Q6.8

a.

$$\mathbf{H} = \begin{pmatrix} 7 & 0 & -3 \\ -9 & -2 & 3 \\ 18 & 0 & -8 \end{pmatrix} \xlongequal[r_1=r_1+3r_2-1.5r_3]{\substack{r_3=2r_2+r_3 \\ r_2=r_1+r_2}} \begin{pmatrix} 1 & 0 & 0 \\ -2 & -2 & 0 \\ 0 & -4 & -2 \end{pmatrix}$$

$$\left|\mathbf{H} - \lambda \mathbf{I}\right| = 0 \Longrightarrow$$

$$\begin{vmatrix} 1-\lambda & 0 & 0 \\ -2 & -2-\lambda & 0 \\ 0 & -4 & -2-\lambda \end{vmatrix} = (1-\lambda)(2+\lambda)^2 = 0$$

So the eigenvalues are $\lambda_1 = 1, \lambda_2 = \lambda_3 = -2$

Then to find eigenvectors,

(1). For $\lambda_1 = 1$,

$$\begin{pmatrix} 6 & 0 & -3 \\ -9 & -3 & 3 \\ 18 & 0 & -9 \end{pmatrix} * \begin{pmatrix} u_1 \\ u_2 \\ u3 \end{pmatrix} = 0 \Longrightarrow 6u_1 - u_3 = 0 \quad and \quad -9u_1 - u_2 + u_3 = 0$$

$$u_3 = r;\ u_1 = 0.5r;\ u2 = -0.5r \Rightarrow \mathbf{u} = r \begin{pmatrix} 0.5 \\ -0.5 \\ 1 \end{pmatrix} \Rightarrow \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ -1 \\ 2 \end{pmatrix}$$

(2). For $\lambda_2 = \lambda_3 = -2$,

$$\begin{pmatrix} 9 & 0 & -3 \\ -9 & 0 & 3 \\ 18 & 0 & -6 \end{pmatrix} * \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = 0 \Longrightarrow 3u_1 - 3u_3 = 0$$

I. when $u_1 = u_3 = 0$, then $u_2 = s$, $\mathbf{u} = s \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

II. when $u_2 = 0$, then $u_1 = t;\ u_3 = 3t$, $\mathbf{u} = t \begin{pmatrix} 1 \\ 0 \\ 3 \end{pmatrix} \Rightarrow \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ 0 \\ 3 \end{pmatrix}$.

Therefore, eigenvalues are $\mathbf{\Lambda} = \begin{pmatrix} 1 & & \\ & -2 & \\ & & -2 \end{pmatrix}$ and eigenvectors are $\mathbf{U} = \begin{pmatrix} \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{10}} \\ -\frac{1}{\sqrt{6}} & 1 & 0 \\ \frac{2}{\sqrt{6}} & 0 & \frac{3}{\sqrt{10}} \end{pmatrix}$

b.

For $\mathbf{H}$, since it's full rank, so $\mathbf{H} = \mathbf{U\Lambda U^{-1}}$. If $\mathbf{U}$ is unitary, then $\mathbf{U}^\dagger = \mathbf{U}^{-1}$. That means $\mathbf{H} = \mathbf{U\Lambda U}^\dagger$.

$$\mathbf{U\Lambda U}^\dagger = \begin{pmatrix} \frac{1}{\sqrt{6}} & 0 & \frac{1}{\sqrt{10}} \\ -\frac{1}{\sqrt{6}} & 1 & 0 \\ \frac{2}{\sqrt{6}} & 0 & \frac{3}{\sqrt{10}} \end{pmatrix} \begin{pmatrix} 1 & & \\ & -2 & \\ & & -2 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{10}} & 0 & \frac{3}{\sqrt{10}} \end{pmatrix}$$

$$= \begin{pmatrix} -1.5 & 0.82 & -1.42 \\ 0.82 & -2 & 0 \\ -1.42 & 0 & -1.7 \end{pmatrix} \neq \mathbf{H}$$

Therefore, $\mathbf{U}$ is not unitary.

