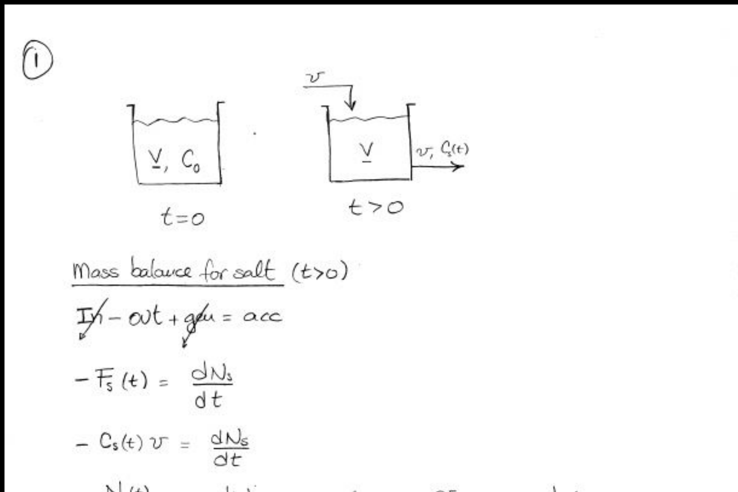
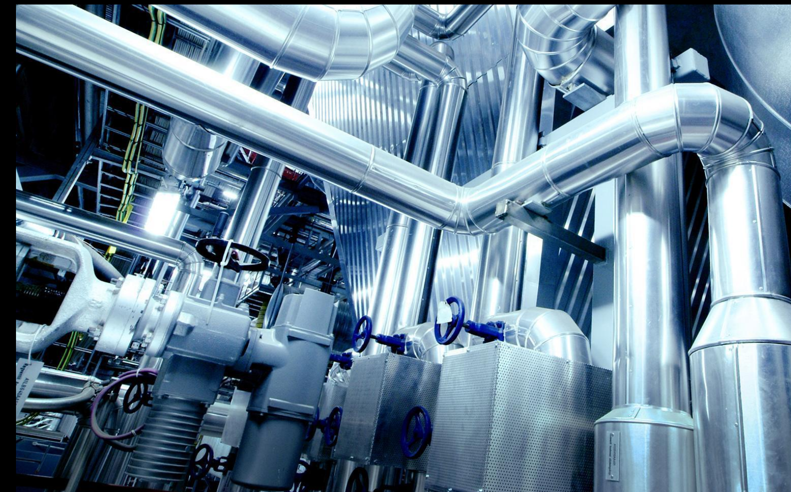
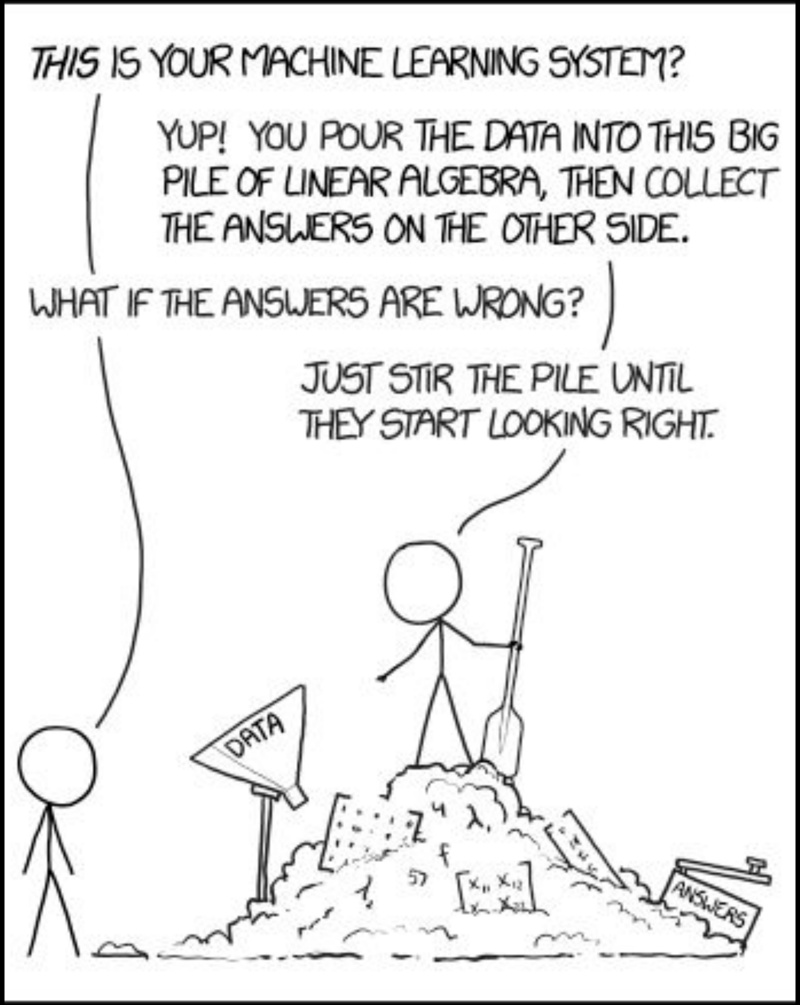




