# The Geometry of Small Chemical Reaction Networks

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## 1 Introduction

Chemical Reaction Network Theory is a branch of mathematics concerned with the modeling of real-world chemical systems. It can also be applied to other systems where objects come together and interact to produce new materials, but the language focuses on applications to chemistry. This area of applied mathematics relies in part on algebraic geometry to better understand the underlying structure of chemical reaction networks. Within this field, these networks are primarily classified according to the total number of species and reactions. Our motivation in conducting this research is to outline and prove a classification system for the positive steady-state varieties of two-species, two-reaction, genuine, at-most-bimolecular chemical reaction networks. Beyond this main result, the report also provides background information on chemical reaction network theory and algebraic geometry, and explores several potential avenues for analyzing chemical reaction networks.

Foremost within the report is the foundational information within chemistry and algebraic geometry upon which our research is based. When attempting to model chemical systems, it is essential to first know some chemical terminology, standard chemistry assumptions, and the general method for graphical modeling of chemical reaction networks. Equally foundational to this research is the algebraic geometry of the mathematical representations of these networks. To create these models, we make assumptions regarding the relationship between the final product and the initial chemical make-up of the system. Here we assume mass-action kinetics, which provides a clear way to construct systems of differential equations from the networks, whose equilibria are used to construct the steady-state varieties of these chemical reaction networks. These equations describe the change in different chemical species with respect to time, and are explained more formally later, along with their other algebraic properties. The equations have visual translations which provide qualitative information about the chemical reaction networks through their geometric characteristics.

Beyond background information, this report covers several algebraic tools that we sought to use to analyze chemical reaction networks. While not all of these tools directly resulted in the main classification theorems, all of them furthered our understanding of the these chemical reaction networks beyond their graphical representations.

One of our initial attempts at classification involved the algebraic analysis of the chemical reaction networks. With the aid of the Macaulay2 software, we calculated various properties of these networks including the degree and dimension of the steady-state and positive steady-state ideals, and the Euclidean distance degree of the steady-state and positive steady-state varieties. These properties aided in our understanding of the networks, but ultimately did not form the basis of the theorems. We explored a few additional areas as well; firstly, the topic of evolutes and how this method of analysis stemmed naturally from our previous algebraic study of the Euclidean

distance degree. Additionally, we investigated mixed volume as a property of chemical reaction networks. While not studied in depth, the mixed volume acts as an upper bound on the number of positive steady-states in most cases, and allowed us to disregard irrelevant networks which had an empty positive steady-state variety. The exact cases in which mixed-volume doesn't provide an accurate upper bound of positive steady-state varieties is also covered briefly, since the details of mixed volume are beyond the scope of our work.

Another attempt at classification was a more geometric approach through the computation of the equation and shape of the steady-state and positive steady-state varieties. This analysis eventually led to the classification theorems, which describe the positive steady-state variety of a reaction network without needing to generate its steady-state equations. We prove the criteria necessary for a network to exhibit each of the four possible non-empty positive steady-state varieties. Additionally, we calculated the same properties for all one-species networks with at most six reactions.

All of the essential Macaulay2 code, along with a spreadsheet of our calculated data, is attached at the end of this report. The thought process behind some of these algorithms is in section 6, *Species Reaction Graphs*, with an example.

# 2 Chemical Reaction Networks

Chemical reaction networks are used to model interactions between sets of objects called *species*. The theory borrows language used in a traditional chemistry course, often describing networks in terms of species, complexes, and the reactions between them. However, chemical reaction networks can model more general phenomena such as biochemical interactions, pattern formation, or disease ecology. Following the formal definition given in [5], we can define a network via its sets of components. A *chemical reaction network* $G = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ is made up of three finite sets. First, a set of species $\mathcal{S} = \{A_1, A_2, \dots A_s\}$, which correspond to the molecules present in a reaction. Second, a set of complexes $\mathcal{C} = \{y_1, y_2, \dots, y_p\}$, which are finite, non-negative, integer combinations of the species. Finally, a set of reactions $\mathcal{R} \subseteq (\mathcal{C} \times \mathcal{C}) \setminus \{(y, y) | y \in \mathcal{C}\}$, which are non-diagonal ordered pairs of complexes. As with typical reactions studied in chemistry, these networks are represented by the set of directed edges between complexes, seen in the following example:

