Geometry of Small Chemical Reaction Networks

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Real-World Example: Rust

$$4Fe + 3O_2 \xrightarrow{\kappa_1} 2Fe_2O_3$$

$$4Fe + 3O_2 \xrightarrow{\kappa_1} 2Fe_2O_3$$

Definition

Species: type of object appearing in the network

Ex: Fe, O_2, Fe_2O_3

Definition

Complex: linear combination of species

Ex: $4Fe + 3O_2$, $2Fe_2O_3$

$$4Fe + 3O_2 \xrightarrow{\kappa_1} 2Fe_2O_3$$

Definition

Reaction: directed edge between complexes

Ex: the single reaction arrow

Definition

Reaction rate: positive parameter κ_i on reaction, describes its speed

Ex: κ_1

$$4Fe + 3O_2 \xrightarrow{\kappa_1} 2Fe_2O_3$$

Definition

Reactant complex: complex at the tail of a reaction arrow

Ex: $4Fe + 3O_2$

Definition

Support: species appearing in a complex

Ex: $\{Fe, O_2\}$, $\{Fe_2O_3\}$

Mathematical Representation

Real-World Example: Rust

$$4Fe + 3O_2 \xrightarrow{\kappa_1} 2Fe_2O_3$$

Definition

Stoichiometric matrix: represents species' net change during reactions

$$\textbf{Ex:}\ N = \begin{bmatrix} -4 \\ -3 \\ 2 \end{bmatrix} \quad \begin{matrix} Fe \\ O_2 \\ Fe_2O_3 \end{matrix}$$

Constructing an ODE System

Real-World Example: Rust

$$4Fe + 3O_2 \xrightarrow{\kappa_1} 2Fe_2O_3$$

Definition

Steady-state equations: differential equations representing species' change in concentration during reactions.

$$f_{Fe} = \frac{d}{dt} x_{Fe} = -4\kappa_1 x_{Fe}^4 x_{O_2}^3$$

$$f_{O_2} = \frac{d}{dt} x_{O_2} = -3\kappa_1 x_{Fe}^4 x_{O_2}^3$$

$$f_{Fe_2O_3} = \frac{d}{dt} x_{Fe_2O_3} = 2\kappa_1 x_{Fe}^4 x_{O_2}^3$$

Definition

Steady-state: points where the concentrations of the species are not changing over time

Formally: a tuple $(x_1, x_2, ..., x_n) \in \mathbb{R}^n$ of species concentrations such that $\frac{d}{dt}x_i$ is zero for all species i.

$$f_{Fe} = -4\kappa_1 x_{Fe}^4 x_{O_2}^3 = 0$$
$$f_{O_2} = -3\kappa_1 x_{Fe}^4 x_{O_2}^3 = 0$$
$$f_{Fe_2O_3} = 2\kappa_1 x_{Fe}^4 x_{O_2}^3 = 0$$

Steady-State Ideal and Variety

Real-World Example: Rust

$$4Fe + 3O_2 \xrightarrow{\kappa_1} 2Fe_2O_3$$

Definition

Steady-state ideal: ideal generated by the steady-state equations

Ex:

$$I = \left\langle -4\kappa_1 x_{Fe}^4 x_{O_2}^3,\ -3\kappa_1 x_{Fe}^4 x_{O_2}^3,\ 2\kappa_1 x_{Fe}^4 x_{O_2}^3 \right\rangle \subseteq \mathbb{R}[x_{Fe}, x_{O_2}, x_{Fe_2O_3}]$$

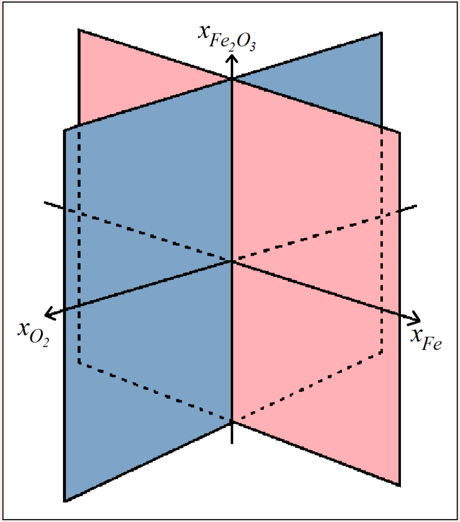
Definition

Steady-state variety: solutions to the system of steady-state equations.

Ex: $x_{Fe} = 0$, $x_{O_2} = 0$

Steady-State Variety

Real-World Example: Rust



$$f_{Fe} = -4\kappa_1 x_{Fe}^4 x_{O_2}^3 = 0$$

$$f_{O_2} = -3\kappa_1 x_{Fe}^4 x_{O_2}^3 = 0$$

$$f_{Fe_2O_3} = 2\kappa_1 x_{Fe}^4 x_{O_2}^3 = 0$$

$$x_{Fe} = 0,\ x_{O_2} = 0$$

What has useful meaning?