ChE352
Numerical Techniques for Chemical Engineers
Professor Stevenson

Lecture 13

Linear Algebra



- Vectors & matrices allow huge calculations to be represented with less code and logic
- Linearity simplifies math
- Because of this, decades of work have gone into framing **every** problem as linear algebra

Example: Stochastic Matrix

A stochastic matrix (also called transition matrix or Markov matrix) summarizes the statistics of a complex system by saying:
Given the current state, what is the probability of each possible next state?

An example current state would be the current letter in a word, and the possible next states are all the letters that could follow it.

Example: Stochastic Matrix

Output

Input

```
        '       X       I              &       E       P
'    [[0.   , 0.   , 0.008, ..., 0.   , 0.059, 0.   ],
X     [0.034, 0.   , 0.243, ..., 0.   , 0.254, 0.073],
I     [0.01 , 0.001, 0.002, ..., 0.   , 0.036, 0.005],
      ...,
&     [0.   , 0.   , 0.   , ..., 0.   , 0.   , 0.   ],
E     [0.006, 0.009, 0.01 , ..., 0.   , 0.041, 0.008],
P     [0.002, 0.   , 0.056, ..., 0.   , 0.16 , 0.034]]
```

Every pair of letters has a probability P(next|current)

AVIMUT WAND MY WHE AD IT
D Y
WOTO T THARSE H F THALS, AY,
IEES LDOM IET COOFUCISCAIUCL CLED.
AMOVE W

Example: Stochastic Matrix

Output

```
               SIR. EARTH BESPEAK CONTAGION LUNACIES DEMAND
  SIR.        [[0.,   0.,   0., ..., 0.,  0.,  0.],
  EARTH        [0.,   0.,   0., ..., 0.,  0.,  0.],
  BESPEAK      [0.,   0.,   0., ..., 0.,  0.,  0.],
                ...,
  CONTAGION    [0.,   0.,   0., ..., 0.,  0.,  0.],
  LUNACIES     [0.,   0.,   0., ..., 0.,  0.,  0.],
  DEMAND       [0.,   0.,   0., ..., 0.,  0.,  0.]]
```

Input

Every pair of words has a probability P(next|current)

"THE FALSE STEWARD, THAT YOU ARE THEY DO SO? PAH! PUTS HIM OUT; SPEAK TO OURSELVES IS IT MUST NOT GUILTY OF WIT, WITH US GO TO WHAT REPLICATION SHOULD HAVE FOUND SO. HAMLET O, TREBLE ON THE CASTLE. ENTER HAMLET SAFELY STOWED. ROSENCRANTZ: GUILDENSTERN:"

Example: Stochastic Matrix

Every pair of word-triplets has a probability
P(next|current two words)

NEW LIGHTED ON A HEAVEN KISSING HILL A COMBINATION AND A FORM INDEED WHERE EVERY GOD DID SEEM TO SET HIS SEAL TO GIVE THE WORLD ASSURANCE OF A MAN THIS WAS YOUR HUSBAND.