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

Complexes at the tail of a reaction arrow are referred to as *reactant complexes*. Complexes at the head of a reaction arrow are called *product complexes*. In this example, $\{A, B, C\}$ is the set of species, $\{A+C, B+C, 2B\}$ is the set of complexes, and $\{A+C \to B+C, B+C \to 2B, 2B \to B+C\}$ is the set of reactions. In addition to these three sets we define the *reaction rates*, one for each reaction, called $\kappa_1$, $\kappa_2$, and $\kappa_3$ above. The $\kappa_i$ are positive, real parameters and can be thought to govern the relative speed of the reactions. In this paper, the main object of study is a set of differential equations describing the change in amount, or concentration, of the species over time. We will use the notation $x = (x_A, x_B, x_C)$ where $x_A$ refers to the concentration of $A$ at a given

time $t$. Then, we generate the system

$$\begin{aligned} f_A &= \frac{d}{dt}x_A = -P_{A+C\to B+C}(x) \\ f_B &= \frac{d}{dt}x_B = P_{A+C\to B+C}(x) + P_{B+C\to 2B}(x) - P_{2B\to B+C}(x) \\ f_C &= \frac{d}{dt}x_C = -P_{B+C\to 2B}(x) + P_{2B\to B+C}(x) \end{aligned}$$

where $P$ is a stand in for the eventual terms of our equation and $f_A$ refers to the change in concentration of $A$ with respect to time $t$. The coefficients are determined by how the concentration of $A$ changes throughout the reactions. Here we see that the coefficient is $-1$ for $P_{A+C\to B+C}(x)$ because as the reaction $A + C \to B + C$ proceeds, it consumes one unit of $A$. Likewise, the other coefficients are 0 since $A$ is not involved in the other reactions. While a helpful demonstrator, these equations are limited in their use. Following the assumption of mass action kinetics, polynomial equations are instead used in the modeling of chemical systems. Mass action kinetics is a chemical proposition dictating that the output of products is proportional to the product of the reacting species' concentrations [2]. Thus, our stand in function amounts would be defined as a product of the corresponding reactant complex and rate constant. In our example, this implies that reactions stemming from $A + C$ are proportional to the monomial $x_A x_C$. Applying this to all equations modeling our network yields the *steady-state equations* of the network shown below:

$$\begin{aligned} f_A &= -\kappa_1 x_A x_C \\ f_B &= \kappa_1 x_A x_C + \kappa_2 x_B x_C - \kappa_3 x_B^2 \\ f_C &= -\kappa_2 x_B x_C + \kappa_3 x_B^2 \end{aligned}$$

These general dynamic equations are of the form

$$f(x) = \begin{Bmatrix} f_A(x) \\ f_B(x) \\ f_C(x) \end{Bmatrix}$$

where $f(x) = N\cdot \operatorname{diag}(k) \cdot x^B$. Here, $N$ denotes the *stoichiometric matrix*, where the columns correspond to reactions, the rows correspond to species, and the entries are $y_j - y_i$ whenever $y_i \to y_j$ is a reaction. For our example,

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

which mimics our set of equations $f$. Following that, we have

$$\operatorname{diag}(k) = \begin{bmatrix} \kappa_1 & 0 & 0 \\ 0 & \kappa_2 & 0 \\ 0 & 0 & \kappa_3 \end{bmatrix}$$

as the diagonal matrix of reaction rates and

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

as the reactant matrix in which the column entries are $y_i$ whenever $y_i \to y_j$ is a reaction. Thus,

$$X^B = \begin{bmatrix} x^{b_1} \\ x^{b_2} \\ x^{b_3} \end{bmatrix} = \begin{bmatrix} x_A^1 & x_B^0 & x_C^1 \\ x_A^0 & x_B^1 & x_C^1 \\ x_A^0 & x_B^2 & x_C^0 \end{bmatrix}$$

has row entries which represent the terms and their respective powers as monomials for each complex. Using this intuition of representing chemical reaction networks as a system of polynomial equations, we introduce an important definition:

