Matlab: Linear Algebraic Systems

1. Background
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MATLAB: Linear Algebraic Systems

Background

Matrix Determinant

- det(X) is the determinant of the square matrix X

```
>> A = [1 2 3; 2 -3 1; 4 1 8];
>> det(A)
ans =
    -7
>> A = [1 2 3; 2 -3 1; 4 1 7];
>> det(A)
ans =
     0
```

Matrix Inverse

- inv(X) is the inverse of the square matrix X. A warning message is printed if X is badly scaled or nearly singular.

```
>> A = [1 2 3; 2 -3 1; 4 1 8];
>> AI = inv(A)
AI =
    3.5714    1.8571   -1.5714
    1.7143    0.5714   -0.7143
   -2.0000   -1.0000    1.0000
>> A*AI
ans =
    1.0000         0         0
    0.0000    1.0000   -0.0000
         0         0    1.0000
>> A = [1 2 3; 2 -3 1; 4 1 7];
>> inv(A)
Warning: Matrix is singular to working precision.
```

Functions for Linear System Solution

- Matlab provides three different ways to solve linear algebraic systems **Ax = b**
- x = inv(A)*b
  - » Only applicable to square systems
- x = A\b
  - » Applicable to square and non-square systems
  - » Provides least-squares solutions if system is non-square
- x = linsolve(A,b)
  - » Similar to x = A\b
  - » Provides additional solution options not discussed here

Square System Example

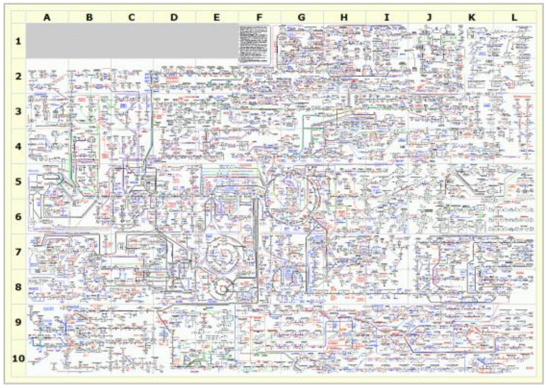
```
>>A=[-1 1 2; 3 -1 1; -1 3 4];
>> b=[2 6 4]';
>> x=inv(A)*b;
>> x=A\b;
>> x=linsolve(A,b)
x =
   1.0000
  -1.0000
   2.0000
```

