

Homework #6

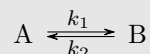
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CBE660: Intermediate Problems in Chemical and Biological Engineering - Fall 2016

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Problem 1. Consider the reversible chemical reaction:



Assume that the reactions are of first-order with constants $k_1, k_2 > 0$ and denote the concentrations at time t as $x_A(t)$ and $x_B(t)$. Express the dynamics of this system as $\dot{x} = Ax$ with arbitrary initial concentrations $x(0) > 0$. Address the following:

- If the system is left to react indefinitely, do the concentrations vanish (converge to zero)? Why?
- What type of dynamic response does this system exhibit (damped, damped oscillations, pure oscillations)?
- Prove that the system always settles at a steady-state defined by the eigenvector corresponding to the zero eigenvalue. Based on this insight, answer the following: If your objective is to produce a given chemical using any type of first-order reaction network, does it make sense to design a network that only has negative eigenvalues?
- Implement your eigenvalue decomposition in Matlab (use function `eig` to perform decomposition) and simulate response for $k_1 = k_2 = 1$ and $x(0) = [1 \ 1]$ over $t \in [0, 10]$. Verify that the system indeed settles at a steady-state defined by the eigenvector with zero eigenvalue.

Solution:

The rate of the chemical reactions can be expressed as

$$\frac{dx_A}{dt} = -k_1 x_A + k_2 x_B$$

$$\frac{dx_B}{dt} = k_1 x_A - k_2 x_B$$

Writing this in matrix notation, $\dot{x} = Ax$ gives

$$\begin{bmatrix} \dot{x}_A \\ \dot{x}_B \end{bmatrix} = \begin{bmatrix} -k_1 & k_2 \\ k_1 & -k_2 \end{bmatrix} \begin{bmatrix} x_A \\ x_B \end{bmatrix}$$

To find the eigenvalues, we use the property $\det(A - \lambda I) = 0$

$$(-k_1 - \lambda)(-k_2 - \lambda) - k_1 k_2 = 0$$

$$\lambda^2 + \lambda(k_1 + k_2) = 0$$

$$\lambda = \frac{-1}{2}(k_1 + k_2) \pm \frac{1}{2}(k_1 + k_2)$$

Thus, $\lambda = 0$ or $\lambda = -(k_1 + k_2)$.

If this system reacts indefinitely, the concentrations go to values defined by the initial condition matrix $x(0)$. It does not make sense for the concentrations to vanish, as mass must be conserved.

Based on the non-zero eigenvalue, the system has $Re(\lambda) < 0$ and $Im(\lambda) = 0$ and therefore exhibits damped behavior with no oscillations.

To find the steady-state solution, we perform a decomposition of matrix A

$$A = S\Lambda S^{-1}$$

$$\dot{x} = Ax = S\Lambda S^{-1}x$$

Let $\dot{y} = S^{-1}\dot{x}$, $y(t) = S^{-1}x$ and $y_0 = S^{-1}x_0$

$$\dot{y} = \Lambda y(t)$$

$$\begin{bmatrix} \dot{y}_1 \\ \dot{y}_2 \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

This yields the solution

$$y(t) = e^{\Lambda t} y_0$$

Using $x(t) = Sy(t)$ and $y_0 = S^{-1}x_0$

$$x(t) = Sy(t) = Se^{\Lambda t}y_0 = Se^{\Lambda t}S^{-1}x_0$$

From the relationship defined above we can prove that the system always settles to the steady-state defined by the eigenvector corresponding to the zero eigenvalue.

$$\begin{aligned} x(t) &= Sy(t) = \sum_{j=1}^n s_j e^{\lambda_j t} s_j^{-1} x_0 \\ x(t) &= s_1 e^{\lambda_1 t} s_1^{-1} x_0 + s_2 e^{\lambda_2 t} s_2^{-1} x_0 \\ x(t) &= s_1 e^{0t} s_1^{-1} x_0 + s_2 e^{-(k_1+k_2)t} s_2^{-1} x_0 \\ \lim_{t \rightarrow \infty} x(t) &= s_1 e^0 s_1^{-1} x_0 + s_2 e^{-\infty} s_2^{-1} x_0 \\ \lim_{t \rightarrow \infty} x(t) &= s_1 s_1^{-1} x_0 \end{aligned}$$