**Definition 1.** A *steady-state* of a system $f$ is any point $x$ such that $f(x) = 0$.

In other words, we can think of a steady-state as a point at which none of the species' concentrations are changing. Intuitively, at a steady-state, the network is like a bathtub with water flowing in and out at the same rate. The water is still flowing, and the reactions are still proceeding, but their relative rates mean that the water level, or the concentrations, remain unchanged. This establishes two additional definitions:

**Definition 2.** A *steady-state ideal* is an ideal generated by the steady-state equations of a reaction network, or the ideal

$$I = \langle f \rangle = \langle f_A, f_B, f_C, \dots \rangle \subseteq \mathbb{R}[x]$$

**Definition 3.** A *steady-state variety* is the variety of a steady-state ideal $I = \langle f \rangle$ or the set

$$V(I) = \{x \in \mathbb{R}^s | f(x) = 0\},$$

where $s$ is the number of species in the reaction network.

When looking at steady-states with useful biological meaning, we disregard those with non-positive concentrations, leading to another definition:

**Definition 4.** A *positive steady-state variety* is the smallest variety containing the intersection of $V(I)$ with the interior of the positive orthant of $\mathbb{R}^s$.

**Example 1.** Consider the reaction network

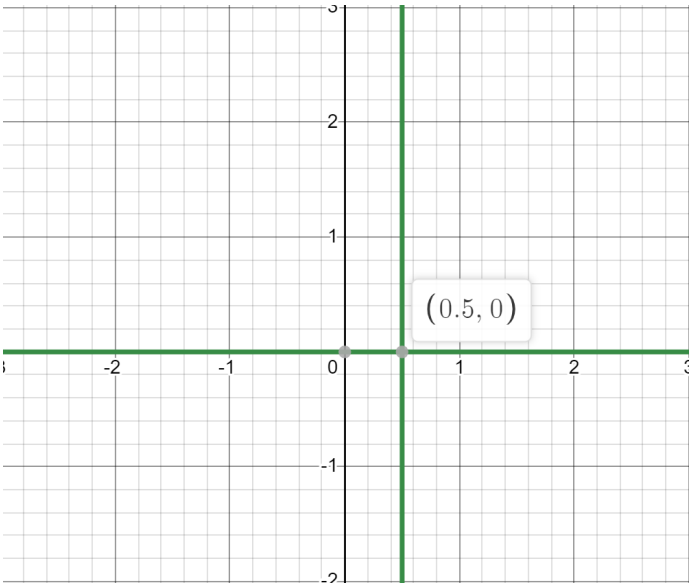
$$B \xrightarrow{\kappa_1} 2B$$
$$A + B \xrightarrow{\kappa_2} A$$

The steady-state equations are then given by

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

When solving for the variety we get $\kappa_1 x_B - \kappa_2 x_A x_B = 0$, factoring to $x_B(\kappa_1 - \kappa_2 x_A) = 0$ as the equation defining the steady-state variety. Thus $x_B = 0$ and $x_A = \frac{\kappa_1}{\kappa_2}$ are the two components

of the variety. Only $x_A = \frac{\kappa_1}{\kappa_2}$ is in our positive steady-state variety since it is a vertical line that intersects the interior of the positive orthant. The line $x_B = 0$ is not included since the x-axis does not intersect the interior of the positive orthant. To illustrate, setting $k_1 = 1, k_2 = 2$, we obtain the graph:




The entire line $x_A = \frac{1}{2}$ is included in the positive steady-state variety, even though it contains points with non-positive concentrations, since it is the smallest variety containing the intersection of the steady-state variety with the positive orthant.

