

The Y A_k Ψ representation

This converts the stoichiometric representation $\frac{dx}{dt} = S v(x)$ of a chemical reaction network to the form $S v(x) = Y A_k \Psi(x) = Y G K \Psi(x)$.

Here A_k is the Laplacian of the complexes graph and Y is the complexes to species matrix. The factoring $A_k = G K$ is found in V. Katsnelson's UCSD undergrad honors thesis. It also computes properties of A_k and the deficiency of the network.

```
(* This notebook presents all the commands available in the
chemYAK.m file. *)

<< "Desktop/chemYAK.m"

chemYAK is loading...

chemYAK has loaded

S = Transpose[{{{-1, 1, 0, 0, 1, 1}, {-1, 1, 0, 0, 0, 0}, {-1, 0, 1, 1, 0, 0}, {-1, 1, -1, 1, 0, 0},
{0, 0, -1, 1, -1, 0}, {1, -1, 0, 0, 0, 0}, {0, 0, 1, -1, 0, 0}}]}(*stoichiometric matrix*];
S //
MatrixForm


$$\begin{pmatrix} -1 & -1 & -1 & -1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & -1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$


(* matrixY takes the Stoichiometric matrix as intput and yields a
list of three matrices.
The first is matrix Y, the second is a list of the input complexes for all
the reactions (with repetitions), and the third is a list of the output
complexes for all the reactions (with repetitions). *)

Y = matrixY[S];

(* Here is the matrix Y. *)
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MatrixForm[Y[[1]]]


$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$


(* Here are the input complexes. They may be identified with
monomials whose exponents are given by the rows of this matrix. *)

MatrixForm[Transpose[Y[[2]]]]


$$\begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$


(* Here are the output complexes. *)

MatrixForm[Transpose[Y[[3]]]]


$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$


(* matrixG takes in matrix Y, the input complexes matrix,
and the output complexes matrix, and yields matrix G. *)

G = matrixG[Y];
G//MatrixForm


$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$


```

- (* Check to make sure YG=S *)

```

Print["YG = ", MatrixForm[Y[[1]].G], ",   S=", MatrixForm[S]];
Y[[1]].G == S

YG = 
$$\begin{pmatrix} -1 & -1 & -1 & -1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & -1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad S = \begin{pmatrix} -1 & -1 & -1 & -1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & -1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 & -1 \\ 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

True

Psi = makeMonomial[-Y[[1]], x];
Print["\u03a8(x) = ", MatrixForm[Psi]]

\Psi(x) = 
$$\begin{pmatrix} x[2] x[5] x[6] \\ x[1] \\ x[2] \\ x[3] x[4] \\ x[2] x[4] \\ x[1] x[3] \\ x[4] \\ x[3] x[5] \\ x[3] \end{pmatrix}$$


(* matrixK takes matrix G as input and yields matrix K. *)

K = matrixK[G];
K//MatrixForm


$$\begin{pmatrix} 0 & k[2, 1] & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & k[2, 3] & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & k[2, 4] & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & k[6, 5] & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & k[8, 7] & 0 \\ 0 & 0 & k[3, 2] & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & k[7, 9] & 0 & 0 \end{pmatrix}$$


Ak = G.K;
Ak // MatrixForm


$$\begin{pmatrix} 0 & k[2, 1] & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -k[2, 1] - k[2, 3] - k[2, 4] & k[3, 2] & 0 & 0 & 0 & 0 & 0 \\ 0 & k[2, 3] & -k[3, 2] & 0 & 0 & 0 & 0 & 0 \\ 0 & k[2, 4] & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & k[6, 5] & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -k[6, 5] & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -k[7, 9] & k[8, 7] \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -k[8, 7] \\ 0 & 0 & 0 & 0 & 0 & k[7, 9] & 0 & 0 \end{pmatrix}$$


