf{a} = \begin{pmatrix} -i & 1 & i \end{pmatrix}\begin{pmatrix} i \\ 1 \\ -i \end{pmatrix} = 1+1+1 = 3$

(ii) $\mathbf{b}^\dagger\mathbf{b} = \begin{pmatrix} -2i & 0 & 3 \end{pmatrix}\begin{pmatrix} 2i \\ 0 \\ 3 \end{pmatrix} = 4+0+9 = 13$

(iii) $\mathbf{a}^\dagger\mathbf{b} = \begin{pmatrix} -i & 1 & i \end{pmatrix}\begin{pmatrix} 2i \\ 0 \\ 3 \end{pmatrix} = 2+3i$

(iv) $\mathbf{b}^\dagger\mathbf{a} = (\mathbf{a}^\dagger\mathbf{b})^\dagger = 2-3i$

40. Which of the matrices in Exercise 36-38 are Hermitian?

$\begin{pmatrix} 2 & i \\ -i & 1 \end{pmatrix}$ in Exercise 37, $\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$ in Exercise 38

41. (i) Show that $\mathbf{A} = \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ -i/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}$ is unitary.

(ii) Confirm that both the columns and the rows of **A** form unitary systems of vectors.

(i) $\mathbf{A} = \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ -i/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \to \mathbf{A}^\dagger = \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ -i/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} \quad (= \mathbf{A})$

Then $\mathbf{A}^\dagger\mathbf{A} = \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ -i/\sqrt{2} & -1/\sqrt{2} \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ -i/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

and **A** in unitary.

(ii) Write $\mathbf{A} = \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ -i/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} = (\mathbf{c}_1 \quad \mathbf{c}_2)$

$$\mathbf{A}^\dagger = \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ -i/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \end{pmatrix}$$

Then
$$\mathbf{c}_1{}^\dagger\mathbf{c}_1 = \left(1/\sqrt{2} \quad i/\sqrt{2}\right)\begin{pmatrix} 1/\sqrt{2} \\ -i/\sqrt{2} \end{pmatrix} = \frac{1}{2} - \frac{i^2}{2} = 1$$

$$\mathbf{c}_1{}^\dagger\mathbf{c}_2 = \left(1/\sqrt{2} \quad i/\sqrt{2}\right)\begin{pmatrix} i/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = \frac{i}{2} - \frac{i}{2} = 0$$

$$\mathbf{c}_2{}^\dagger\mathbf{c}_2 = \left(-i/\sqrt{2} \quad -1/\sqrt{2}\right)\begin{pmatrix} i/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = -\frac{i^2}{2} + \frac{1}{2} = 1$$

and the columns are orthonormal.

For the rows, write $\mathbf{A} = \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ -i/\sqrt{2} & -1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \end{pmatrix}$

Then
$$\mathbf{r}_1\mathbf{r}_1{}^\dagger = \left(1/\sqrt{2} \quad i/\sqrt{2}\right)\begin{pmatrix} 1/\sqrt{2} \\ -i/\sqrt{2} \end{pmatrix} = 1$$

$$\mathbf{r}_2\mathbf{r}_1{}^\dagger = \left(1/\sqrt{2} \quad i/\sqrt{2}\right)\begin{pmatrix} i/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = 0$$

$$\mathbf{r}_2\mathbf{r}_2{}^\dagger = \left(-i/\sqrt{2} \quad -1/\sqrt{2}\right)\begin{pmatrix} i/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = 1$$

and the rows are orthonormal.

42. Repeat Exercise 41 for $\mathbf{A} = \begin{pmatrix} i/\sqrt{3} & i/\sqrt{2} & i/\sqrt{6} \\ i/\sqrt{3} & -i/\sqrt{2} & i/\sqrt{6} \\ i/\sqrt{3} & 0 & -2i/\sqrt{6} \end{pmatrix}$.

