ABE 201
Biological Thermodynamics 1

Module 5:

Linear Algebra for Mass Balances

Topics for Today

Using Linear Algebra and Computer Tools to Solve Mass (and Energy) Balances

- Writing and solving systems of linear equations

- Using computer tools to solve systems of linear equations

System of Linear Equations

- A <u>set</u> of equations that share the same variables (definition of system)

- Variables are all of 1st order in the set of equations (definition of linear)

$$3\,x + 7 = 15$$

$$3\,x^1 + 7 = 15$$

$$\cancel{3\,x^2 + 7 = 15}$$

<u>System</u> of Linear Equations

$$3x + 4y = 35$$

$$2x - y = 15$$

2 variables – 2 equations = 0 DOF

Generalized

$$a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n = b_2$$

$$\begin{array}{ccc} . & . & . \\ . & . & . \\ . & . & . \end{array}$$

$$a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n = b_m$$

$x_1 \ldots x_n$ = variables $a_{11} \ldots a_{mn}$ = coefficients

$b_1 \ldots b_m$ = constants

Vector Form

$$\begin{bmatrix} a_{11} \\ a_{21} \\ \cdots \\ a_{m1} \end{bmatrix} x_1 + \begin{bmatrix} a_{12} \\ a_{22} \\ \cdots \\ a_{m2} \end{bmatrix} x_2 + \cdots + \begin{bmatrix} a_{1n} \\ a_{2n} \\ \cdots \\ a_{mn} \end{bmatrix} x_n = \begin{bmatrix} b_1 \\ b_2 \\ \cdots \\ b_m \end{bmatrix}$$

$$\overrightarrow{a_1} x_1 + \overrightarrow{a_2} x_2 + \cdots + \overrightarrow{a_n} x_n = \vec{b}$$

Matrix Form

$$Ax = b$$

$$A = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix}$$

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \qquad b = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$$

Solving Using Invertible Matrix

$$Ax = b$$
$$A^{-1}Ax = A^{-1}b$$
$$x = A^{-1}b$$

$$A^{-1}A = I$$

$$I = \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & 1 & \vdots \\ 0 & \cdots & 1 \end{bmatrix}$$

$$5^{-1}5 = 1$$

$$\mathbf{A} = \begin{pmatrix} a & b & c \\ p & q & r \\ u & v & w \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} \alpha & \beta & \gamma \\ \lambda & \mu & \nu \\ \rho & \sigma & \tau \end{pmatrix},$$

$$\mathbf{AB} = \begin{pmatrix} a & b & c \\ p & q & r \\ u & v & w \end{pmatrix} \begin{pmatrix} \alpha & \beta & \gamma \\ \lambda & \mu & \nu \\ \rho & \sigma & \tau \end{pmatrix} :$$

$$= \begin{pmatrix} a\alpha + b\lambda + c\rho & a\beta + b\mu + c\sigma & a\gamma + b\nu + c\tau \\ p\alpha + q\lambda + r\rho & p\beta + q\mu + r\sigma & p\gamma + q\nu + r\tau \\ u\alpha + v\lambda + w\rho & u\beta + v\mu + w\sigma & u\gamma + v\nu + w\tau \end{pmatrix}$$

$$\mathbf{A} = \begin{pmatrix} a & b & c \\ p & q & r \\ u & v & w \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} \alpha & \beta & \gamma \\ \lambda & \mu & \nu \\ \rho & \sigma & \tau \end{pmatrix},$$

$$\mathbf{AB} = \begin{pmatrix} a & b & c \\ p & q & r \\ u & v & w \end{pmatrix} \begin{pmatrix} \alpha & \beta & \gamma \\ \lambda & \mu & \nu \\ \rho & \sigma & \tau \end{pmatrix} :$$

$$= \begin{pmatrix} a\alpha + b\lambda + c\rho & a\beta + b\mu + c\sigma & a\gamma + b\nu + c\tau \\ p\alpha + q\lambda + r\rho & p\beta + q\mu + r\sigma & p\gamma + q\nu + r\tau \\ u\alpha + v\lambda + w\rho & u\beta + v\mu + w\sigma & u\gamma + v\nu + w\tau \end{pmatrix}$$