# 3 Introduction to Euclidean Distance Degree (EDD)

The Euclidean Distance degree of a variety was first defined in [3], and measures the algebraic complexity of solving the nearest-point problem. In other words, if we have some variety $V \subseteq \mathbb{R}^n$ and we pick some generic point $u$, the EDD describes how difficult it is to calculate the point $x \in V$ with the minimal Euclidean distance to $u$. Before examining the Euclidean Distance Degree in detail, we introduce some notation used in this paper:

- $V$ will denote a *variety*
- $I$ will denote an *ideal*
- $J_f(x)$ will denote the Jacobian matrix of $f$ with respect to the variables $x$
- $r$ will denote the *maximal rank* of a Jacobian matrix
- $T_x$ will denote the *tangent space* of a curve at a the point $x$

The Euclidean Distance Degree of a variety builds upon a foundational understanding of several topics. We will examine these topics individually, providing both an intuitive explanation and

mathematical definitions for each, before finally defining Euclidean Distance Degree. The first foundational concept is the singular point. In the context of curves in the plane, singular points may be thought of as cusps and points of self-intersection. Although our definition allows for abstraction beyond this specific context, the visual intuition will be foundational later when rigorously defining singular points and their relationship to tangent lines.

Given an ideal $I$ and an arbitrary complex polynomial $f_i \in C[x_1, \ldots, x_n]$, let us compile all potential $f_i$ to a single map $f$:

$$f : \mathbb{C}^n \to \mathbb{C}^s; f(x) = (f_1(x), f_2(x), \ldots, f_s(x))$$

Note, $x$ is any combination of the variables $(x_1, \ldots, x_n)$. Thus, given $n$ variable inputs, our new function $f$ outputs the $s$ - dimensional vector composed of our respective function outputs. Examine the Jacobian matrix of $f$ constructed below:

$$J_f(x) = \begin{bmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_s(x) \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1(x)}{\partial x_1} & \cdots & \frac{\partial f_1(x)}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_s(x)}{\partial x_1} & \cdots & \frac{\partial f_s(x)}{\partial x_n} \end{bmatrix}$$

From this we can formulate the following definition:

**Definition 5.** Let $X$ be a variety. A point $x \in X$ is *regular* if the rank of $J_f(x)$ is maximal. Otherwise, the point is *singular*.

A non-maximal rank in the Jacobian of $f$ indicates linear dependence between rows or columns. This builds upon our intuition from earlier which suggested that a singular point $x$ would have a poorly defined tangent, or more rigorously, result in a non maximal rank of $J_f(x)$. Checking linear dependence between columns and rows can be accomplished by comparing the ratios of columns to one another. Through algebraic manipulation, this corresponds to checking the $r \times r$ minors of the matrix where $r$ is the generic rank of $J_f$. If the generic rank of the Jacobian is maximal, the majority of points $x \in X$ are regular; that is, the rank of $J_f(x)$ is maximal for all $x \in X$ except for points in a set of Lebesgue measure zero. For these problematic points, the rank of $J_f(x)$ will be non-maximal. If the $r \times r$ minors are all zero for some point $x$, then the rank of the Jacobian evaluated at $x$ is strictly less than $r$, meaning that $x$ is a singular point.

Now that we have defined singular points and found a way to identify them, we may compile them into a single mathematical object.

**Definition 6.** The *singular locus* of an ideal $I$ is the collection of all singular points in $V(I)$ and will be denoted as $X_{sing}$. The singular locus is the variety of the ideal

$$I_{sing} = (f_1, f_2, \ldots, f_s, \{r \times r \text{ minors of } J_f\}).$$

In other words, our singular locus is defined as the variety of the ideal generated not only by our polynomial set, but also by every $r \times r$ minor, thereby restricting the variety to contain only the singular points of the curve. Our singular locus, in turn, helps us define something called the *tangent space* of a function at a point.

