Geometry of Small Chemical Reaction Networks

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Pomona Research in Mathematics Experience (PRiME)

Abstract

Chemical reaction networks are used to model interactions between sets of objects called species. The theory is based in traditional chemistry, however, it has applications to mathematical biology and pattern formation.

Our studies were focused on how these objects form steady-state ideals after being turned into systems of ordinary differential equations. From there we created classifications of each distinct positive steady-state variety form. This project was done as a part of the Pomona Research in Mathematics Experience (DMS-2113782).

Definitions

Given a **chemical reaction network**, G, we can describe it in terms of species, reactions, and complexes. For the network below, our species are A, B, C while the complexes are $A+C$, $B+C$, and $2B$.

$$A+C \xrightarrow{\kappa_1} B+C \underset{\kappa_3}{\overset{\kappa_2}{\rightleftarrows}} 2B$$

Edges representing reactions are drawn as arrows, with their positive reaction rates written as κ_i.

Steady-State Equations: ordinary differential equations representing species' change in concentration during reactions.
Steady-State: 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.
Positive Steady-State Variety: the smallest variety containing the intersection of the steady-state variety and the interior of the positive orthant.

Motivating Question

How can we formally classify all positive steady-state varieties of genuine, at-most-bimolecular, 2-species, 2-reaction networks?

Looking for Patterns

For clarity, we will explain how to find the steady-state variety of a network with this example.

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

We construct each steady-state equation to equal the change in concentration of a species in the network. They have one term per reaction in the network, and the monomials are composed by the reaction complex. Here, f_A has coefficient $2\kappa_1$ since it has a net change of 2 across the reaction. Thus,

$$\frac{dx_A}{dt} = f_A = 2\kappa_1 x_B^2 + \kappa_2 x_B$$
$$\frac{dx_B}{dt} = f_B = -2\kappa_1 x_B^2 - \kappa_2 x_B$$

We find the steady-state variety by calculating the solutions to $f_A, f_B = 0$. In this case, it is $x_B = 0, \frac{-\kappa_2}{2\kappa_1}$.

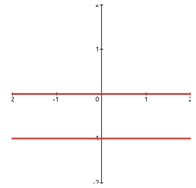

Figure: Steady-State Variety

Since $\kappa_1, \kappa_2 \neq 0$, these lines will never intersect for any reaction-rate values and will also never cross the axis.

Despite its nonempty steady-state variety, this network has an empty positive-steady state variety as neither component intersects the positive orthant. This relationship is essential for the results of this project.

For contrast, consider the network $A+B \underset{\kappa_2}{\overset{\kappa_1}{\rightleftarrows}} 0$ which will have terms of the form $x_A x_B$ plus a constant, creating a hyperbola. Since it consists of a single component, the whole figure composes the positive steady-state variety.

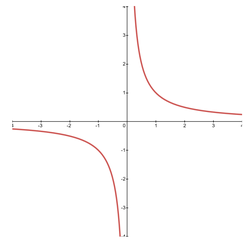

Figure: Hyperbolic Positive Steady-State Variety

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

Our project is closely tied with applications to not only chemical but other biological processes, and in these contexts having negative values does not make sense. Hence, our focus on the positive steady-state variety.

Results

After studying all 210 genuine, at-most-bimolecular, 2-species, 2-reaction networks, the following theorems were created to classify the positive steady-state variety of each network based on the chemical reaction network's properties.

Horizontal & Vertical Lines ($F_2H_2, 2023$)

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

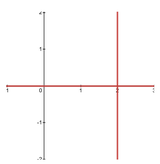

Figure: Steady-State Variety

A Vertical Line Network:

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

Steady-State Equations:

$$f_A = 0$$
$$f_B = \kappa_1 x_B - \kappa_2 x_A x_B$$

Theorem on Slanted Lines ($F_2H_2, 2023$)

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

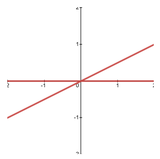

Figure: Steady-State Variety

A Slanted Line Network:

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

Steady-State Equations:

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

Theorem on Parabolas ($F_2H_2, 2023$)

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

Proof Outline (Forwards Direction)

Let x, y represent x_A, x_B, then we have $V(y-kx^2) = V(f_A) \cap V(f_B)$. Since G is at-most-bimolecular, $\Rightarrow \deg(f_A), \deg(f_B) \leq 2$, and

$$f_A = c_1(y - kx^2)$$
$$f_B = c_2(y - kx^2)$$

With x^2, y exactly $\Rightarrow G$ must have a bimolecular complex and a monomolecular complex which are disjoint (1), (2). When neither $c_1, c_2 \neq 0$, $f_B = \frac{c_2}{c_1} f_A$. From these equations,

$$f_A = ak_1 y - bk_2 x^2$$
$$f_B = ck_1 y - dk_2 x^2$$

we can make the matrix N

$$\det N = \det \begin{pmatrix} a & -b \\ c & -d \end{pmatrix} = -ad + bc = -a\left(\frac{c_2}{c_1}b\right) + b\left(\frac{c_2}{c_1}a\right) = 0.$$

With $\det N = 0$, the columns must be negative linear multiples (3).

Parabola Network Example:

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

Steady-State Equations:

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

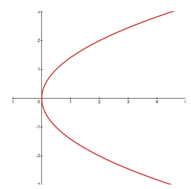

Figure: Positive Steady-State Variety

Theorem on Hyperbolas ($F_2H_2, 2023$)

Given any chemical reaction network, the positive steady-state variety will be a hyperbola if and only if all of 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.

Future Work

- Investigating and classifying other types of chemical reaction networks, especially the following:
  - not at-most bimolecular networks
  - 3-species, 2-reaction networks
  - n-species and higher networks where n is at least 4
- Considering other applications of these techniques, such as complicated biochemical reactions.

References

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Acknowledgements

We would like to thank:

- Our research advisor Dr. Luis David Garcia Puente
- Dr. Edray Goins, Dr. Alex Barrios, and our fellow PRiME participants
- PRiME 2023 and those who made it possible

Research at PRiME was supported by the National Science Foundation award DMS-2113782. Any opinions, findings, and conclusions or recommendations expressed in this poster are those of the authors and do not necessarily reflect the views of the National Science Foundation.