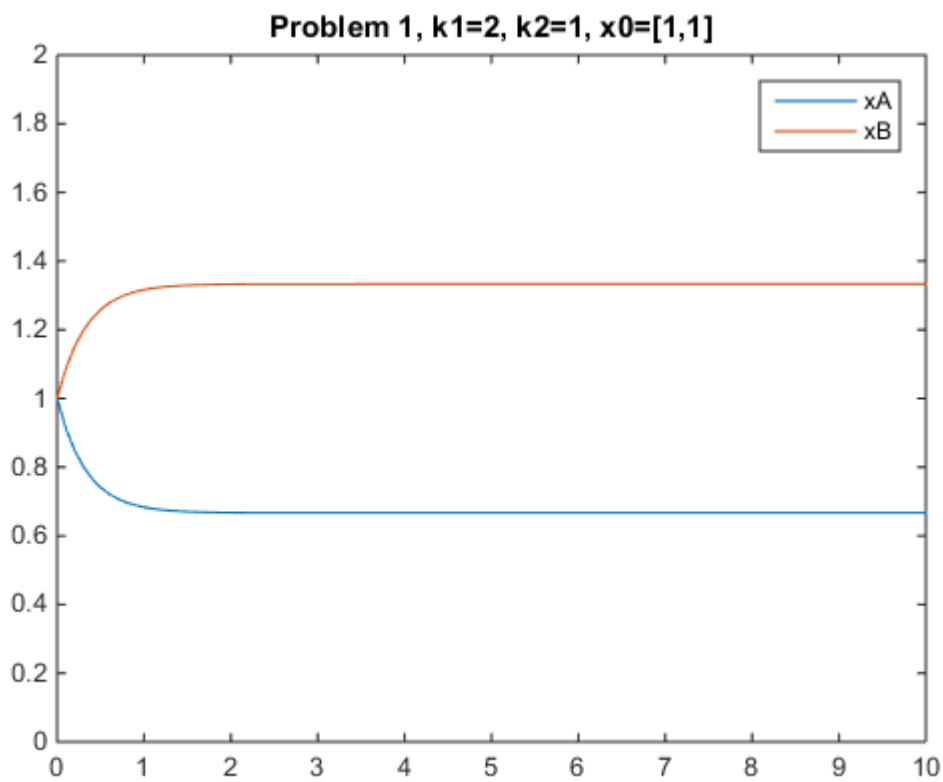
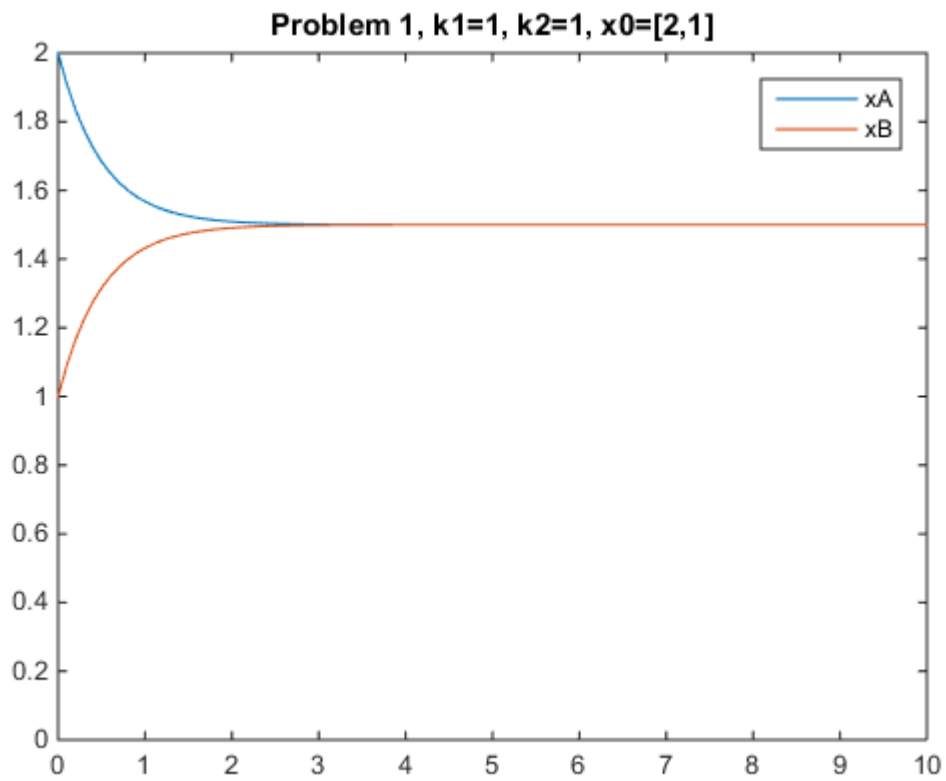
In the limit where $t \rightarrow \infty$ we see that $x(t) \rightarrow s_1 s_1^{-1} x_0$. Therefore the system always settles at the steady state defined by the zero eigenvalue. Note, s^{-1} does not actually exist because you cannot take the inverse of a vector. This notation refers to the vector s_i produced by taking the inverse of the matrix S .