Definition

Positive steady-state variety: positive solutions to the system of steady-state equations.

Formally: The smallest variety containing the intersection of the steady-state variety and the interior of the positive orthant.

Ex: For rust reaction, empty.

General CRN Example

$$2A \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} A + B$$

Species: $\{A,\ B\}$

Complexes: $\{2A,\ A+B\}$

Reactions: Forward and reverse arrows

Reaction Rates: $\kappa_1,\ \kappa_2$

$$2A \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} A + B$$

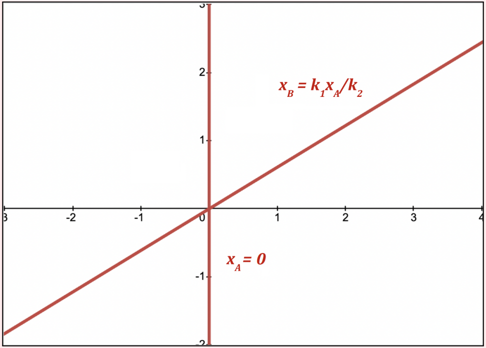
Supports: $\{A\}$ and $\{A, B\}$

Stoichiometric matrix:

$$N = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$2A \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} A + B$$

Steady-state variety:



Steady-state equations:

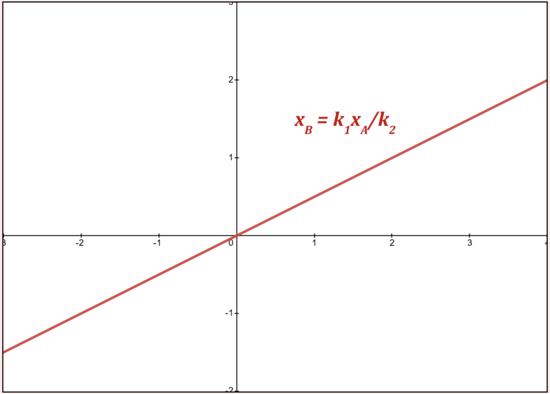
$$f_A = -\kappa_1 {x_A}^2 + \kappa_2 x_A x_B$$

$$f_B = \kappa_1 {x_A}^2 - \kappa_2 x_A x_B$$

Since $f_A = -f_B$, the zero sets overlap completely.

$$2A \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} A + B$$

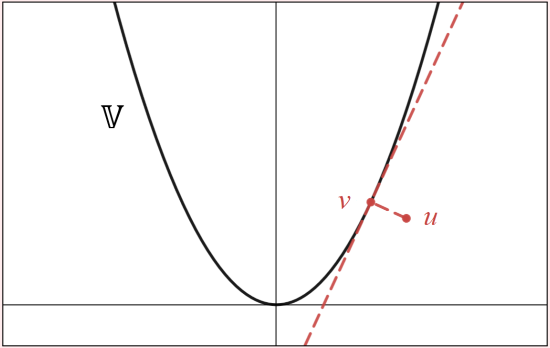
Positive steady-state variety:



Closest Point Problem

Algebraic Analysis

Motivating Question: Given an arbitrary point u, and an algebraic set $\mathbb{V}$, what's the closest point $v \in \mathbb{V}$ to u?



- $\frac{\partial}{\partial x}[d_u(v)] = \frac{(x - u_x)}{\sqrt{(x-u_x)^2 + (y-u_y)^2}}$
- $\frac{\partial}{\partial y}[d_u(v)] = \frac{(y - u_y)}{\sqrt{(x-u_x)^2 + (y-u_y)^2}}$

Definition

Singular points: places where the tangent is not well-defined, i.e. cusps and points of self-intersection.

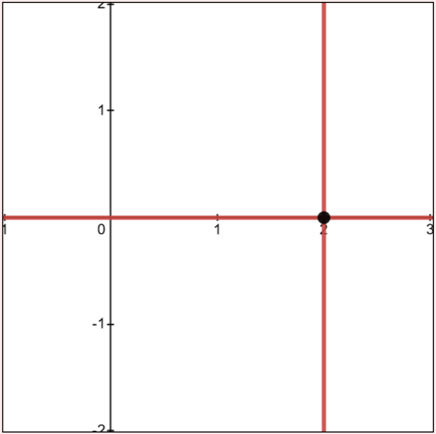
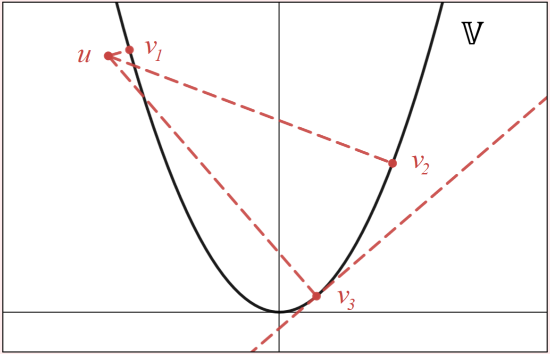