6.9

Calculate eigenvectors and eigenvalues of $\mathbf{H_1}$ in MATLAB by:

```
H1= [3 0 -1; 0 1 0; -1 0 2];
[V,D]=eig(H1);
```

Then eigenvalues are $\mathbf{D} = \begin{pmatrix} 1 & & \\ & 1.382 & \\ & & 3.618 \end{pmatrix}$, and eigenvectors are $\mathbf{V} = \begin{pmatrix} 0 & -0.5257 & -0.8507 \\ 1 & 0 & 0 \\ 0 & -0.8507 & 0.5257 \end{pmatrix}$. Therefore, using `V*D*V'`, $\mathbf{VDV}^\dagger = \begin{pmatrix} 3 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 2 \end{pmatrix} = \mathbf{H_1}$. It indicates eigenvectors matrix $\mathbf{V}$ is unitary matrix.

6.10

(1). For $\mathbf{V} \in \mathbb{C}_{2\times 2}$, $\mathbf{HH}^\dagger = \begin{pmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{pmatrix} \begin{pmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 11 & 1 \\ 1 & 11 \end{pmatrix}$.

To calculate its eigenvalues, $\begin{vmatrix} 11-\lambda & 1 \\ 1 & 11-\lambda \end{vmatrix} = 0 \Rightarrow (11-\lambda)^2 - 1 = 0 \Rightarrow$ $(\lambda - 10)(\lambda - 12) = 0$, then the eigenvalues is $\lambda_1 = 10$ and $\lambda_2 = 12$.

I. For $\lambda_1 = 10$, $(\mathbf{AA}^\dagger - 10\mathbf{I})\mathbf{v} = \mathbf{0} \Rightarrow \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = 0 \Rightarrow v_1 + v_2 = 0$

So $v_1 = r;\ v_2 = -r \Rightarrow \mathbf{v} = r \begin{pmatrix} 1 \\ -1 \end{pmatrix} \overset{orthonormalize}{\Longrightarrow} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

II. For $\lambda_2 = 12$, $(\mathbf{AA}^\dagger - 12\mathbf{I})\mathbf{v} = \mathbf{0} \Rightarrow \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = 0 \Rightarrow v_1 - v_2 = 0$

So $v_1 = s; v_2 = s \Rightarrow \mathbf{v} = s \begin{pmatrix} 1 \\ 1 \end{pmatrix} \overset{orthonormalize}{\Longrightarrow} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

Therefore, $\mathbf{V} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

(2). For $\mathbf{U} \in \mathbb{C}_{3\times 3}$, $\mathbf{H}^\dagger\mathbf{H} = \begin{pmatrix} 3 & -1 \\ 1 & 3 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{pmatrix} = \begin{pmatrix} 10 & 0 & 2 \\ 0 & 10 & 4 \\ 2 & 4 & 2 \end{pmatrix}$

To get its eigenvalues, $\begin{vmatrix} 10-\lambda & 0 & 2 \\ 0 & 10-\lambda & 4 \\ 2 & 4 & 2-\lambda \end{vmatrix} = \lambda(\lambda-10)(\lambda-12) = 0$
$\Rightarrow \lambda_1 = 0;\ \lambda_2 = 10; \lambda_3 = 12$.

I. For $\lambda_1 = 0$, $(\mathbf{H}^\dagger\mathbf{H} - \mathbf{0})\mathbf{u} = \begin{pmatrix} 10 & 0 & 2 \\ 0 & 10 & 4 \\ 2 & 4 & 2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = 0 \Rightarrow$
$10u_1 + 2u_3 = 0; \quad 10u_2 + 4u_3 = 0; \quad 2u_1 + 4u_2 + 2u_3 = 0;$
Let $u_1 = r$, then $u_2 = 2r$ and $u_2 = -5r$.

$$\mathbf{u} = r \begin{pmatrix} 1 \\ 2 \\ -5 \end{pmatrix} \overset{orthonormalize}{\Longrightarrow} \frac{1}{\sqrt{30}} \begin{pmatrix} 1 \\ 2 \\ -5 \end{pmatrix}$$

II. For $\lambda_2 = 10$, $(\mathbf{H}^\dagger\mathbf{H} - 10\mathbf{I})\mathbf{u} = \begin{pmatrix} 0 & 0 & 2 \\ 0 & 0 & 4 \\ 2 & 4 & -8 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = 0 \Rightarrow$