(Following the path of highest probability for the starting word-triplet "NEW LIGHTED", the model has directly copied these lines from Hamlet Act 3, Scene 4.)

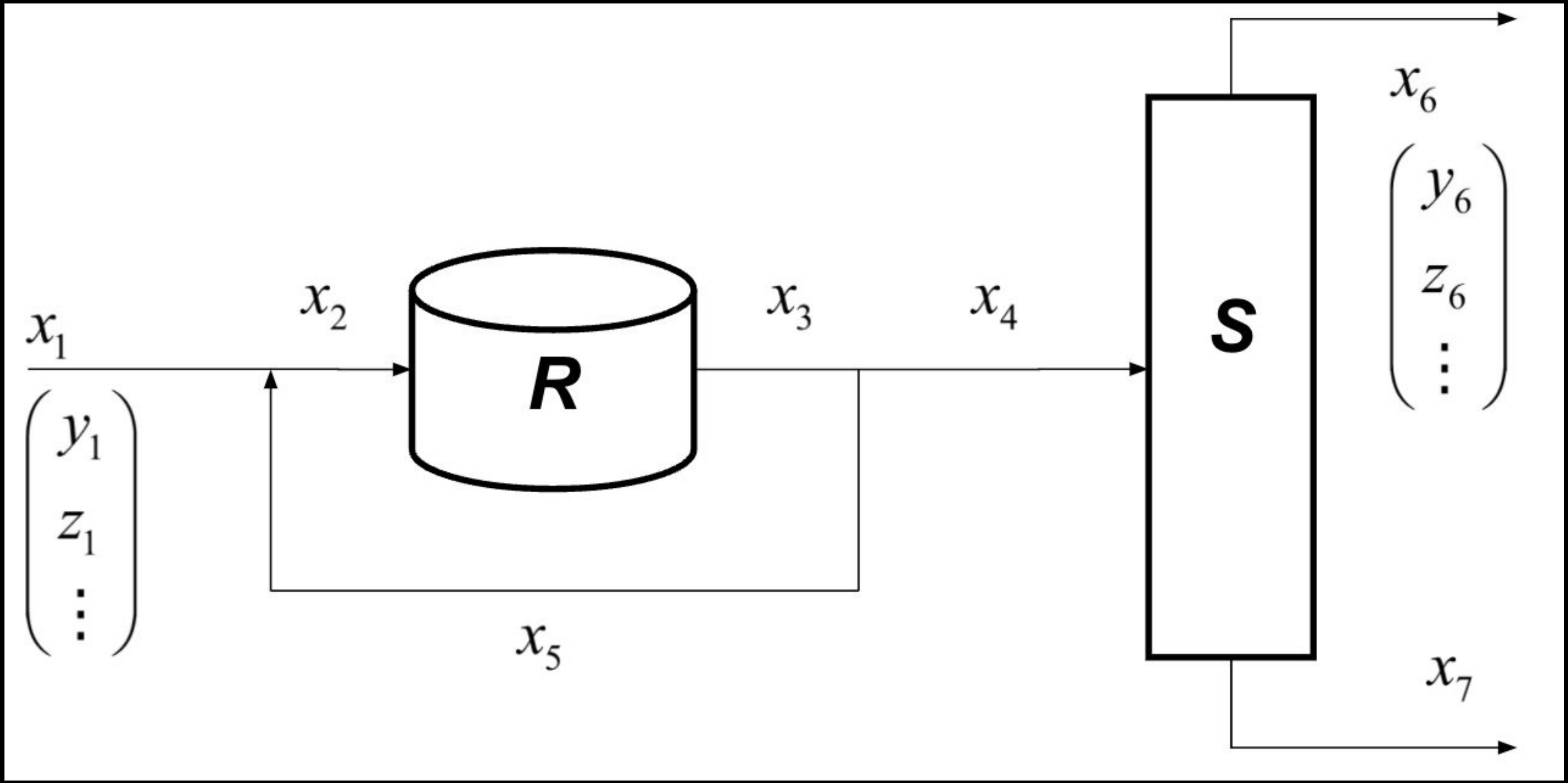
Linear Systems Vocabulary

- Linear system / matrix / vector
- Row vector / column vector
- Gaussian Elimination
- Row operation / augmented matrix