Figure: Singular point at (2,0), self-intersection

Euclidean Distance Degree

Algebraic Analysis



Definition

The ***Euclidean Distance Degree*** (EDD) is the number of non-singular critical points of the distance formula.

Ex: The EDD of a parabola is 3.

Standard Definition of an Evolute

Algebraic Analysis

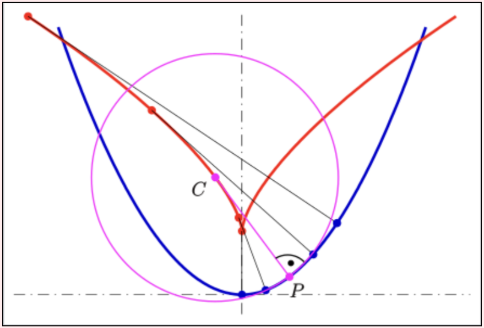
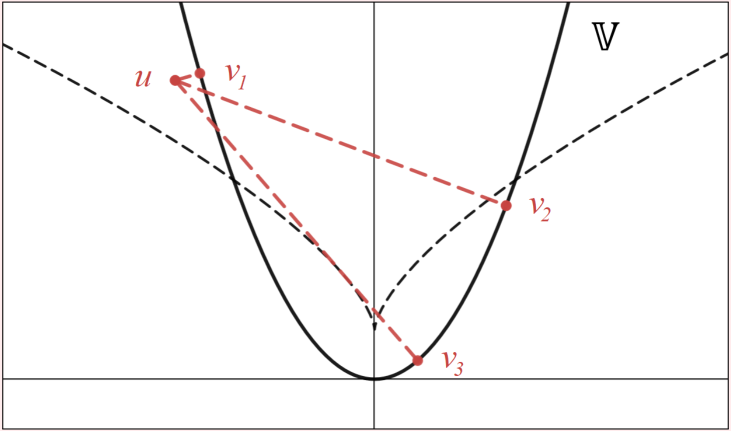


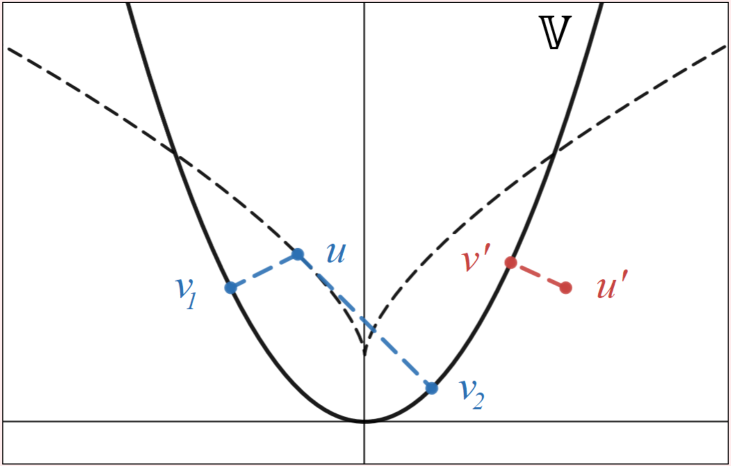
Figure: Evolute of a parabola, made from centers of curvature

Connection to EDD
Algebraic Analysis



- EDD is constant with respect to complex solutions
- Number of real solutions varies, evolute acts as a discriminant
- Divides the plane into regions with a constant number of real solutions

Connection to EDD
Algebraic Analysis



- For u on the evolute, solutions have multiplicity

Original 25 Networks

List of genuine at-most bimolecular 2-species, 2-reaction networks from a paper by Obatake, Shiu, & Sofia.