It does not make sense to have exclusively negative eigenvalues for the situation described in the problem statement. In this case, the $x(t) \rightarrow 0$ as $t \rightarrow \infty$. However, the concentrations cannot all go to zero at steady state because mass must be conserved.

These results were verified using Matlab. The results and methods are given below.

When $k_1 = 1$, $k_2 = 1$ and $x_0 = [2, 1]$ the system begins at the initial concentrations defined by x_0 and converges to the equilibrium concentrations of $x_A = x_B = 1.5$.

When $k_1 = 2$, $k_2 = 1$ and $x_0 = [1, 1]$ the system begins at the initial concentrations defined by x_0 and converges to the equilibrium concentrations of $x_A = 1.3$ and $x_B = 0.7$. Because k_1 is defined as twice as large as k_2 , it is logical that the final concentration of x_A is twice the final concentration of x_B .



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1 clear
2
3 k1=1;
4 k2=1;

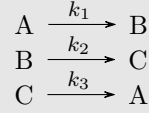
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5
6 A=[-k1 k2; k1 -k2];
7 [S,E,W]=eig(A);
8 x0=[2;1];
9 A1=S*E*W^(-1); % This check my eigen decomp
10
11 t=linspace(0,10);
12 %x=x0(1)*S(:,1)*exp(E(1,1)*t)+x0(2)*S(:,2)*exp(E(2,2)*t);
13
14 xt=[];
15 for i=1:100
16     x=S*expm(E*t(i))*S^(-1)*x0;
17     xt(1,i)=x(1);
18     xt(2,i)=x(2);
19 end
20
21
22 figure
23 plot(t,xt)
24 axis([0,10,0,2])
25 title('Problem 1, k1=1, k2=1, x0=[2,1]')
26 legend('xA','xB')

```

Problem 2. Consider the "loop" reaction network:



Assume that the reactions are of first-order with constants $k_1, k_2, k_3 \geq 0$ and denote the concentrations at time t as $x_A(t)$, $x_B(t)$, and $x_C(t)$. Express the dynamics of this system as $\dot{x} = Ax$ with arbitrary initial concentrations $x(0) > 0$. Address the following:

- Assume that the first and third reactions have equal rate constants. Establish a critical value for k_2 leading to damped oscillatory behavior.
- Is it possible to find a combination for the rate constants k_1, k_2, k_3 (say by designing new catalysts) that make the system oscillate indefinitely?

Solution:

First, the reaction rate expressions can be written in matrix notation

$$\begin{bmatrix} \dot{x}_A \\ \dot{x}_B \\ \dot{x}_C \end{bmatrix} = \begin{bmatrix} -k_1 & 0 & k_3 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & -k_3 \end{bmatrix} \begin{bmatrix} x_A \\ x_B \\ x_C \end{bmatrix}$$

Use the property $\det|A - \lambda I| = 0$ to find the eigenvalues

$$(-k_1 - \lambda)(-k_2 - \lambda)(-k_3 - \lambda) + k_1 k_2 k_3 = 0$$

Expanding this expression out, canceling $k_1 k_2 k_3$ and dividing through by $-\lambda$ yields

$$\lambda^2 + \lambda(k_1 + k_2 + k_3) + k_1 k_2 + k_1 k_3 + k_2 k_3 = 0$$

We can then use the quadratic equation to solve for λ