```

■ ** We finally obtain our desired formula **

```

Print["YGK\Psi(x) = ", MatrixForm[Y[[1]]], MatrixForm[G], MatrixForm[K], MatrixForm[Psi]]

YGK\Psi(x) = 

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \end{pmatrix}$$



$$\begin{pmatrix} 0 & k[2, 1] & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & k[2, 3] & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & k[2, 4] & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & k[6, 5] & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & k[8, 7] & 0 & 0 \\ 0 & 0 & k[3, 2] & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & k[7, 9] & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x[2] x[5] x[6] \\ x[1] \\ x[2] \\ x[3] x[4] \\ x[2] x[4] \\ x[1] x[3] \\ x[4] \\ x[3] x[5] \\ x[3] \end{pmatrix}$$


(* The desired decomposition Y Ak \Psi(x). *)

decomposition[S]

```

$$\{\{0, 1, 0, 0, 0, 1, 0, 0, 0\}, \{1, 0, 1, 0, 1, 0, 0, 0, 0\}, \{0, 0, 0, 1, 0, 1, 0, 1, 1\},$$

$$\{0, 0, 0, 1, 1, 0, 1, 0, 0\}, \{1, 0, 0, 0, 0, 0, 1, 0\}, \{1, 0, 0, 0, 0, 0, 0, 0, 0\}\},$$

$$\{\{0, k[2, 1], 0, 0, 0, 0, 0, 0, 0\}, \{0, -k[2, 1] - k[2, 3] - k[2, 4], k[3, 2], 0, 0, 0, 0, 0, 0\},$$

$$\{0, k[2, 3], -k[3, 2], 0, 0, 0, 0, 0, 0\},$$

$$\{0, k[2, 4], 0, 0, 0, 0, 0, 0, 0\}, \{0, 0, 0, 0, 0, k[6, 5], 0, 0, 0\},$$

$$\{0, 0, 0, 0, 0, -k[6, 5], 0, 0, 0\}, \{0, 0, 0, 0, 0, 0, -k[7, 9], k[8, 7], 0\},$$

$$\{0, 0, 0, 0, 0, 0, -k[8, 7], 0\}, \{0, 0, 0, 0, 0, 0, k[7, 9], 0, 0\}\},$$

$$\{x[2] x[5] x[6], x[1], x[2], x[3] x[4], x[2] x[4], x[1] x[3], x[4], x[3] x[5], x[3]\}\}$$

(* linkageClasses takes the Laplacian of a graph (e.g. the A_k matrix in the Y A_k Φ(x)) as an input. It returns a vector with two components. The first component gives a list of all the linkage classes. For example, {1,3,4} would be a linkage class where the first, third and fourth complex participate in reactions with each other. By definition, the linkage classes are disjoint.

The second component in our output is a list of 3-tuples for each different complex in our chemical network. A 3-tuple will list all the reactions a certain complex participates in. The first vector in the 3-tuple gives the index i of a particular complex y_i . The second vector in the 3-tuple gives indices for each complex that y_i participates in a reaction with, and where y_i is an input for that reaction.

The third vector in the 3-tuple gives indices for each complex that y_i participates in a reaction with, and where y_i is an output for that reaction. For example, the 3-tuple $\{5\}, \{1,2\}, \{2,4,6\}$ means we have the reactions $y_5 \rightarrow y_1$, $y_5 \rightarrow y_2$, $y_2 \rightarrow y_5$, $y_4 \rightarrow y_5$, and $y_6 \rightarrow y_2$. *)

```
components = linkageClasses [Ak]
```

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{{{1, 2, 3, 4}, {5, 6}, {7, 8, 9}},
{{{1}, {}, {2}}, {{2}, {1, 3, 4}, {3}}, {{3}, {2}, {2}}, {{4}, {}, {2}},
{{5}, {}, {6}}, {{6}, {5}, {}}, {{7}, {9}, {8}}, {{8}, {7}, {}}, {{9}, {}, {7}}}}

```