**Proposition 7.** *When $f_i \in \mathbb{R}[x_i, \ldots, x_n]$. The tangent space $T_x(X \setminus X_{sing})$ is given by the kernel of $J_f(x)$*

$$T_x(X \setminus X_{sing}) = ker J_f(x)$$

More specifically, since the Jacobian matrix of $f$ is composed of gradients, this matrix is defined by the its rows of orthogonal vectors to $f$. Thus, the kernel of this matrix may be interpreted as the matrix whose column vectors lie perpendicular to each respective gradient. From the orthogonal properties of a gradient, it follows that this matrix is the matrix whose columns are tangent to $f$.

With the background knowledge of singular points and the tangent space in place, we can finally define the Euclidean Distance Degree of a variety.

**Definition 8.** For a complex algebraic set $X$, the *Euclidean Distance Degree* with respect to a generic point $u$ is the cardinality of the solution set to

$$x \notin X_{sing} \quad (x-u) \perp T_x X$$

This definition captures the property that Euclidean distance is minimized when the vector from $u$ to $x$ is perpendicular to the tangent space at $x$. Finding the solutions to this system gives the set of non-singular points $x \in X$ which are critical points of the derivative of the distance function. In turn, these are points on the variety where distance to $u$ is potentially minimized. We can study the ideal containing the critical points as well, but to understand its definition we need another tool.

**Definition 9.** For ideals $I, J \subseteq R$, the *saturation* of $I$ by $J$ is

$$I : J^{\infty} = \{g \in R : gJ^m \subseteq I, m \geq 0\}.$$

The technique of saturation allows us to manipulate ideals and their varieties in the following manner:

**Proposition 10.** *For ideals $I$ and $J$ and their respective varieties $V$ and $Z$, the smallest variety containing the set $V \backslash Z$ is the variety of $I : J^{\infty}$.*

So, saturating lets us "remove" components from a variety without inadvertently producing a set that is not a variety. Now, we return to the definition of a critical ideal.

**Proposition 11.** *Given a point $u$, let*

$$I_T = (f_1, \ldots, f_s\{(c+1) \times (c+1) \text{ minors of } J'_f\})$$
$$I_{X_{sing}} = (f_1, \ldots, f_s, \{c \times c \text{ minors of } J_f\})$$

*Then, the smallest variety containing the set of solutions $S$ to the equation*

$$x \notin X_{sing} \; (x-u) \perp T_x X$$

*is given by*

$$\overline{S} = \mathcal{V}(I_T : X_{sing}^{\infty})$$

*The ideal $(I_T : X_{sing}^{\infty})$ is the **critical ideal** of $I$ and its zero locus is the set of **critical points** [4].*

Using saturation here allows us to remove singular points from the set of critical points, and only consider critical points with well-defined tangent spaces. In the context of the EDD, this means we discard potential closest points which are singular. However, depending on the properties of $I$, we might calculate different singular ideals. In particular, components generating $I$ which have multiplicity can falsely indicate a singular point where, for example, a cusp or self-intersection does not actually occur. This will result in a falsely low EDD and lost information about potential closest points. Connecting back to reaction networks, we have defined the positive steady-state in terms of the variety thus far, but we can also consider the ideal that generates that variety.

**Definition 12.** Let $I$ be an ideal of the ring $R$. The *radical ideal*, denoted $\sqrt{I}$, is defined as

$$\sqrt{I} = \{r \in R | r^n \in I \text{ for some } n \in \mathbb{N}\}.$$

Considering the radical of $I$ eliminates the multiplicity of components, and improves the EDD calculation.

**Example 2.** Consider the following network:

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

The steady-state equations are

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

The zero sets of these equations are two distinct upward-opening parabolas, and thus the intersection of these zero sets, which is precisely the steady-state variety, is the origin. However, the multiplicity of $x_B$ in the steady-state equations means that the origin is counted a singular point, and we discard it when calculating the EDD using the ideal $I = \langle x_A, x_B^2 \rangle$, getting a value of 0. But, when picking a random point $u$ and solving for the closest point in the variety, there is clearly one solution. Looking at the radical ideal $\sqrt{I} = \langle x_A, x_B \rangle$ instead gives the proper EDD of 1.