$u_3 = 0 \quad and \quad 2u_1 + 4u_2 - 8u_3 = 0$

Let $u_1 = s$, then $u_2 = -0.5s$. $\mathbf{u} = s \begin{pmatrix} 1 \\ -0.5 \\ 0 \end{pmatrix} \overset{orthonormalize}{\Longrightarrow} \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ -1 \\ 0 \end{pmatrix}$

III. For $\lambda_3 = 12$, $(\mathbf{H}^\dagger\mathbf{H} - 12\mathbf{I})\mathbf{u} = \begin{pmatrix} -2 & 0 & 2 \\ 0 & -2 & 4 \\ 2 & 4 & -10 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = 0 \Rightarrow$

$-2u_1 + 2u_3 = 0; \; -2u_2 + 4u_3 = 0; \quad and \quad 2u_1 + 4u_2 - 10u_3 = 0$

Let $u_3 = t$, then $u_1 = t$; $u_2 = 2t$. $\mathbf{u} = t \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix} \overset{orthonormalize}{\Longrightarrow} \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix}$

Therefore, $\mathbf{U} = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{5}} & \frac{1}{\sqrt{30}} \\ \frac{2}{\sqrt{6}} & -\frac{1}{\sqrt{5}} & \frac{2}{\sqrt{30}} \\ \frac{1}{\sqrt{6}} & 0 & -\frac{5}{\sqrt{30}} \end{pmatrix}$ and $\mathbf{\Sigma^{1/2}} = \begin{pmatrix} \sqrt{12} & 0 & 0 \\ 0 & \sqrt{10} & 0 \end{pmatrix}$

In this case, $\mathbf{V\Sigma^{1/2}U}^\dagger = \begin{pmatrix} 3 & 1 & 1 \\ -1 & 3 & 1 \end{pmatrix} = \mathbf{H}$

6.11

Since $x_1 + x_2 \underset{f_2}{\overset{f_1}{\rightleftharpoons}} x_3$, then

$x_1/dt = -f_1 + f2; \quad x_2/dt = -f_1 + f2; \quad x_3/dt = f_1 - f_2 \Rightarrow$

$\mathbf{s_1} = \begin{pmatrix}-1 & 1\end{pmatrix}; \ \mathbf{s_2} = \begin{pmatrix}-1 & 1\end{pmatrix}; \ \mathbf{s_3} = \begin{pmatrix}1 & -1\end{pmatrix}$

Then the stoichiometric matrix $\mathbf{S} = (\mathbf{s_1}\ \mathbf{s_2}\ \mathbf{s_3}) = \begin{pmatrix}-1 & 1\\ -1 & 1\\ 1 & -1\end{pmatrix}$

(1). For $\mathbf{V} \in \mathbb{C}_{3\times 3}$, $\mathbf{SS}^\dagger = \begin{pmatrix}-1 & 1\\ -1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}-1 & -1 & 1\\ 1 & 1 & -1\end{pmatrix} = \begin{pmatrix}2 & 2 & -2\\ 2 & 2 & -2\\ -2 & -2 & 2\end{pmatrix} \Longrightarrow$ its eigenvalues are $\lambda_1 = 6$, $\lambda_2 = \lambda_3 = 0$.

I. when $\lambda_1 = 6$, then $(\mathbf{SS}^\dagger - 6\mathbf{I})\mathbf{v} = \begin{pmatrix}-4 & 2 & -2\\ 2 & -4 & -2\\ -2 & -2 & -4\end{pmatrix}\begin{pmatrix}v_1\\ v_2\\ v_3\end{pmatrix} = 0$. Like problem 6.10, its eigenvectors are $\mathbf{v} = r\begin{pmatrix}-1\\ -1\\ 1\end{pmatrix} \Rightarrow \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\ -1\\ 1\end{pmatrix}$ (orthonormal)

II. when $\lambda_2 = \lambda_3 = 0$, then $\begin{pmatrix}2 & 2 & -2\\ 2 & 2 & -2\\ -2 & -2 & 2\end{pmatrix}\begin{pmatrix}v_1\\ v_2\\ v_3\end{pmatrix} = 0$. Similarly, its eigenvectors should be

$\mathbf{v_2} = s\begin{pmatrix}0\\ 1\\ 1\end{pmatrix} \Rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix}0\\ 1\\ 1\end{pmatrix}$ and $\mathbf{v_3} = t\begin{pmatrix}1\\ 0\\ 1\end{pmatrix} \Rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 0\\ 1\end{pmatrix}$ (orthonormal)