$$\lambda = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$a = 1$$

$$b = k_1 + k_2 + k_3$$

$$c = k_1 k_2 + k_1 k_3 + k_2 k_3$$

To decay with damped oscillations, the $Re(\lambda) < 0$ and $Im(\lambda) \neq 0$. Therefore $\frac{-b}{2a} < 0$ and $b^2 - 4ac < 0$. The final solution is obtained by allowing $k_1 = k_3 = K$

From the criteria $Re(\lambda) < 0$

$$\frac{b}{a} > 0$$

$$k_1 + k_2 k_3 > 0$$

$$2K + k_2 > 0$$

$$-k_2 < 2K$$

From the criteria $Im(\lambda) \neq 0$

$$b^2 - 4ac < 0$$

$$b^2 < 4ac$$

$$(k_1 + k_2 + k_3)^2 < 4(Kk_2 + K^2 + Kk_2)$$

$$k_2^2 < 4Kk_2$$

$$k_2 < 4K$$

From the criteria that $Re(\lambda) < 0$, we define that $-k_2 < 2K$. However, because we define in the problem statement that $k_1, k_2, k_3 > 0$ we know that $2K$ is a positive value and k_2 is a positive value. By definition, $-k_2$ will *always* be less than $2K$, regardless of the magnitude of k_2 .

From the criteria that $Im(\lambda) \neq 0$ we see that $k_2 < 4K$ in order to give a negative within the square root and thus, produce an imaginary component.

Thus,

$$0 \leq k_2 < 4K$$

It is NOT possible to have a combination that oscillates indefinitely ($Re(\lambda) = 0$ and $Im(\lambda) \neq 0$). From the above equations, we can see that for $Re(\lambda) = 0$ then $b = k_1 + k_2 + k_3 = 0$ must be satisfied. With $k_1, k_2, k_3 \geq 0$, $Re(\lambda) = 0$ only when $k_1 = k_2 = k_3 = 0$. In this situation, the $Im(\lambda)$ would also be zero, resulting in a system that does not react (straight horizontal line).

Problem 3: When working in the complex domain is the only way to go. Consider a linear dynamical system in the Laplace domain $\bar{x}(s) = \bar{f}(s)\bar{u}(s)$ where $\bar{f}(s)$ is its transfer function and $\bar{u}(s)$ is the input (forcing). Recall that the Fourier representation of this system is simply $\bar{x}(j\omega) = \bar{f}(j\omega)\bar{u}(j\omega)$. Address the following:

- Apply the convolution property to $\bar{x}(s) = \bar{f}(s)\bar{u}(s)$ to prove that, when subjected to a sinusoidal input $u(t) = \sin(\omega t)$, any dynamical system $\bar{f}(s)$ will ultimately converge to a sinusoidal signal of the form $\lim_{t \rightarrow \infty} x(t) = |\bar{f}(j\omega)| \sin(\omega t + \phi)$ where $\phi = \angle \bar{f}(j\omega)$.
- Congrats, you just proved one of the most powerful results in control theory. The response $|\bar{f}(j\omega)| \sin(\omega t + \phi)$ is called the ultimate periodic response. This result is useful because we can anticipate the amplitude and phase shift of the response $x(t)$ by knowing the algebraic structure of the transfer function $\bar{f}(j\omega)$. This result is used to estimate unknown parameters of a dynamical system by exciting it using a sinusoidal signal. Now apply your result to the first-order system $\tau \dot{x}(t) + x(t) = Ku(\tau)$ to get an algebraic form of the magnitude and phase shift of the response in terms of the gain K and the time constant τ .