More Linear Systems Vocabulary

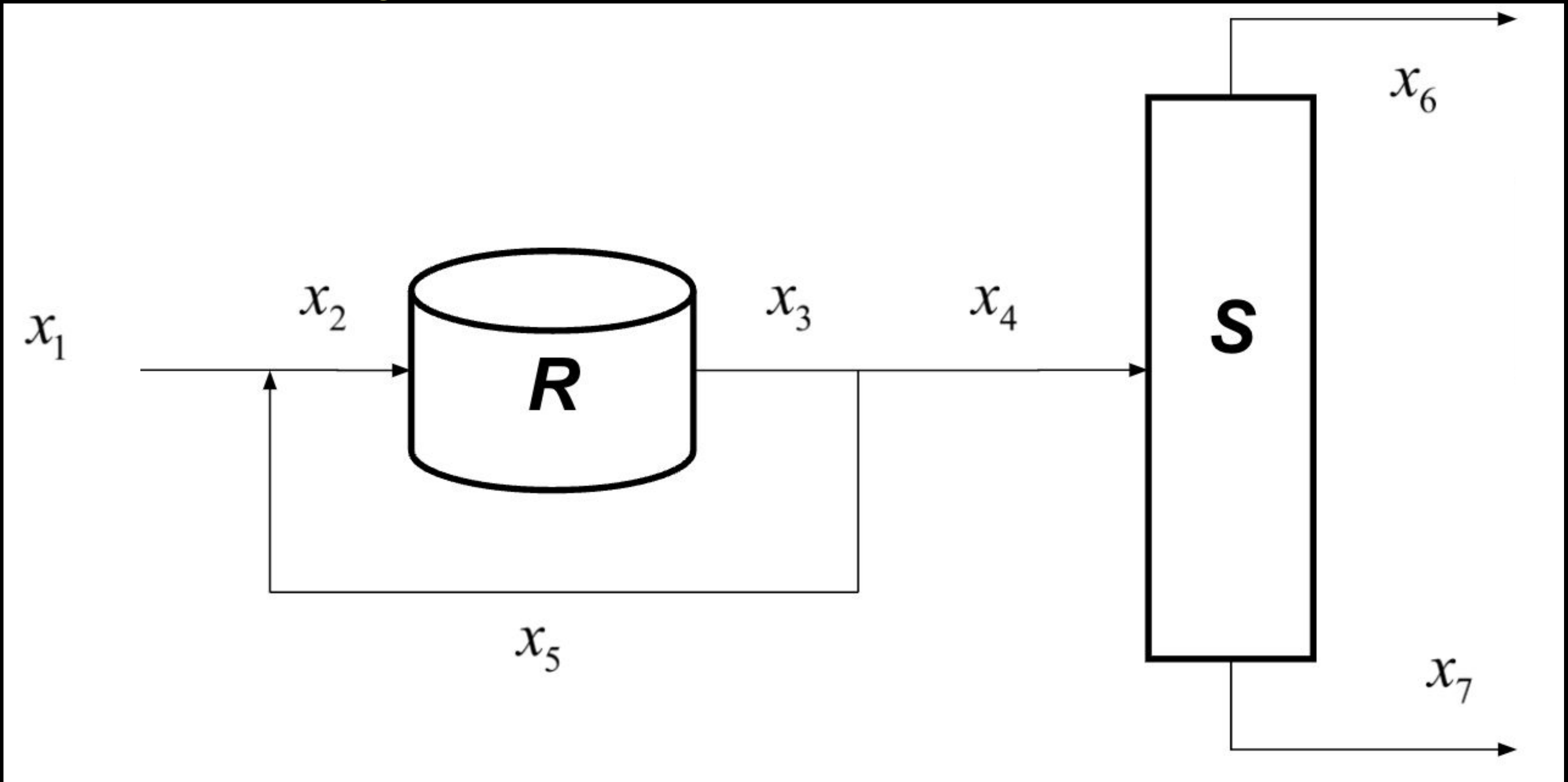
- Square
- Linearly independent / dependent
- Rank
- Full rank / rank deficient

Motivation: Example PFD



- What are *R* and *S* in this diagram?
- What could x_i represent?
- What if there are y_i, z_i, w_i, ..., what are those?