$$Ix = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$= \begin{bmatrix} x_1 + 0 + 0 \\ 0 + x_2 + 0 \\ 0 + 0 + x_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Identity and Determinants

$$A^{-1} \cdot A = I$$

Any square matrix A has an inverse iff det A ≠ 0

The Determinant

$$A = \begin{vmatrix} a & b \\ c & d \end{vmatrix}$$

$$\det A = a \cdot d - b \cdot c$$

Inverse Matrices

$$A = \begin{vmatrix} a & b \\ c & d \end{vmatrix}$$

$$\det A = a \cdot d - b \cdot c$$

$$A^{-1} = \frac{1}{\det A} \cdot \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = \frac{1}{ad - bc} \cdot \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

Matrices – a short review

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\det A = ??$$

Inverse Matrices

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\mathsf{A}^{-1} = \frac{1}{|\mathsf{A}|} \begin{bmatrix} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} & \begin{vmatrix} a_{13} & a_{12} \\ a_{33} & a_{32} \end{vmatrix} & \begin{vmatrix} a_{12} & a_{13} \\ a_{22} & a_{23} \end{vmatrix} \\ \begin{vmatrix} a_{23} & a_{21} \\ a_{33} & a_{31} \end{vmatrix} & \begin{vmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{vmatrix} & \begin{vmatrix} a_{13} & a_{11} \\ a_{23} & a_{21} \end{vmatrix} \\ \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix} & \begin{vmatrix} a_{12} & a_{11} \\ a_{32} & a_{31} \end{vmatrix} & \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} \end{bmatrix}.$$