- Criteria for the 25:
  - Non-zero mixed volume
- 17 had non-empty positive steady-state varieties

	Network	Mixed vol.		Network	Mixed vol.
(1)	$2A \longrightarrow 2B \longrightarrow A+B$	2	(14)	$2A \longrightarrow A\ ,\ A+B \longrightarrow B$	1
(2)	$2A \longrightarrow 2B\ ,\ B \longrightarrow A$	2	(15)	$A+B \rightleftharpoons 0$	2
(3)	$2A \longrightarrow A\ ,\ B \longrightarrow A+B$	2	(16)	$B \longrightarrow A\ ,\ A+B \longrightarrow 2A$	1
(4)	$B \longrightarrow A\ ,\ 2A \longrightarrow A+B$	2	(17)	$0 \longrightarrow 2B\ ,\ A+B \longrightarrow A$	1
(5)	$B \longrightarrow A\ ,\ 2B \longrightarrow A+B$	1	(18)	$2B \longrightarrow 0\ ,\ A+B \longrightarrow A$	1
(6)	$2A \rightleftharpoons 2B$	2	(19)	$A+B \longrightarrow 2A \longrightarrow 2B$	1
(7)	$2A \longrightarrow A+B \longleftarrow 2B$	2	(20)	$A+B \longrightarrow 2B \longrightarrow A+B$	1
(8)	$B \longrightarrow A\ ,\ 2B \longrightarrow 2A$	1	(21)	$A+B \longrightarrow 2B\ ,\ B \longrightarrow A$	1
(9)	$B \longrightarrow 2B\ ,\ A \longrightarrow A+B$	1	(22)	$A \longrightarrow 0\ ,\ B \longrightarrow A+B$	1
(10)	$2B \longrightarrow 0\ ,\ A \longrightarrow A+B$	2	(23)	$A \rightleftharpoons B$	1
(11)	$A \rightleftharpoons 2B$	2	(24)	$A+B \longrightarrow A\ ,\ 0 \longrightarrow B$	1
(12)	$A+B \longrightarrow 2B \longleftarrow 2A$	1	(25)	$A+B \rightleftharpoons A$	1
(13)	$2A \longrightarrow A+B \longrightarrow 2B$	1			

Figure: Networks with non-zero mixed volume

Data and Findings

Original 25 Networks

	A	B	C	D	E	F	G	H	I	J	K	L
1	networks	EDD	degree	dim	weakly reversible	deficiency	dim of sing locus	shape of graph	relationship with rate constants	eqn of SS variety (xa=x, xb=y)	positive SS variety	EDD of PSSV
2	R22: A-->0, B-->A+B	1	1	1	F	1	-1	line	slope k1/k2	y= k1/k2 x	y=k1/k2 x	1
3	R23: A-->B, B-->A	1	1	1	T	0	-1	line	slope k1/k2	y= k1/k2 x	y=k1/k2 x	1
4	R9: B-->2B, A-->B+A	1	1	1	F	1	-1	line	slope -k2/k1	y= -k2/k1 x	empty	0
5	R5: B-->A, 2B-->B+A	2	2	1	F	1	-1	horizontal parallel lines	lines y=0, -k1/k2	y(k1+k2 y)=0	empty	0
6	R8: B-->A, 2B-->2A	2	2	1	F	1	-1	horizontal parallel lines	lines y=0, -k1/2k2	y(k1+2 k2 y)=0	empty	0
7	R16: B-->A, B+A-->2A	2	2	1	F	1	0	plus sign	lines y=0, x=-k1/k2	y(k1+k2 x)=0	empty	0
8	R21: A+B-->2B, B-->A	2	2	1	F	1	0	plus sign	lines y=0, x=k2/k1	y(k1 x-k2)=0	x=k2/k1 (vertical)	1
9	R25: A+B-->A, A-->A+B	2	2	1	T	0	0	plus sign	lines x=0, y=k2/k1	x(k2-k1 y)=0	y=k2/k1 (horizontal)	1
10	R12: A+B-->2B, 2A-->2B	2	2	1	F	1	0	rotated X at origin	lines x=0 and y=-2k2/k1 x	x(k1 y+2 k2 x)=0	empty	0
11	R14: 2A-->A, A+B-->B	2	2	1	F	1	0	rotated X at origin	lines x=0 and y=-k1/k2 x	x(k1 x+k2 y)=0	empty	0
12	R13: 2A-->A+B, A+B-->2B	2	2	1	F	1	0	rotated X at origin	lines x=0 and y=-k1/k2 x	x(k1 x+k2 y)=0	empty	0
13	R18: 2B-->0, B+A-->A	2	2	1	F	1	0	rotated X at origin	lines y=0 and y=-k2/2k1 x	y(2 k1 y+k2 x)=0	empty	0
14	R19: A+B-->2A, 2A-->2B	2	2	1	F	1	0	rotated X at origin	lines x=0 and y=2k2/k1 x	x(k1 y-2 k2 x)=0	y=2 k2/k1 x	1
15	R20: A+B-->2B, 2B-->A+B	2	2	1	T	0	0	rotated X at origin	lines y=0 and y=k1/k2 x	y(k1 x-k2 y)=0	y=k1/k2 x	1
16	R6: 2A-->2B, 2B-->2A	2	2	1	T	0	0	X at origin	slopes are pm sqrt(k1/k2)	y^2=k1/k2 x^2	y=sqrt(k1/k2)x	1
17	R1: 2A-->2B, 2B-->A+B	2	2	1	F	1	0	X at origin	slopes are pm sqrt(2k1/k2)	y^2=2 k1/k2 x^2	y=sqrt(2 k1/k2)x	1
18	R7: 2A-->A+B, 2B-->A+B	2	2	1	F	1	0	X at origin	slopes are pm sqrt(k1/k2)	y^2=k1/k2 x^2	y=sqrt(k1/k2)x	1
19	R2: 2A-->2B, B-->A	3	2	1	F	1	-1	parabola	through (1,2k1/k2)	y=2 k1/k2 x^2	y=2 k1/k2 x^2	3
20	R3: 2A-->A, B-->A+B	3	2	1	F	1	-1	parabola	through (1,k1/k2)	y=k1/k2 x^2	y=k1/k2 x^2	3
21	R4: B-->A, 2A-->B+A	3	2	1	F	1	-1	parabola	through (1,k2/k1)	y=k2/k1 x^2	y=k2/k1 x^2	3
22	R10: 2B-->0, A-->B+A	3	2	1	F	1	-1	sideways parabola	through (2k1/k2,1)	x=2 k1/k2 y^2	x=2 k1/k2 y^2	3
23	R11: A-->2B, 2B-->A	3	2	1	T	0	-1	sideways parabola	through (k2/k1,1)	x=k2/k1 y^2	x=k2/k1 y^2	3
24	R15: A+B-->0, 0-->A+B	4	2	1	T	0	-1	hyperbola	through (k2/k1, 1) and (-k2/k1, -1)	xy=k2/k1	xy=k2/k1	4
25	R17: 0-->2B, B+A-->A	4	2	1	F	1	-1	hyperbola	through (2k1/k2, 1) and (-2k1/k2, -1)	xy=2 k1/k2	xy=2 k1/k2	4
26	R24: A+B-->A, 0 -->B	4	2	1	F	1	-1	hyperbola	through (k2/k1, 1) and (-k2/k1, -1)	xy=k2/k1	xy=k2/k1	4
27												

- Originally focused on EDD
- Moved on to categorizing by steady-state and positive steady-state varieties

Steady-State Varieties
Original 25 Networks

Steady-state variety types:

- parallel lines, plus sign, X shape
- parabola, hyperbola

Positive steady-state variety types:

- slanted line, vertical or horizontal line, parabola, hyperbola

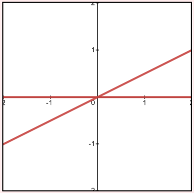


Figure: X shape

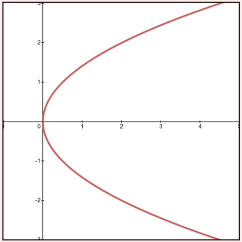


Figure: Parabola

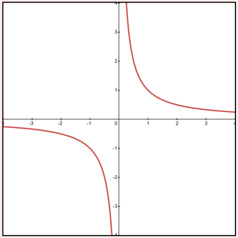


Figure: Hyperbola

Expanding Beyond 2S2R

Table enumerating CRNs

from `https://reaction-networks.net/networks/`

Table 2: Genuine networks (no unused species)

	1 Reaction	2 Reactions	3 Reactions	4 Reactions	5 Reactions	6 Reactions	Total
1 Species	6	15	20	15	6	1	63
2 Species	10	210	2,024	13,740	71,338	297,114	384,436
3 Species	5	495	17,890	414,015	7,262,666 (zip: 12.5 MB, unzip: 473 MB)	103,511,272 (zip: 197 MB, unzip: 7.97 GB)	111,206,343
4 Species	1	451	47,323	2,900,934	128,328,834 (zip: 196 MB, unzip: 8.88 GB)		131,277,543
5 Species	0	204	55,682	7,894,798 (zip: 10.6 MB, unzip: 466 MB)			7,950,684
6 Species	0	54	35,678	10,704,289 (zip: 15.1 MB, unzip: 650 MB)			10,740,021
Total	22	1,429	158,617	21,927,791	135,662,844	103,808,387	261,559,090

1-species networks, 3S2R, 2S2R with higher molecularity

Rate-Dependent Varieties

$$A \xrightarrow{\kappa_1} 2A$$

$$A \xrightarrow{\kappa_2} 0$$

$$2A \xrightarrow{\kappa_3} 0$$

Steady-state equation:

$$\begin{aligned} f_A &= \kappa_1 x_A - \kappa_2 x_A - 2\kappa_3 x_A^2 \\ &= x_A(\kappa_1 - \kappa_2 - 2\kappa_3 x_A) \end{aligned}$$

Steady-state variety:

$$x_A = 0,\ x_A = \frac{\kappa_1 - \kappa_2}{2\kappa_3}$$

Positive steady-state variety nonempty when $\kappa_1 > \kappa_2$

Coming Back with a Broader Perspective

Expanding Beyond 2S2R

- How can we categorize these steady-state varieties using the new info we have?
- Is mixed volume the best way to determine which networks have positive steady-state varieties?
- Applying code developed with larger databases to solve computational problems in 2S2R

Let's check all 210 chemical reaction networks!

Translation Algorithm

- All 210 networks were listed as strings of numbers in a .txt file
- first digit, m, is the number of reactions
- second digit, n, is the number of species
- all numbers after are listed as pairs
- here, we have $m, n = 2$, and 4 pairs after

$$2203032121$$

Networks were derived from the database at *https://reaction-networks.net/networks/.*

Translation Algorithm

$$2203032121$$

- Our string, omitting the m & n entries, is described by the set
$$H = \{0, 1, 2, 3\}$$
- The pairs are made of one *species number* and one *reaction number*.
  - These numbers are all entries, h_i, in H
  - Reaction numbers: $0 \leq h_i \leq m - 1$
  - Species numbers: $m \leq h_i \leq m + n - 1$
- Here, the set of reaction and species numbers are
$$R = \{0, 1\},\ S = \{2, 3\}.$$

Translation Algorithm

$$2203032121$$

- Individual reactions and species are labeled sequentially.
  - $R = \{0, 1\} \Rightarrow r_0, r_1$ are our reactions
  - $S = \{2, 3\} \Rightarrow 2 = A = s_1$, $3 = B = s_2$
- The ordering of r_i, s_i in a pair tells you if s_i is in the product or reactant complex.
  - $(s_i, r_i) \Rightarrow s_i$ is in the reactant complex
  - $(r_i, s_i) \Rightarrow s_i$ is in the product complex

Example: $(0, 3)$ is (r_0, s_2), and $(2, 1)$ is (s_1, r_1) which becomes

$$(0, 3) : \longrightarrow B$$

$$(2, 1) : A \longrightarrow$$

Translation Algorithm

$$2203032121$$

- In this network, the pairs $(0,3)$ and $(2,1)$ have multiplicity 2
- So, "multiply" these reactions each by 2
- Combine like reactions, "adding" complexes.

$$(0,3) : \longrightarrow B$$

$$(0,3) : \longrightarrow B$$

$$(2,1) : A \longrightarrow$$

$$(2,1) : A \longrightarrow$$

$$0 \longrightarrow 2B$$

$$2A \longrightarrow 0$$

Now add the respective reaction rates κ_1, κ_2:

$$0 \xrightarrow{\kappa_1} 2B$$

$$2A \xrightarrow{\kappa_2} 0$$

Further Coding and Calculations

- Made a function, called superEDD, to compute various qualities
  - EDD, codim(I), deg(I), generators and dimensions of the singular locus, steady-state equations
- Noticed errors whenever the ideal was equal to the entire plane.
  - correspond to empty steady-state varieties
- Graphed and recorded all of the other networks.

New Steady-State Varieties

Among the rest of the 210 networks, four new steady-state variety classes emerged:

1. Empty
2. The origin
3. Single coordinate axis
4. Both coordinate axes

Only one of the 185 new reactions had a nonempty positive steady-state variety.

Positive Steady-State Varieties

There are four possible shapes of a nonempty positive steady-state variety:

1. Horizontal/vertical line
2. Line through the origin
3. Parabola
4. Hyperbola

We proved classifications of all networks producing each type of variety.

Lines
Positive Steady-State Varieties

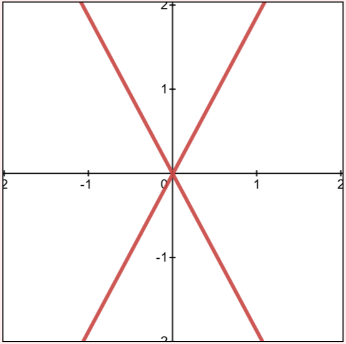


Figure: Line through origin

$$2A \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} 2B$$

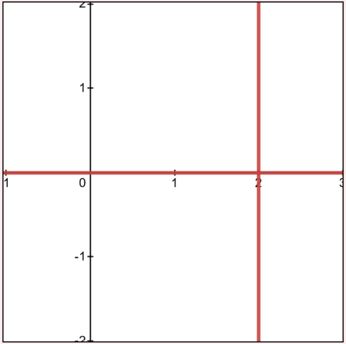


Figure: Vertical line

$$B \xrightarrow{\kappa_1} 2B$$

$$A + B \xrightarrow{\kappa_2} A$$

Degree 2 Conics

Positive Steady-State Varieties

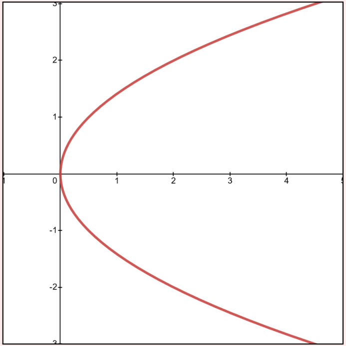


Figure: Parabola

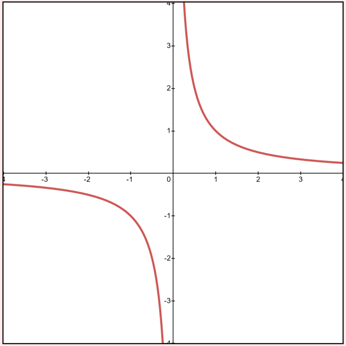


Figure: Hyperbola

$$A \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} 2B$$

$$A + B \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} 0$$

Horizontal/Vertical Lines

Looking for Patterns

$$A + B \xrightarrow{\kappa_1} 2B$$
$$B \xrightarrow{\kappa_2} A$$

$$N = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$A + B \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} A$$

$$N = \begin{bmatrix} 0 & 0 \\ -1 & 1 \end{bmatrix}$$

Horizontal/Vertical Lines

Categorization Theorem

Theorem (F_2H_2, 2023)

Given a chemical reaction network, the positive steady-state variety will be non-axis horizontal or vertical line if and only if the following criteria are true:

1. *One reactant complex is $A + B$ and the other is monomolecular*
2. *The columns of the stoichiometric matrix are negative multiples of one another.*

Horizontal/Vertical Lines

Worked Example

$$A + B \xrightarrow{\kappa_1} 2B$$
$$B \xrightarrow{\kappa_2} A$$

- Reactant complexes are $A + B$ and B

$$N = \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}$$

- The columns differ by a factor of -1

$$f_A = -\kappa_1 x_A x_B + \kappa_2 x_B$$
$$f_B = \kappa_1 x_A x_B - \kappa_2 x_B$$

- $f_A = -f_B$

$$x_B = 0, \; x_B = \frac{\kappa_2}{\kappa_1}$$

- Positive portion of the variety is a vertical line

Three examples of slanted line networks:

$$A + B \xrightarrow{\kappa_1} 2A$$
$$2A \xrightarrow{\kappa_2} 2B$$

$$N = \begin{bmatrix} 1 & -2 \\ -1 & 2 \end{bmatrix}$$

$$A \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} B$$

$$N = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$2A \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} 2B$$

$$N = \begin{bmatrix} -2 & 2 \\ 2 & -2 \end{bmatrix}$$

Slanted Lines
Categorization Theorem

Theorem (F_2H_2, 2023)

Given a chemical reaction network, the positive steady-state variety will be a line through the origin if and only if the following hold:

1. *The two reactant complexes have the same number of molecules*
2. *The supports of the reactant complexes are nonempty and distinct (not necessarily disjoint).*
3. *The columns of the stoichiometric matrix are negative multiples of each other.*

Slanted Lines

Worked Example

$$A + B \xrightarrow{\kappa_1} 2A$$
$$2A \xrightarrow{\kappa_2} 2B$$

$$N = \begin{bmatrix} 1 & -2 \\ -1 & 2 \end{bmatrix}$$

$$f_A = \kappa_1 x_A x_B - 2\kappa_2 x_A^2$$
$$f_B = -\kappa_1 x_A x_B + 2\kappa_2 x_A^2$$

$$x_A = 0, \; x_B = \frac{2\kappa_2}{\kappa_1} x_A$$

- Reactant complexes have the same number of molecules and distinct supports
- Columns differ by a factor of -2
- $f_A = -f_B$
- Positive portion of the variety is a slanted line

Three examples of parabola networks:

$$2A \xrightarrow{\kappa_1} A \qquad B \xrightarrow{\kappa_2} A + B \qquad N = \begin{bmatrix} -1 & 1 \\ 0 & 0 \end{bmatrix}$$

$$2B \xrightarrow{\kappa_1} 0 \qquad A \xrightarrow{\kappa_2} A + B \qquad N = \begin{bmatrix} -2 & 1 \\ 0 & 0 \end{bmatrix}$$

$$2A \xrightarrow{\kappa_1} 2B \qquad B \xrightarrow{\kappa_2} A \qquad N = \begin{bmatrix} -2 & 1 \\ 2 & -1 \end{bmatrix}$$

Theorem (F_2H_2, 2023)

Given a chemical reaction network, the positive steady-state variety will be a parabola if and only if the following hold:

1. *One reactant complex is bimolecular and the other is monomolecular*
2. *The supports of the reactant complexes are disjoint*
3. *The columns of the stoichiometric matrix are negative linear multiples of each other.*

Parabolas

Worked Example

$$2A \xrightarrow{\kappa_1} 2B$$

$$B \xrightarrow{\kappa_2} A$$

$$N = \begin{bmatrix} -2 & 1 \\ 2 & -1 \end{bmatrix}$$

$$f_A = -2\kappa_1 x_A^2 + \kappa_2 x_B$$
$$f_B = 2\kappa_1 x_A^2 - \kappa_2 x_B$$

$$x_B = \frac{2\kappa_1}{\kappa_2} x_A^2$$

- Supports of the reactant complexes are disjoint; bimolecular & monomolecular.
- Columns differ by a factor of -2
- $f_A = -f_B$
- Variety is defined by the equation of a parabola

All hyperbola networks:

$$0 \xrightarrow{\kappa_1} 2B$$
$$A + B \xrightarrow{\kappa_2} A$$

$$N = \begin{bmatrix} 0 & 0 \\ 2 & -1 \end{bmatrix}$$

$$A + B \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} 0$$

$$N = \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}$$

$$A + B \xrightarrow{\kappa_1} A$$
$$0 \xrightarrow{\kappa_2} B$$

$$N = \begin{bmatrix} 0 & 0 \\ -1 & 1 \end{bmatrix}$$

Theorem ($F_2 H_2$, 2023)

Given a chemical reaction network, the positive steady-state variety will be a hyperbola if and only if the following hold:

1. *The reactant complexes are* $A + B$ *and* 0
2. *The columns of the stoichiometric matrix are negative linear multiples of each other.*

Hyperbolas

Worked Example

$$A + B \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} 0$$

- Reactant complexes are $A + B$ and 0

$$N = \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}$$

- Columns differ by a factor of -1

$$f_A = -\kappa_1 x_A x_B + \kappa_2$$
$$f_B = -\kappa_1 x_A x_B + \kappa_2$$

- $f_A = f_B$

$$x_A x_B = \tfrac{\kappa_2}{\kappa_1}$$

- Variety is defined by the equation of a hyperbola

Future Directions - Higher Molecularity

Conjecture

For slanted lines:

Molecularity of distinct supports is even $\Rightarrow$ *2 lines in SSV*

odd $\Rightarrow$ *1 line in SSV*

Conjecture

For horizontal/vertical lines:

Molecularity of non-shared reactant species is:

even $\Rightarrow$ *0, 2 lines in SSV*

odd $\Rightarrow$ *1 line in SSV*

Ex:

$$2A + 2B \xrightarrow{\kappa_1} 3A + B$$

$$2B + A \xrightarrow{\kappa_2} 3B$$

Future Directions - Higher Molecularity

Conjecture

The variety types of networks only depend on reactant complexes, as long as columns of stoichiometric matrix are negative multiples of each other

$$2A + 2B \xrightarrow{\kappa_1} 3A + B \qquad 2A + 2B \xrightarrow{\kappa_1} B$$

$$2B + A \xrightarrow{\kappa_2} 3B \qquad 2B + A \xrightarrow{\kappa_2} 3A + 3B$$

Future Directions - Larger Networks

Table 2: Genuine networks (no unused species)

	1 Reaction	2 Reactions	3 Reactions	4 Reactions	5 Reactions	6 Reactions	Total
1 Species	6	15	20	15	6	1	63
2 Species	10	210	2,024	13,740	71,338	297,114	384,436
3 Species	5	495	17,890	414,015	7,262,666 (zip: 12.5 MB, unzip: 473 MB)	103,511,272 (zip: 197 MB, unzip: 7.97 GB)	111,206,343
4 Species	1	451	47,323	2,900,934	128,328,834 (zip: 196 MB, unzip: 8.88 GB)		131,277,543
5 Species	0	204	55,682	7,894,798 (zip: 10.6 MB, unzip: 466 MB)			7,950,684
6 Species	0	54	35,678	10,704,289 (zip: 15.1 MB, unzip: 650 MB)			10,740,021
Total	22	1,429	158,617	21,927,791	135,662,844	103,808,387	261,559,090

Figure: There remains a lot left to explore...

Thank you Professor Luis & Mark!

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