```
Print["The number of linkage classes is ", Length[components[[1]]]]
```

The number of linkage classes is 3

(*This gives the topological deficiency of a chemical reaction network. The input is the stoichiometric matrix. *)

topDeficiency [s]

1

(* The next formula gives the chemical deficiency of a chemical reaction network. Its input is the stoichiometric matrix. *)

`matDeficiency [S]`

1

(* Another example done from scratch: t.brucei. *)

$$\left(\begin{array}{c} \mathbf{x}[38] \\ \mathbf{x}[2] \\ \mathbf{x}[1] \\ \mathbf{x}[3] \mathbf{x}[7] \\ \mathbf{x}[2] \mathbf{x}[6] \\ \mathbf{x}[4] \\ \mathbf{x}[3] \\ \mathbf{x}[5] \mathbf{x}[7] \\ \mathbf{x}[4] \mathbf{x}[6] \\ \mathbf{x}[9] \mathbf{x}[10] \\ \mathbf{x}[5] \\ \mathbf{x}[10] \\ \mathbf{x}[9] \\ \mathbf{x}[10] \mathbf{x}[24] \\ \mathbf{x}[12] \mathbf{x}[25] \\ \mathbf{x}[6] \mathbf{x}[14] \\ \mathbf{x}[7] \mathbf{x}[12] \\ \mathbf{x}[32] \\ \mathbf{x}[14] \\ \mathbf{x}[34] \\ \mathbf{x}[15] \\ \mathbf{x}[16] \mathbf{x}[17] \\ \mathbf{x}[15] \mathbf{x}[18] \\ \mathbf{x}[27] \\ \mathbf{x}[16] \\ \mathbf{x}[11] \mathbf{x}[24] \\ \mathbf{x}[9] \mathbf{x}[25] \\ \mathbf{x}[9] \mathbf{x}[21] \\ \mathbf{x}[11] \mathbf{x}[20] \\ \mathbf{x}[20] \mathbf{x}[22] \\ \frac{1}{2} \mathbf{x}[21] \mathbf{x}[23] \\ \mathbf{x}[6] \mathbf{x}[13] \\ \mathbf{x}[7] \mathbf{x}[11] \\ \mathbf{x}[39] \\ \mathbf{x}[13] \\ \mathbf{x}[26] \\ \mathbf{x}[18] \mathbf{x}[37] \\ \mathbf{x}[17] \\ \mathbf{x}[6] \mathbf{x}[8] \\ \mathbf{x}[7]^2 \\ \mathbf{x}[17] \mathbf{x}[19] \\ \mathbf{x}[18]^2 \end{array} \right)$$

The topological deficiency is 0

The matrix deficiency is 0

The linkage classes:

```

{{1, 2, 3}, {4, 5}, {6, 7}, {8, 9}, {10, 11}, {12, 13}, {14, 15}, {16, 17}, {18, 19, 20, 21}, {22, 23},
{24, 25}, {26, 27}, {28, 29}, {30, 31}, {32, 33}, {34, 35, 36}, {37, 38}, {39, 40}, {41, 42}},
{{{1}, {2, 3}, {2, 3}}, {{2}, {1}, {1}}, {{3}, {1}, {1}}, {{4}, {}, {5}}, {{5}, {4}, {}},
{6}, {7}, {7}}, {{7}, {6}, {6}}, {{8}, {}, {9}}, {{9}, {8}, {}}, {{10}, {11}, {11}},
{11}, {10}, {10}}, {{12}, {13}, {13}}, {{13}, {12}, {12}}, {{14}, {15}, {15}},
{15}, {14}, {14}}, {{16}, {17}, {17}}, {{17}, {16}, {16}}, {{18}, {19, 20}, {19, 20}},
{19}, {18}, {18}}, {{20}, {18, 21}, {18, 21}}, {{21}, {20}, {20}}, {{22}, {}, {23}},
{23}, {22}, {}}, {{24}, {}, {25}}, {{25}, {24}, {}}, {{26}, {27}, {27}},
{27}, {26}, {26}}, {{28}, {29}, {29}}, {{29}, {28}, {28}}, {{30}, {31}, {31}},
{31}, {30}, {30}}, {{32}, {33}, {33}}, {{33}, {32}, {32}}, {{34}, {35, 36}, {35, 36}},
{35}, {34}, {34}}, {{36}, {34}, {34}}, {{37}, {38}, {38}}, {{38}, {37}, {37}},
{39}, {40}, {40}}, {{40}, {39}, {39}}, {{41}, {42}, {42}}, {{42}, {41}, {41}}}}

```

(* A (too) big example *)