(i) $$\mathbf{A} = \begin{pmatrix} i/\sqrt{3} & i/\sqrt{2} & i/\sqrt{6} \\ i/\sqrt{3} & -i/\sqrt{2} & i/\sqrt{6} \\ i/\sqrt{3} & 0 & -2i/\sqrt{6} \end{pmatrix} \rightarrow \mathbf{A}^\dagger = \begin{pmatrix} -i/\sqrt{3} & -i/\sqrt{3} & -i/\sqrt{3} \\ -i/\sqrt{2} & i/\sqrt{2} & 0 \\ -i/\sqrt{6} & -i/\sqrt{6} & 2i/\sqrt{6} \end{pmatrix}$$

Then $$\mathbf{A}^\dagger\mathbf{A} = \begin{pmatrix} i/\sqrt{3} & i/\sqrt{2} & i/\sqrt{6} \\ i/\sqrt{3} & -i/\sqrt{2} & i/\sqrt{6} \\ i/\sqrt{3} & 0 & -2i/\sqrt{6} \end{pmatrix}\begin{pmatrix} -i/\sqrt{3} & -i/\sqrt{3} & -i/\sqrt{3} \\ -i/\sqrt{2} & i/\sqrt{2} & 0 \\ -i/\sqrt{6} & -i/\sqrt{6} & 2i/\sqrt{6} \end{pmatrix}$$
$$= \begin{pmatrix} 1/3+1/2+1/6 & 1/3-1/2+1/6 & 1/3-1/3 \\ 1/3-1/2+1/6 & 1/3+1/2+1/6 & 1/3-1/3 \\ 1/3-1/3 & 1/3-1/3 & 1/3+2/3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and **A** in unitary.

(ii) For the columns, write $\mathbf{A} = \begin{pmatrix} i/\sqrt{3} & i/\sqrt{2} & i/\sqrt{6} \\ i/\sqrt{3} & -i/\sqrt{2} & i/\sqrt{6} \\ i/\sqrt{3} & 0 & -2i/\sqrt{6} \end{pmatrix} = \begin{pmatrix} \mathbf{c}_1 & \mathbf{c}_2 & \mathbf{c}_3 \end{pmatrix}$

Then $$\mathbf{c}_1{}^\dagger\mathbf{c}_1 = \begin{pmatrix} -i/\sqrt{3} & -i/\sqrt{3} & -i/\sqrt{3} \end{pmatrix}\begin{pmatrix} i/\sqrt{3} \\ i/\sqrt{3} \\ i/\sqrt{3} \end{pmatrix} = \frac{1}{3}+\frac{1}{3}+\frac{1}{3} = 1$$
$$\mathbf{c}_1{}^\dagger\mathbf{c}_2 = \begin{pmatrix} -i/\sqrt{3} & -i/\sqrt{3} & -i/\sqrt{3} \end{pmatrix}\begin{pmatrix} i/\sqrt{2} \\ -i/\sqrt{2} \\ 0 \end{pmatrix} = \frac{1}{\sqrt{6}}-\frac{1}{\sqrt{6}} = 0$$
$$\mathbf{c}_1{}^\dagger\mathbf{c}_3 = \begin{pmatrix} -i/\sqrt{3} & -i/\sqrt{3} & -i/\sqrt{3} \end{pmatrix}\begin{pmatrix} i/\sqrt{6} \\ i/\sqrt{6} \\ -2i/\sqrt{6} \end{pmatrix} = \frac{1}{3\sqrt{2}}+\frac{1}{3\sqrt{2}}-\frac{2}{3\sqrt{2}} = 0$$

Similarly for the other pairs of columns and for the rows:

$$\mathbf{c}_2{}^\dagger\mathbf{c}_2 = 1,\ \mathbf{c}_2{}^\dagger\mathbf{c}_3 = 0,\ \mathbf{c}_3{}^\dagger\mathbf{c}_3 = 1$$
$$\mathbf{r}_1\mathbf{r}_1{}^\dagger = 1,\ \mathbf{r}_1\mathbf{r}_2{}^\dagger = 0,\ \mathbf{r}_1\mathbf{r}_3{}^\dagger = 0,\ \mathbf{r}_2\mathbf{r}_2{}^\dagger = 1,\ \mathbf{r}_2\mathbf{r}_3{}^\dagger = 0,\ \mathbf{r}_3\mathbf{r}_3{}^\dagger = 1$$

(note: $\mathbf{r}_i = \mathbf{c}_1{}^\dagger,\ \mathbf{r}_i{}^\dagger = \mathbf{c}_1$)