Solution:

Beginning with the convolution property

$$\mathcal{L}^{-1}[\bar{f}(s)\bar{u}(s)] = \int_0^t f(t')u(t-t')dt' = x(t)$$

And using the Euler identities

$$e^{j\omega t} = \cos(\omega t) + j\sin(\omega t)$$

$$e^{-j\omega t} = \cos(\omega t) - j\sin(\omega t)$$

$$e^{-j\omega t} - e^{j\omega t} = -2j\sin(\omega t)$$

$$\sin(\omega t) = \frac{-1}{2j}(e^{-j\omega t} - e^{j\omega t})$$

Substituting this result into $u(t) = \sin(\omega t)$ for $t = (t - t')$

$$u(t) = \sin(\omega(t - t'))$$

$$x(t) = \int_0^t f(t')\sin(\omega(t - t'))dt'$$

$$x(t) = \int_0^t f(t') \left[\frac{-1}{2j}(e^{-j\omega(t-t')} - e^{j\omega(t-t')}) \right] dt'$$

$$x(t) = \int_0^t f(t') \left[\frac{-1}{2j}(e^{-j\omega t} e^{j\omega t'}) \right] dt' + \int_0^t f(t') \left[\frac{-1}{2j}(e^{j\omega t} e^{-j\omega t'}) \right] dt'$$

Using the Fourier Transform

$$\bar{f}(s) = \int f(t')e^{-j\omega t'} dt'$$

$$x(t) = \frac{1}{2j}e^{j\omega t}\bar{f}(j\omega) - \frac{1}{2j}e^{-j\omega t}\bar{f}(-j\omega)$$

From the properties of the magnitude

$$|\bar{f}(j\omega)| = |\bar{f}(-j\omega)|$$

$$|\bar{f}(j\omega)| = \sqrt{\text{Re}(\bar{f}(j\omega))^2 + \text{Im}(\bar{f}(j\omega))^2}$$

$$\bar{f}(j\omega) = |\bar{f}(j\omega)|e^{j\phi}$$

We can substitute this expression into our $x(t)$ to get

$$x(t) = \frac{1}{2j} [e^{j\omega t} |\bar{f}(j\omega)| e^{j\phi} - e^{-j\omega t} |\bar{f}(j\omega)| e^{-j\phi}]$$

$$x(t) = \frac{1}{2j} |\bar{f}(j\omega)| [e^{j(\omega t + \phi)} - e^{-j(\omega t + \phi)}]$$

From the Euler identity

$$\sin(s) = \frac{-1}{2j} (e^{-js} - e^{js})$$

$$2j \sin(s) = e^{js} - e^{-js}$$

Substituting then gives the final equation

$$x(t) = \frac{1}{2j} |\bar{f}(j\omega)| 2j \sin(\omega t + \phi)$$

$$x(t) = |\bar{f}(j\omega)| \sin(\omega t + \phi)$$

Beginning by taking the Laplace transform of $\tau \dot{x}(t) + x(t) = Ku(t)$

$$\mathcal{L}[\tau \dot{x}(t) + x(t) = Ku(t)] \longrightarrow \tau(s\bar{x}(s) - \bar{x}(0)) + \bar{x}(s) = K\bar{u}(s)$$

Setting $x(0) = 0$ and solving for $\bar{x}(s)$

$$\bar{x}(s)(\tau s + 1) = K\bar{u}(s)$$

$$\bar{x}(s) = \frac{K}{\tau s + 1} \bar{u}(s)$$

To determine the magnitude where $s = j\omega$

$$\bar{f}(j\omega) = \frac{K}{\tau s + 1} = \frac{K}{\tau j\omega + 1} = \frac{N(j\omega)}{D(j\omega)}$$

$$|\bar{f}(j\omega)| = \frac{K}{|\tau j\omega + 1|} = \frac{K}{\sqrt{(\omega\tau)^2 + 1}}$$

To determine the phase shift

$$\phi = \phi_N - \phi_D$$

$$\phi = \tan^{-1} \frac{Im}{Re}$$

$$\phi_N = \tan^{-1} \left(\frac{0}{K} \right)$$

$$\phi_D = \tan^{-1} \left(\frac{\omega\tau}{1} \right)$$

$$\phi = \tan^{-1}(\omega\tau)$$