```
x[9] x[10]
x[6] x[14]
x[43]
x[15]
x[6] x[41]
x[7] x[42]
2 x[18] x[21] x[47]
4 x[8] x[41] x[48]
x[10]^2
x[13] x[14]
x[16] x[48] x[68]
x[11] x[18] x[47]
x[11] x[41]
x[12] x[42]
x[10] x[41] x[57]
x[14] x[39]
3 x[14] x[39] x[41]
```

```
| 4 x[10] x[42] x[57]
| x[16]
| x[17]
| x[15] x[18] x[41]
| x[8] x[39] x[55]
| 2 x[39] x[42] x[61]
| 0.5 x[41]^2 x[53] x[62]
| x[41] x[44]
| x[42] x[45]
| x[39] x[56]
| x[2]
| x[21] x[41]
| x[22] x[42]
| x[19] x[31]
| x[26]
| x[23] x[57]
| x[26] x[39]
| x[27]
| x[28]
| x[24] x[66]
| x[25] x[29]
| x[46]
| x[29] x[39]
| 2 x[29] x[41]
| 2 x[30] x[42]
| x[5] x[41] x[50]
| x[32] x[49]
| x[1] x[41] x[48]
| x[31] x[47] x[57]
| x[32] x[59]
| x[33] x[56]
| x[10] x[34] x[41] x[57]
| x[14] x[36] x[51]
| x[14] x[35] x[39]
| x[11] x[41] x[50] x[51]
| x[36] x[39] x[49]
| x[36] x[51]
| x[34] x[39]
| x[36]^2 x[49]
| x[11] x[34] x[41] x[50]
| x[36] x[41]
| x[37] x[42]
| x[16] x[50] x[64]
| x[4] x[49]
| x[39]
| x[40]
| x[11] x[16] x[50]
| x[43] x[49]
| x[38] x[66]
| x[41] x[48] x[59]
| x[44] x[47]
| x[18] x[41] x[46]
| x[81] x[381] x[391]
```

x[41] x[48] x[55]
x[46] x[47]
x[16] x[48] x[59]
x[16] x[50] x[59]
x[46] x[49]
x[42]² x[47] x[62]
x[41]³ x[48] x[61]
x[48] x[49]
x[47] x[50]
x[51]
x[52]
x[53]
x[54]
x[8] x[16] x[48]
x[18] x[47] x[59]
x[10] x[26] x[41]
x[14] x[23]
x[8] x[27]
x[18] x[59]
x[23]
x[32]
x[1] x[10]
x[3] x[14]
x[4] x[41]
x[5] x[39]
x[3]
x[41] x[57]
x[42] x[58]
x[41] x[55] x[57]
x[16] x[39] x[56]
x[10] x[16] x[56]
x[14] x[55]
2 x[13] x[41] x[56] x[57]
x[14] x[39] x[59]
x[9] x[18]
x[8] x[57]
x[14] x[59]
x[10] x[41] x[56]
x[41] x[59]
x[42] x[60]
x[69]
x[64]
x[63]
x[41]² x[66]
x[42]² x[67]
x[41] x[67]
x[42] x[66]
x[24] x[62]
x[25] x[61]
x[10] x[57] x[68]
x[14] x[18] x[66]
x[20] x[23]

```
| x[31] x[65]
| x[41]2 x[47] x[50]
| x[42]2 x[48] x[49]
| x[63] x[69]
| x[23] x[31]
| x[20] x[69]
| x[31]
| x[19]
```

The topological deficiency is 11