

Part I: Linear Algebra

This part of the assignment will review important concepts from linear algebra that you will need to know for this course. For each problem, first solve by hand and then check your answer with MATLAB. Please show and hand in all of your work by hand, all of the MATLAB commands required to solve each problem, and the answers that MATLAB gives. Specifically indicate which problem each set of MATLAB commands is solving. Use the built in Help command to aid in solving the problems if needed.

1. Matrix Multiplication

$$A = \begin{bmatrix} 2 & 4 \\ 0 & -1 \end{bmatrix} \quad B = \begin{bmatrix} 8 & 3 \\ 5 & 1 \end{bmatrix} \quad C = \begin{bmatrix} -6 & 0 \\ 3 & 2 \end{bmatrix}$$

- a. Find ABC

Matlab: A*B*C

$$ABC = \begin{bmatrix} -186 & 20 \\ 27 & -2 \end{bmatrix}$$

- b. Find CAB

Matlab: C*A*B

$$CAB = \begin{bmatrix} -216 & -60 \\ 98 & 28 \end{bmatrix}$$

2. Null Space

- a) Find a linear basis for the null space of E. That is, find a linearly independent set of vectors x_i that span the null space of E and for which any linear combination of x_i will satisfy $Ex=0$.

Hint #1: 0 is a column vector containing 3 elements in this case.

Hint #2: MATLAB may find a different linear basis than you do by hand. If your answer does not match MATLAB's, use MATLAB to show that you have found a linear basis for the null space.

$$E = \begin{bmatrix} -1 & 0 & 2 & 1 & 4 \\ -1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 2 \end{bmatrix}$$

Matlab:

$$\text{null}(E, 'r') = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & -2 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \text{ or } \text{null}(E) = \begin{bmatrix} 0.6591 & 0.2562 \\ 0 & 0 \\ 0.3241 & -0.8336 \\ 0.6591 & 0.2562 \\ -0.1620 & 0.4168 \end{bmatrix}$$

3. Solving Linear Equations

Solve the following set of linear equations represented by:

$$\begin{bmatrix} 2 & 0 & 3 \\ 1 & 4 & -1 \\ -5 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 6 \\ -1 \\ -16 \end{bmatrix}$$

Hint: check your answer in MATLAB using the “\” command.

Matlab: $x = [2, 0, 3; 1, 4, -1; -5, 1, 1] \setminus [6; -1; -16]$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ -1 \\ 0 \end{bmatrix}$$

4. Determinants

$$D = \begin{bmatrix} 3 & 4 \\ 5 & 6 \end{bmatrix}$$

- a. Find the determinant of D.

Matlab: $\det(D) = -2$

- b. Is the matrix singular or nonsingular, and how can you tell from part (a)?

5. Column Space

Find a linear basis for the column space of F.

$$F = \begin{bmatrix} -3 & -2 & 1 & 3 \\ 2 & 4 & 1 & -2 \\ -1 & 2 & 2 & 1 \\ -1 & 4 & -3 & 1 \end{bmatrix}$$

Hint: you may have to use MATLAB to creatively verify that you have solved the problem correctly.

$$\text{Matlab: } \text{rref}(F') = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

where the first three rows represent the linear basis for the column space of F.

6. Row Space

Find a linear basis for the row space of F.

See hint for #5.

$$\text{Matlab: } \text{rref}(F) = \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

7. Subspaces

- What is the relationship between the rank of a matrix and the dimension of its column space?
- What is the relationship between the dimension of the column and row spaces?

8. Eigenvalues & Eigenvectors

- In your own words explain what an eigenvector/eigenvalue pair is?
- Recall that if $Gx = \lambda x$, x is an eigenvector of G and λ is an eigenvalue of G . Find the eigenvalues and corresponding eigenvectors of G . Match each eigenvalue to an eigenvector.

$$G = \begin{bmatrix} 3 & 6 \\ 2 & 2 \end{bmatrix}$$

Matlab:

$$[V, L] = \text{eig}(G)$$

$$V = \begin{bmatrix} 0.8944 & -0.8321 \\ 0.4472 & 0.5547 \end{bmatrix}$$

$$L = \begin{bmatrix} 6 & 0 \\ 0 & -1 \end{bmatrix}$$

Part II: Metabolic Reconstructions

The Kegg Database contains genome annotation information for sequenced organisms. For this part of the assignment you will use the Kegg Database to collect reaction information about a set of reactions from the TCA Cycle in *Saccharomyces cerevisiae*, the yeast that ferments sugars to ethanol. From the information you collect you will create both the Stoichiometric and Elemental matrices, and ensure that all reactions are balanced.

1. Visit <http://www.genome.jp/kegg/>. Where it says "Organism-specific entry points" type "SCE"; this is the Kegg abbreviation for *S. cerevisiae*.
2. Using the "Pathway Maps" link in the top toolbar, navigate to the "Citrate Cycle".
3. Generate the stoichiometric (S) matrix for the reactions converting *Pyruvate* to *Succinyl-CoA*. The reactions for this organism are represented by "EC #s", highlighted in green. Clicking on each green box will bring you a screen containing information about the SCE gene encoding that reaction. Click on the link for the EC# in this page and you will find information about the reaction taking place. Specifically, include the following reactions in your S matrix:
 - a. EC-6.4.1.1
 - b. EC-1.1.1.37
 - c. EC-4.2.1.2
 - d. EC-1.3.5.1
 - e. EC-6.2.1.5

Include only the forward version of these reactions (i.e., assume they are irreversible). When collecting reaction information, be careful about which direction the reaction is written. Sometimes the reactions described in the Kegg files are in the reverse direction. Use the direction depicted on the TCA Cycle pathway map. This may mean you need to flip the direction of the reaction you see when you click on the EC# link.

4. Generate the elemental (E) matrix for the metabolites in the S matrix. The molecular formulas for each metabolite can be found by clicking on the link for the reaction ID (Rxxxxx) for the reaction depicted on the EC# page. Note that some molecular formulas may represent a polymer and thus look like (xxx)n. For these, assume that n = 1.
5. Find the product of $E \cdot S$. What does the result tell you?
6. Make any necessary changes to S to ensure balanced reactions, and validate using $E \cdot S$.
7. Explain what each of the numbers tells us in the EC# 6.2.1.5, representing the conversion of *Succinate* to *Succinyl-CoA*.
8. What other pathways (in *S. cerevisiae*) does the reaction represented by EC-6.2.1.5 participate in? What is the ID of the gene encoding for this reaction.

For this problem, turn in your initial S and E matrices, the initial product of $E \cdot S$, your corrected S matrix, and the corrected product of $E \cdot S$, as well as answers to the conceptual questions. For S and E, please label all columns and rows with their corresponding reactions and metabolites names. For reaction names, use the EC# for the reaction.