Methods to invert matrix

- Gauss-Jordan elimination
- Gaussian elimination
- LU decomposition

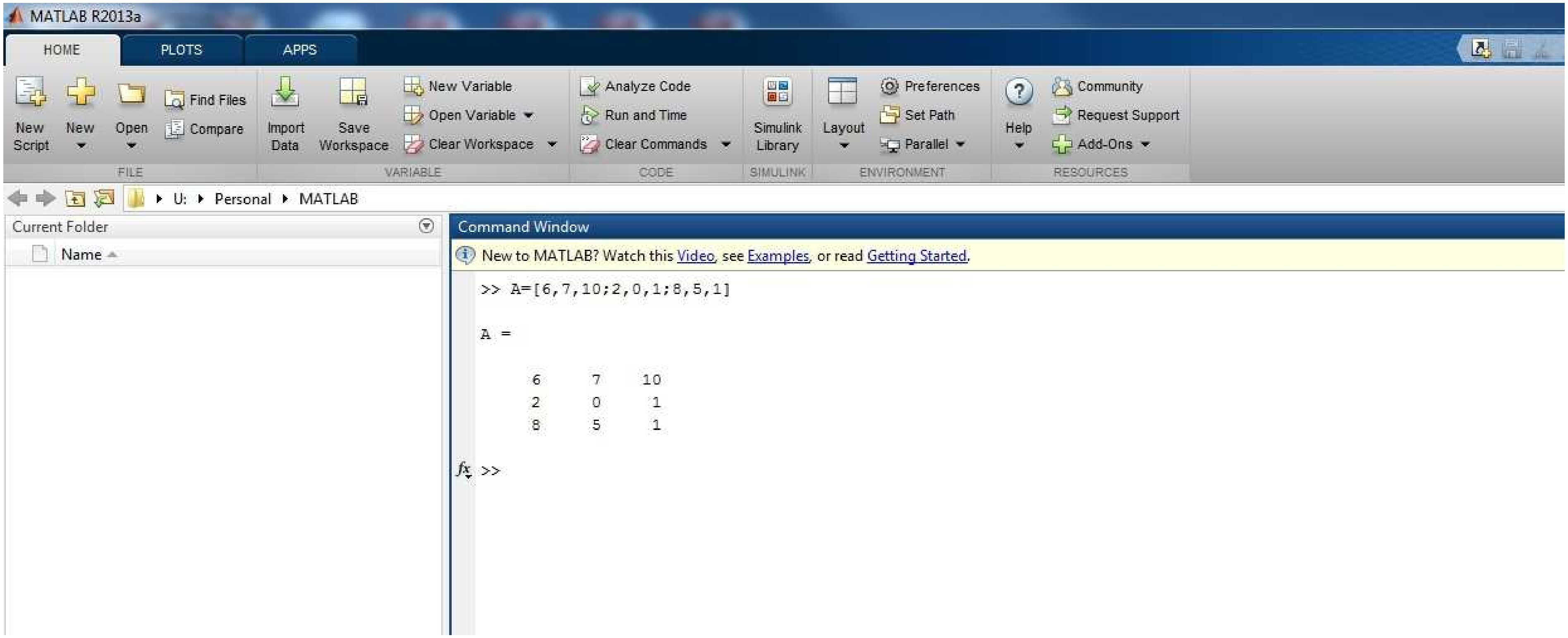
Using MatLAB to Solve Linear Systems

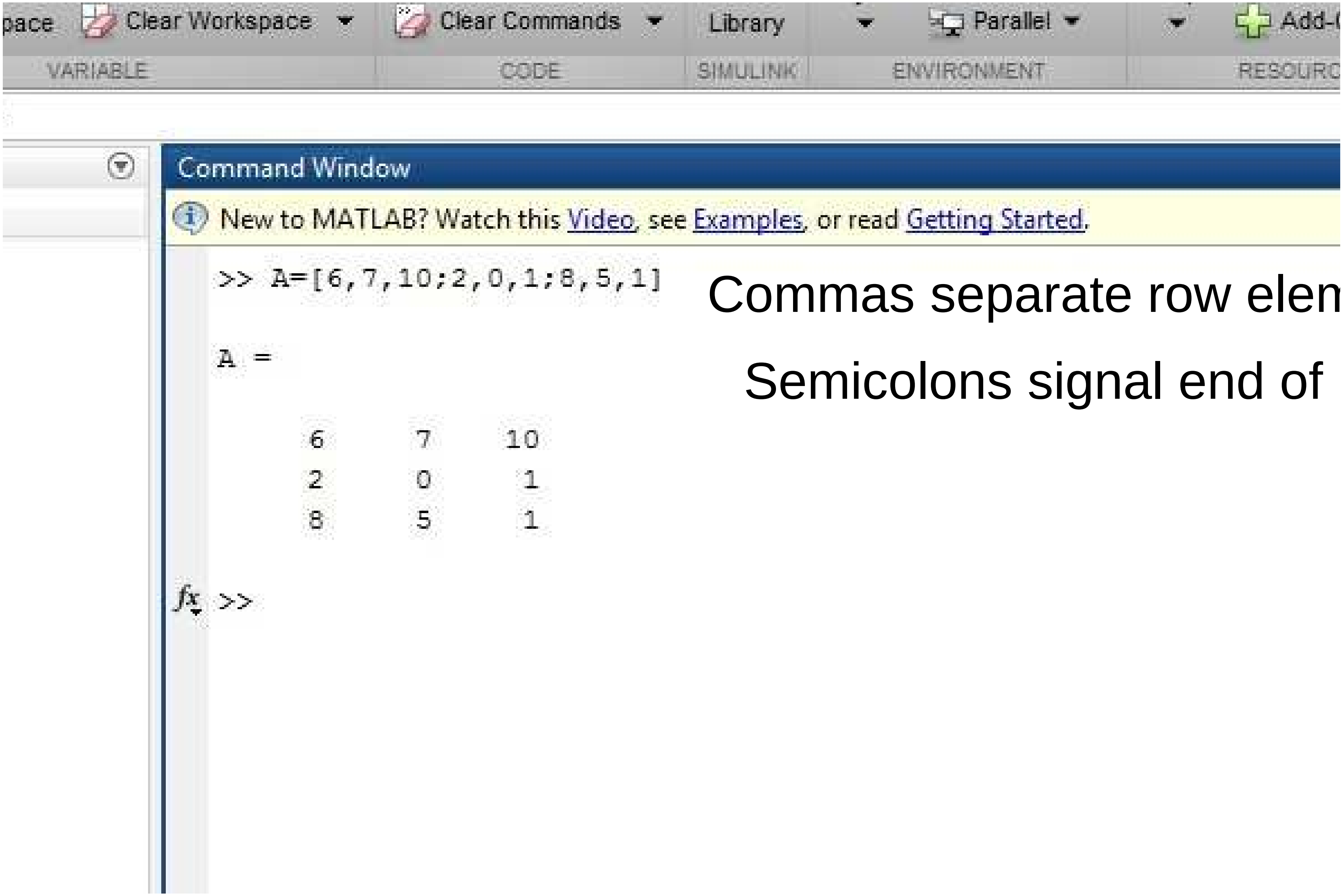
$$6x_1 + 7x_2 + 10x_3 = 35$$

$$2x_1 + x_3 = 15$$

$$8x_1 + 5x_2 + x_3 = 22$$

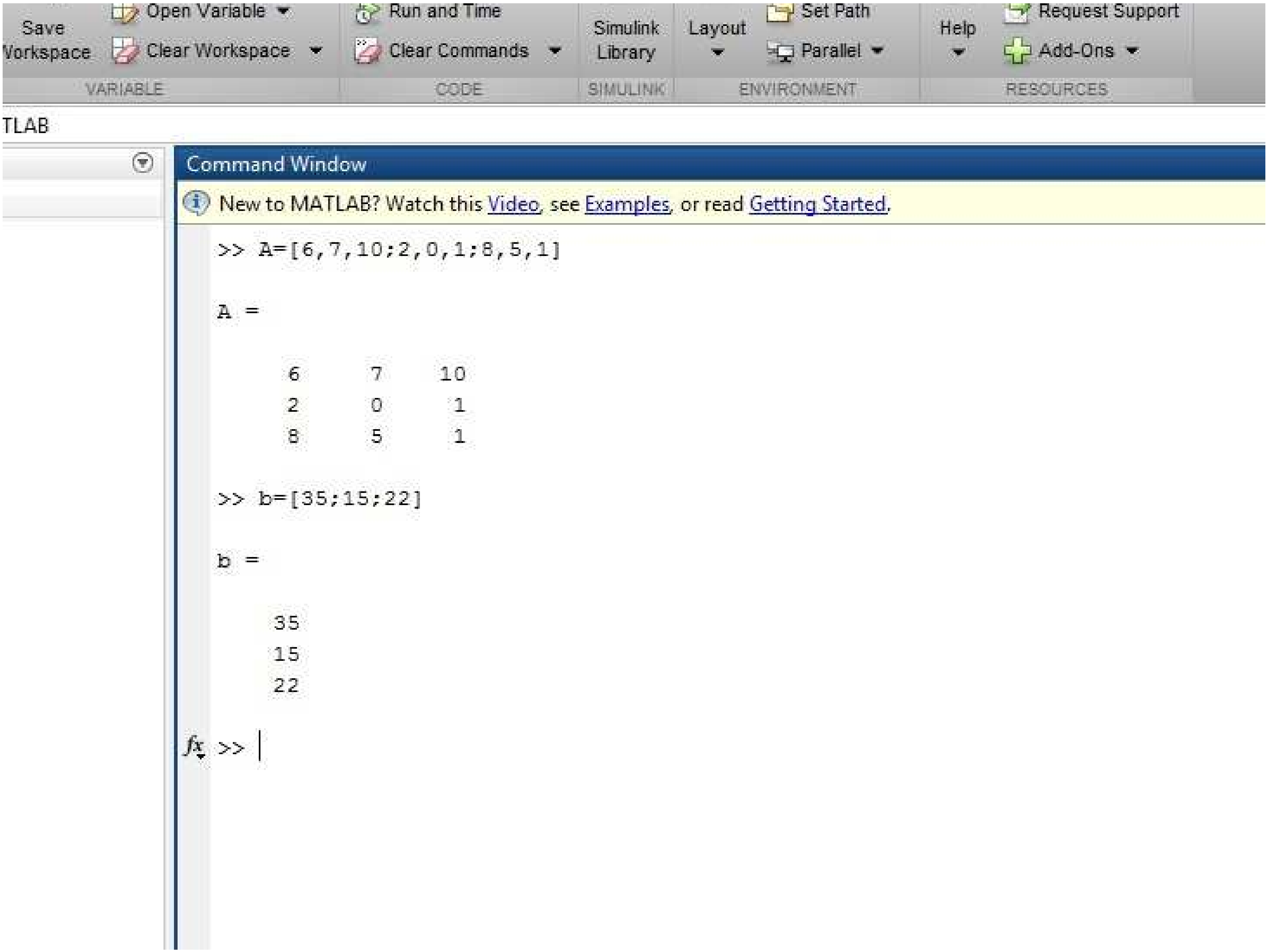
$$A = \begin{bmatrix} 6 & 7 & 10 \\ 2 & 0 & 1 \\ 8 & 5 & 1 \end{bmatrix} \qquad x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \qquad b = \begin{bmatrix} 35 \\ 15 \\ 22 \end{bmatrix}$$


MATLAB R2013a
HOME
PLOTS
APPS
New Script
New
Open
Find Files
Compare
Import Data
Save Workspace
New Variable
Open Variable
Clear Workspace
Analyze Code
Run and Time
Clear Commands
Simulink Library
Layout
Preferences
Set Path
Parallel
Help
Community
Request Support
Add-Ons
FILE
VARIABLE
CODE
SIMULINK
ENVIRONMENT
RESOURCES
U: Personal MATLAB
Current Folder
Name
Command Window
New to MATLAB? Watch this Video, see Examples, or read Getting Started.
>> A=[6,7,10;2,0,1;8,5,1]
A =
6 7 10
2 0 1
8 5 1
fx >>



Commas separate row elen

Semicolons signal end of


Save
Workspace
Open Variable
Clear Workspace
VARIABLE
Run and Time
Clear Commands
CODE
Simulink
Library
SIMULINK
Layout
Set Path
Parallel
ENVIRONMENT
Help
Request Support
Add-Ons
RESOURCES
TLAB
Command Window
New to MATLAB? Watch this Video, see Examples, or read Getting Started.
>> A=[6,7,10;2,0,1;8,5,1]
A =
6 7 10
2 0 1
8 5 1
>> b=[35;15;22]
b =
35
15
22
fx >>

```
>> A=[6,7,10;2,0,1;8,5,1]

A =

     6     7    10
     2     0     1
     8     5     1

>> b=[35;15;22]

b =

    35
    15
    22

>> x=inv(A)*b

x =

    5.5714
   -5.2857
    3.8571

>>
```

Inv(A) is the command to compute the inverse of A

* is the symbol for dot product

ABE Fermentation

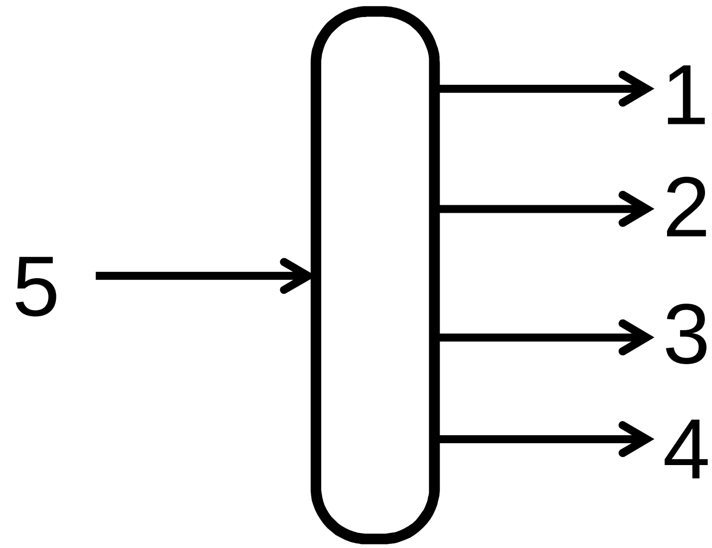
Clostridium acetylbutylicum is used to ferment sugar to a mixture of acetone, butanol, and ethanol. Distillation is used to recover and purify the products from the fermentation liquid (water).

At steady state, 1,575 kg of liquid enters the distillation column per minute. The fermentation liquid is 3.5% (w/w) acetone, 4.5% (w/w) butanol, 3.7% (w/w) ethanol, and the remainder water.

Four streams leave the column with the following compositions:

1. 94.2% acetone, 3.1% ethanol, 1.5% butanol, remainder water
2. 92.5% ethanol, 3.8% butanol, remainder water
3. 93.3% butanol, remainder water
4. 1.0% butanol, remainder water

What are the rates of production for each stream?



	1	2	3	4	5
m (kg/min)	m_1	m_2	m_3	m_4	1575
x_a	0.942	0	0	0	0.035
x_e	0.031	0.925	0	0	0.037
x_b	0.015	0.038	0.933	0.010	0.045
x_w	0.012	0.037	0.067	0.990	0.883

acc = in – out + gen - con

0 = (m_5) – (m_1 + m_2 + m_3 + m_4)

m_5 = (m_1 + m_2 + m_3 + m_4)

$$\begin{bmatrix} x_{5a} \\ x_{5e} \\ x_{5b} \\ x_{5w} \end{bmatrix} m_5 = \begin{bmatrix} x_{1a} & x_{2a} & x_{3a} & x_{4a} \\ x_{1e} & x_{2e} & x_{3e} & x_{4e} \\ x_{1b} & x_{2b} & x_{3b} & x_{4b} \\ x_{1w} & x_{2w} & x_{3w} & x_{4w} \end{bmatrix} \bullet \begin{bmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \end{bmatrix}$$

$$\begin{bmatrix} 0.035 \\ 0.037 \\ 0.045 \\ 0.883 \end{bmatrix} 1575 = \begin{bmatrix} 0.942 & 0 & 0 & 0 \\ 0.031 & 0.925 & 0 & 0 \\ 0.015 & 0.038 & 0.933 & 0.01 \\ 0.012 & 0.037 & 0.067 & 0.990 \end{bmatrix} \bullet \begin{bmatrix} m_1 \\ m_2 \\ m_3 \\ m_4 \end{bmatrix}$$

$$b = a \bullet \overrightarrow{m}$$

$$\overrightarrow{m} = a^{-1} b$$

Command Window

```
>> b=[0.035;0.037;0.045;0.883]*1575

b =

   1.0e+03 *

    0.0551
    0.0583
    0.0709
    1.3907

>> a=[0.945,0,0,0;0.031,0.925,0,0;0.015,0.038,0.933,0.01;0.012,0.037,0.067,0.99]

a =

    0.9450         0         0         0
    0.0310    0.9250         0         0
    0.0150    0.0380    0.9330    0.0100
    0.0120    0.0370    0.0670    0.9900

>> m=inv(a)*b

m =

   1.0e+03 *

    0.0583
    0.0610
    0.0576
    1.3979

fx >>
```

m_1= 58.3 kg/min

m_2= 61.0 kg/min

m_3= 57.6 kg/min

m_4= 1397.9 kg/min

Summary

- Material (and energy!) balances are systems of linear equations
- Systems of linear equations can be represented and solved in matrix form
- MatLAB and other computer tools make easy the tedious and repetitive work of solving
- The challenge is <u>translating</u> an engineering problem into mathematics