Activity: Mole/Mass Balance

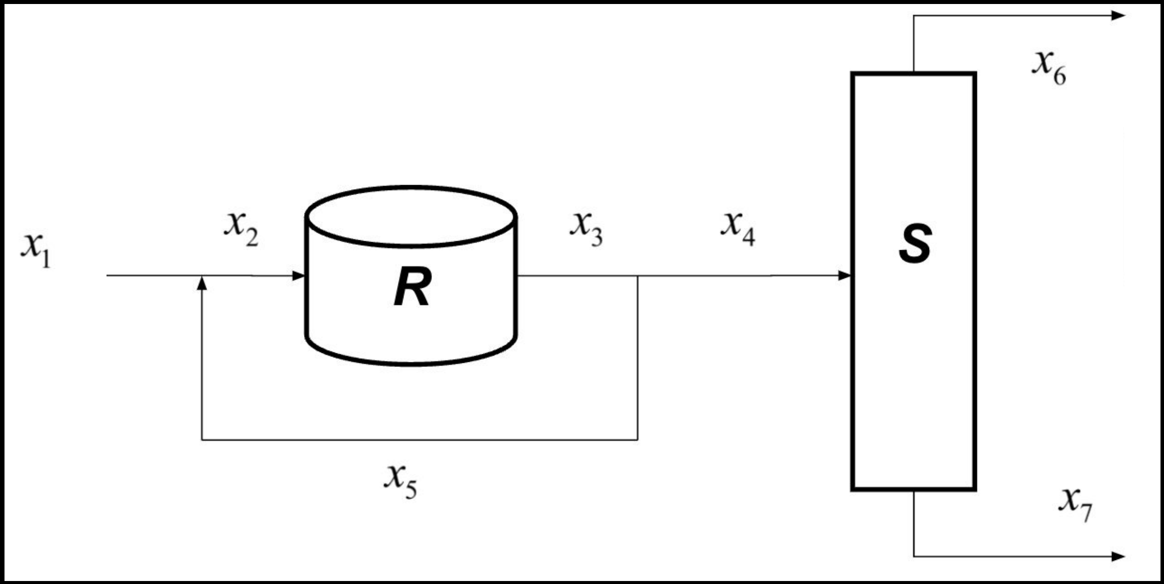


Set up the mole balance equations for this PFD, given that R & S operate so $x_3 = Rx_2$ and $x_6 + x_7 = Sx_4$. Then arrange in the form $Ax = b$.

Answer: Mole/Mass Balance

Write out the equations with variables in order (x_1, x_2, x_3, ...):

$$-x_1 + x_2 - x_5 = 0$$
$$-Rx_2 + x_3 = 0$$
$$x_3 - x_4 - x_5 = 0$$
$$Sx_4 - x_6 - x_7 = 0$$



Expand into matrix form with each equation as a row (any absent variable = coefficient zero)

Answer: Mole/Mass Balance

$$x = \begin{bmatrix} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 \end{bmatrix}^T$$

Why 0?

$$A = \begin{bmatrix} -1 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -R & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & S & 0 & -1 & -1 \end{bmatrix}, \quad b = 0$$

- How many degrees of freedom do we have?
- What if the reactor equation is nonlinear? What about the separator?
- How could we solve this linear system?

Gaussian Elimination for Ax = b

- Want to reduce matrix to identity matrix
- Three permissible row operations:
  1. Multiply equation/row by scalar
  2. Add scaled row to another equation/row
  3. Move rows/equations around
- The pivot element is the entry in A used to scale the row operations to remove variables
- The number of operations for solving $Ax = b$ is $O(n^3)$ if A has size $n \times n$ (that's a lot for big n)
- Does A have to be square? What rank?

Gaussian Elimination Example

$$A = \begin{bmatrix} 1 & 2 \\ 4 & 5 \end{bmatrix}, \quad b = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

How would you start turning matrix A into an identity matrix?

(Remember, you have to do the same operations to b.)

Gaussian Elimination Example

$$A=\begin{bmatrix}1 & 2\\ 4 & 5\end{bmatrix},\quad b=\begin{bmatrix}3\\ 4\end{bmatrix},\quad A|b0=\begin{bmatrix}1 & 2 & 3\\ 4 & 5 & 4\end{bmatrix}$$

Augmented matrix
(A mashed into b)

$$-4*row1+row2:\quad A|b1=\begin{bmatrix}1 & 2 & 3\\ 0 & -3 & -8\end{bmatrix}$$

○ = pivot

$$\frac{2}{3}*row2+row1:\quad A|b2=\begin{bmatrix}1 & 0 & 3-\frac{16}{3}\\ 0 & -3 & -8\end{bmatrix}$$

$$-\frac{1}{3}*row2:\quad A|b3=\begin{bmatrix}1 & 0 & -\frac{7}{3}\\ 0 & 1 & \frac{8}{3}\end{bmatrix}\quad\rightarrow\quad x=\frac{1}{3}\begin{bmatrix}-7\\ 8\end{bmatrix}$$

Example usage: cubic splines

For datapoints y_0, y_1, etc, the cubic spline coefficients can be found by solving:

$$\begin{bmatrix} 2 & 1 & & & & & \\ 1 & 4 & 1 & & & & \\ & 1 & 4 & 1 & & & \\ & & 1 & 4 & 1 & & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & & & 1 & 4 & 1 \\ & & & & & 1 & 2 \end{bmatrix} \begin{bmatrix} D_0 \\ D_1 \\ D_2 \\ D_3 \\ \vdots \\ D_{n-1} \\ D_n \end{bmatrix} = \begin{bmatrix} 3(y_1 - y_0) \\ 3(y_2 - y_0) \\ 3(y_3 - y_1) \\ \vdots \\ 3(y_{n-1} - y_{n-3}) \\ 3(y_n - y_{n-2}) \\ 3(y_n - y_{n-1}) \end{bmatrix}$$

A *tridiagonal* matrix

Boundary conditions

Matrix Pivoting Strategies

- There are a combinatorial # of ways to do any given Gaussian elimination - Why?
- If the matrix A is ill-conditioned (one variable is much smaller/bigger than the others) then it's hard to find the exact solution due to round-off error (see p. 241 in F&B)
- Methods such as partial pivoting, scaled partial pivoting, and total/full/maximal pivoting can be used to reduce round-off error, using $O(N^3)$ extra flops (Is that a lot in this context?)
- Iterative methods (coming soon) are better...

Linear algebra is easy in numpy

```
b = np.array([1, 1, 1])  # Define vector b
A = np.array([[4, -1, 1], [-1, 4.25, 2.75],
[1, 2.75, 3.5]])  # Define matrix A
x = np.linalg.solve(A, b)  # Find Ax = b
C = A + B  # Find A plus B
D = A @ B  # Find A times B (matrix multiply)
E = A * B  # Find A times B COMPONENT-WISE
Bsq = B**2  # Square each element of B (≠B@B)
L = np.linalg.cholesky(A)  # Cholesky factor
Ainv = np.linalg.inv(A)  # Inverse (unwise)
Apnv = np.linalg.pinv(A)  # pseudo-inverse
```

Summary and Problems

- Open Python Numerical Methods, go to Chapter 14.7: Summary and Problems

https://pythonnumericalmethods.berkeley.edu/notebooks/chapter14.07-Summary-and-Problems.html

- Solve the problem beginning "*Write a function my_make_lin_ind(A) . . .*"
    - You might want to start with printing the input matrix *A* column by column