$$-x_1 + x_2 + 2x_3 = 2$$

$$3x_1 - x_2 + x_3 = 6$$

$$-x_1 + 3x_2 + 4x_3 = 4$$

Cellular Metabolic Network Models

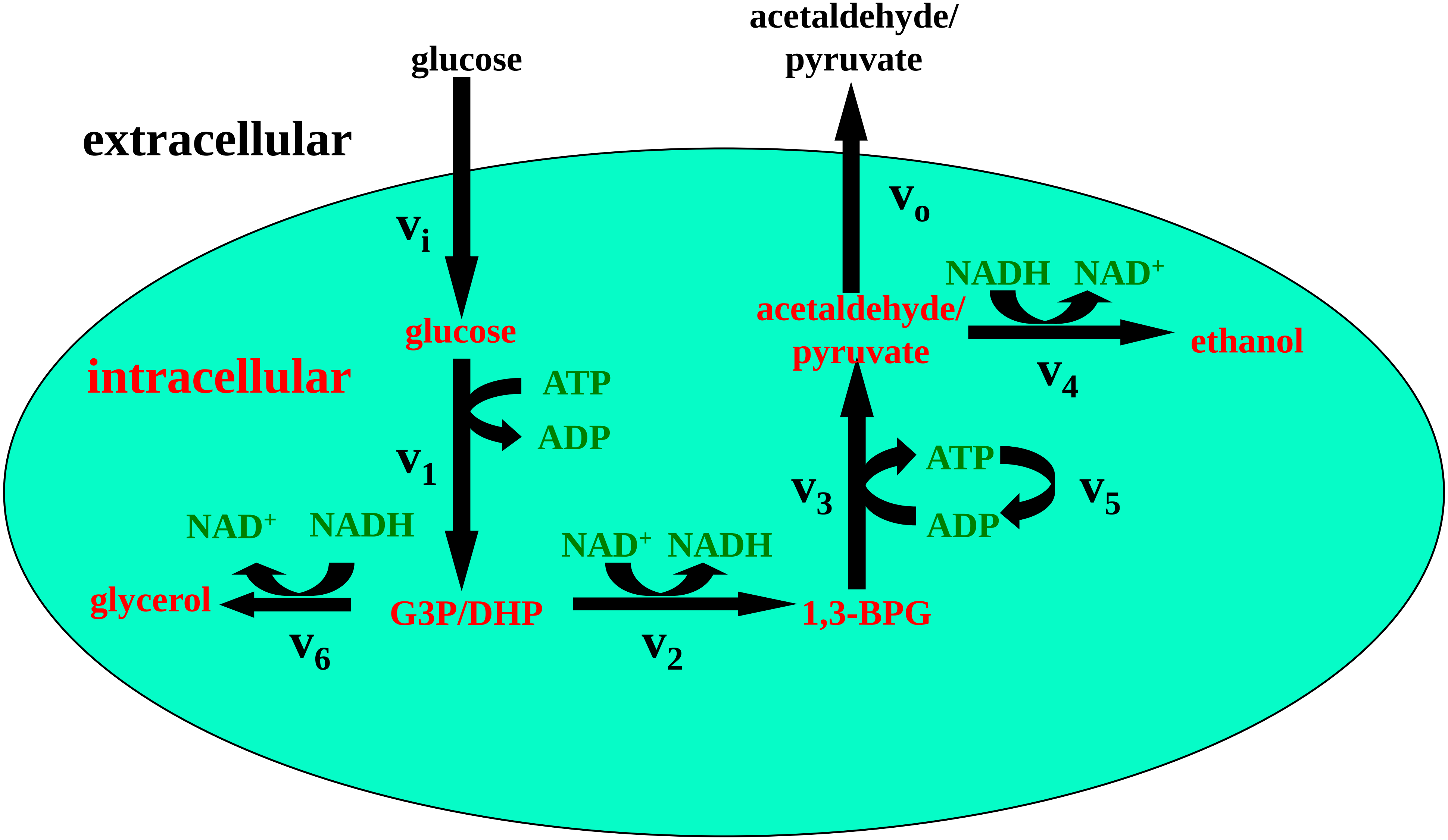


$$S \xrightarrow{v_1} M \xrightarrow{v_2} P$$

$$0 = a_1 v_1 - a_2 v_2$$

- Stoichiometric coefficients (a_1,a_2)
  - » Determines number of product molecules produced per molecule of substrate consumed
  - » Often known from biochemistry literature
- Reaction rates (v_1,v_2)
  - » Also called reaction velocity or flux
  - » Can be determined computationally
- Metabolic flux balance analysis
  - » Assume no intracellular metabolite accumulation
  - » Calculate unknown fluxes from available measurements

Yeast Energy Metabolism



Wolf & Heinrich, Biochemical Journal, 345, 321-334, 2000.

Steady-State Mass Balances

Membrane transport (v_i)	Glucose (extracellular) → Glucose
Reaction 1 (v_1)	Glucose + 2ATP → 2G3P/DHP + ADP
Reaction 2 (v_2)	G3P/DHP+NAD^+ → 1,3-BPG + NADH
Reaction 3 (v_3)	1,3-BPG+ADP → Acetaldehyde/Pyruvate + 2ATP
Reaction 4 (v_4)	Acetaldehyde/Pyruvate+NADH → Ethanol + NAD^+
Reaction 5 (v_5)	ATP → ADP
Reaction 6 (v_6)	G3P/DHP+NADH → glycerol + NAD^+
Membrane transport (v_o)	Acetaldehyde/Pyruvate → Acetaldehyde/Pyruvate (extracellular)

$$\text{Glucose}: \ 0 = v_i - v_1 \qquad \text{G3P/DHP}: \ 0 = 2v_1 - v_2 - v_6$$

$$1-3-\text{BPG}: \ 0 = v_2 - v_3 \qquad \text{Acetaldeyde/Pyruvate}: \ 0 = v_3 - v_4 - v_0$$

$$\text{NADH}: \ 0 = v_2 - v_4 - v_6 \qquad \text{ATP}: \ 0 = -2v_1 + 2v_3 - v_5$$

Linear System Representation

- Assume measurements of glucose influx v_i and acetaldehyde/pyruvate efflux v_0 are available

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 2 & -1 & 0 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & -1 \\ -2 & 0 & 2 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \end{bmatrix} = \begin{bmatrix} v_i \\ 0 \\ 0 \\ v_o \\ 0 \\ 0 \end{bmatrix}$$

Compute Matrix Rank

```
>> A = [1 0 0 0 0 0; 2 -1 0 0 0 -1; 0 1 -1 0 0 0; 0 0 1 -1 0 0; 0 1 0 -1 0 -1; -2 0 2 0 -1 0]

A =

     1     0     0     0     0     0
     2    -1     0     0     0    -1
     0     1    -1     0     0     0
     0     0     1    -1     0     0
     0     1     0    -1     0    -1
    -2     0     2     0    -1     0

>> rank(A)

ans =

     6
```

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In-class Exercise