Therefore, $\mathbf{V} = \begin{pmatrix}-\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & 0\\ -\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix}$

(2). For $\mathbf{U} \in \mathbb{C}_{2\times 2}$, $\mathbf{S}^\dagger\mathbf{S} = \begin{pmatrix}3 & -3\\ -3 & 3\end{pmatrix}$, whose eigenvalues are $\lambda_1 = 6$ and $\lambda_2 = 0$. Likewise, the eigenvectors are $\mathbf{U} = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}$

And $\mathbf{\Sigma}^{1/2} = \begin{pmatrix} \sqrt{6} & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$ so that $\mathbf{V\Sigma^{1/2}U} = \begin{pmatrix} -1 & 1 \\ -1 & 1 \\ 1 & -1 \end{pmatrix} = \mathbf{S}$

$\mathbf{S}$ is only rank 1, with 1 dynamic mode. Since $\mathbf{u_1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ and $\mathbf{Su_1} = \sqrt{\varsigma_1}\mathbf{v_1}$ as equation 6.19, apply $\mathbf{u_1}$ to $\mathbf{S}$ by multiplying $\sqrt{2}$ at each side of the equation.

$$\mathbf{S} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \sqrt{2} * \sqrt{6} \frac{1}{\sqrt{3}} \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} = 2 \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}$$

Therefore, like the example illustrated in the textbook section 6.9, this reaction's flux mode changes the concentrations of x in the opposite direction at twice the magnitude of flux. The $1\times$ fold change in flux generate $2\times$ fold change in concentration rate.

6.12

(a). Because these is 5 components and 5 fluxes in this reaction, the stoichiometric matrix $\mathbf{S} \in \mathbb{R}_{5\times 5}$.

$\mathbf{x_1} = \begin{pmatrix} -1 & 0 & -1 & 0 & 0 \end{pmatrix} \mathbf{f}$

$\mathbf{x_2} = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \end{pmatrix} \mathbf{f}$

$\mathbf{x_3} = \begin{pmatrix} 0 & 0 & 1 & -1 & 0 \end{pmatrix} \mathbf{f}$

$\mathbf{x_4} = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 \end{pmatrix} \mathbf{f}$

$\mathbf{x_5} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \end{pmatrix} \mathbf{f} \Longrightarrow$

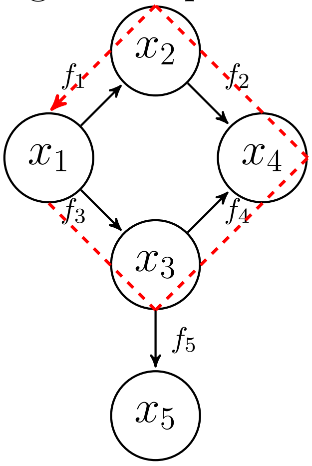
$$\mathbf{S} = \begin{pmatrix} -1 & 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

(b). Apply eigenanalysis to $\mathbf{S}$ by `[V, E]=eig(S)`, get eigenvalues $\mathbf{E}$ and eigvectors $\mathbf{V}$:

$$\mathbf{V} = \begin{pmatrix} -0.3536 & -0.5 & 0.5 & 0.3536 & 0 \\ 0.8536 & -0.5 & 0.5 & 0.1464 & 0 \\ -0.1464 & 0.5 & -0.5 & -0.8536 & 0 \\ -0.3536 & 0.5 & -0.5 & 0.3536 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \text{ and } \mathbf{E} = \begin{pmatrix} -\sqrt{2} & & & & \\ & 0 & & & \\ & & 0 & & \\ & & & \sqrt{2} & \\ & & & & 1 \end{pmatrix}$$

So $\mathbf{v_1} = \begin{pmatrix} -0.5 \\ -0.5 \\ 0.5 \\ 0.5 \\ 0 \end{pmatrix}$ and $\mathbf{v_2} = \begin{pmatrix} 0.5 \\ 0.5 \\ -0.5 \\ -0.5 \\ 0 \end{pmatrix}$ are the eigvectors corresponding to homogeneous pathway. They look like this:

$\mathbf{v_1}$:



$\mathbf{v_2}$: