Stoichiometric matrix

The stoichiometric matrix corresponds to adjacency matrix (graph theory). All kinetic laws can be expressed as

$$\frac{dx}{dt} = Sv$$

We have: m reactions and n molecular species

$$x = (x_1 x_2 ... x_n)^T \in R^n$$
$$v = (v_1 v_2 ... v_n)^T \in R^m$$

typical example: $A + B \to C, C \to A + B$

$$\frac{d}{dt}[A] = k_2[C] - k_1[A][B]$$
$$\frac{d}{dt}[B] = k_2[C] - k_1[A][B]$$
$$\frac{d}{dt}[C] = k_1[A][B] - k_2[C]$$

Singular value decomposition

Let A be an mxn matrix. Then, there exist orthogonal matrices U and V and a matrix Σ such that $A = U\Sigma V^T$

Steady states

A steady state is a state x of the syste for which

$$\frac{dx}{dt} = Sv = 0$$

Solving for $v = (V_1 V_2 ... V_m)^T$ will give us the possible reaction rates at equilibrium

Matlab code

```
% Solving linear systems in Matlab
A = [1 2, 0 1]
Y = [1, 2]

% If we want to solve the equation Ax = y, we do...
x=A\y

S = [-1 1 -1, 1 -1 0, 0 0 1]
v = S\zeros(3,1) % uh oh...singular matrix
null(S)
```

We want to describe all possible solutions of $Sv = 0$ (equation *). It turns out that ever solution v of * can be written as

$$v = c_1 v_1 + c_2 v_2 + ... + c_k v_k$$

where $v_1 ... v_k$ are some special solutions of *.

```
S = [-1 1 0 0 -1 1, 0 -1 1 0 0 0, 0 0 -1 1 -1 1]
A = S'
null(A)
```

Conservation relations

$$\frac{dx}{dt} = Sv$$

S is nxm

Consider a vector x such that $x^T S = 0$

$$y^T \frac{dx}{dt} = y^T(Sv) \rightarrow \frac{dy^T x}{dt} = y^T S_v = 0 \rightarrow \frac{d}{dt} y^T x = 0$$

This implies that $y^T x$ is constant. $y^T x = [y_1 ... y_n][x_1 ... x_n]^T = y_1 x_1 + y_2 x_2 + ... + y_n x_n =$ constant

Example

```
glucose --(ATP -> ADP)--> gluc_6P  <----> fruc_6P --(ATP -> ADP)--> fruc-1,6P

          S_1                     S_2          S_3                      S_4
                S_5    S_6
                   V_1                 V_2             V_3


S = |  -1  0  0  |
    |   1 -1  0  |
    |   0  1 -1  |
    |   0  0  1  |
    |  -1  0 -1  |
    |   1  0  1  |

Matlab code starts here
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A = [-1 1 0 0 -1 1, 0 -1 1 0 0 0, 0 0 -1 1 -1 1]
null(A)
% if you scale, you get this vector
[ 2 1 1 0 0 1, 0 0 0 0 1 1, 1 1 1 1 0 0 ]

% first column y_1, second y_2, third y_3
% additional conservation relation
% -y_1 + 3*y_2 + 2*y_3 = [0 1 1 2 3 2]^T
```