

The $Y A_k \Psi$ representation

This converts the stoichiometric representation $dx/dt = S v(x)$ 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
```

```
(-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)
```

```
(* matrixY takes the Stoichiometric matrix as input 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. *)
```

```
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["Ψ(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
```

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

```
Ak = G.K;
```

```
Ak // MatrixForm
```

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

■ **** We finally obtain our desired formula ****

```
Print["YGKΨ(x)= ", MatrixForm[Y[[1]]], MatrixForm[G], MatrixForm[K], MatrixForm[Psi]]
```

$$YGK\Psi(x) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

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

(* The desired decomposition Y Ak Ψ(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, 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, 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]}}
```


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


```
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[8] x[38] x[39]
```

```
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]
```

$$\left(\begin{array}{l} x[31] x[65] \\ x[41]^2 x[47] x[50] \\ x[42]^2 x[48] x[49] \\ x[63] x[69] \\ x[23] x[31] \\ x[20] x[69] \\ x[31] \\ x[19] \end{array} \right)$$

The topological deficiency is 11