Using the radical ideal, we can then consider only the components of the variety that intersect the positive orthant.

**Definition 13.** The *positive radical ideal* is the set of all polynomials that vanish when evaluated at the positive steady-states.

This definition gives a group-theoretic perspective on the positive steady-state variety.

**Example 3.** Returning to the reaction in Example 1, we have the steady-state equations

$$f = \left\{ \begin{array}{l} f_A = 0 \\ f_B = \kappa_1 x_B - \kappa_2 x_A x_B \end{array} \right\}$$

Our positive steady-state is then $x_A = \frac{k1}{k2}$. Thus, $< x_A - \frac{\kappa_1}{\kappa_2} >$ is the positive radical ideal because it vanishes over the positive steady-state.

In practice, it is difficult to compute the positive radical ideal; in this report, the positive steady-state varieties were calculated by hand.

# 4 The Evolute

Over $\mathbb{R}^s$, the EDD is constant when examining the total number of complex solutions to the relevant system of equations. However, the number of real solutions may vary based on our choice of the generic point $u$. In applications of network theory, only real solutions have useful meaning, and so we would like a method to determine the number of real solutions to the EDD system for some generic point $u$. As defined in [3], the *ED discriminant* divides $\mathbb{R}^s$ into connected regions over which

the number of real critical points is constant. For plane curves, this allows us to determine the number of real solutions to the system for large regions of the plane rather than individual points. In particular, the Euclidean distance discriminant is the evolute of the variety; this will be made clear by building up from the most common definition of the evolute.

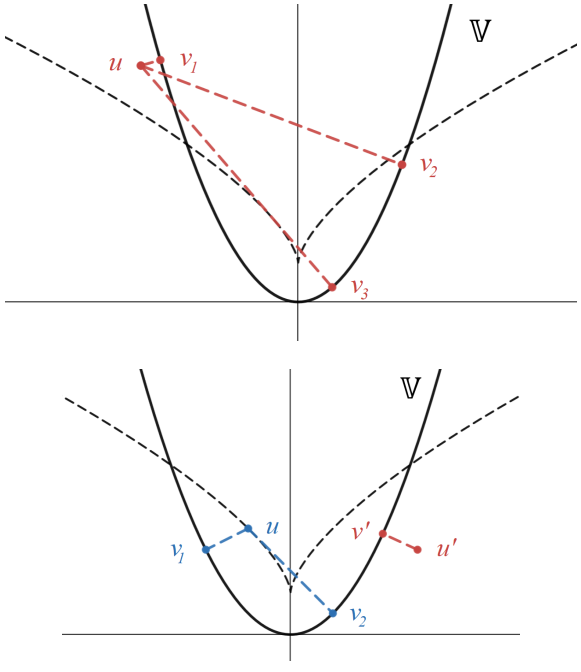
**Definition 14.** The *evolute* of a curve is the locus of all of its centers of curvature. More specifically, given an arbitrary point on the curve, there exists a circle of non-zero radius with equal curvature at that point. The set of every circle's center is the *evolute*.

However, it's important to note that while the circle of equal curvature defines the evolute, it does not define curvature. Rather, given a parametrized curve, we craft the circle of equivalent curvature using the normal vector to the curve at our specified point. This provides some intuition for an equivalent definition of the evolute:

**Definition 15.** The *evolute* of a curve is the envelope of normal vectors to the curve. Equally, given the family of normal vectors to our curve at various points, the envelope is tangent to each normal exactly once.

From this new definition, some properties of the evolute are revealed. Namely, why the evolute divides the plane into areas with a constant number of real solutions. Through our construction of the evolute as the envelope of normals we can think of the ED Degree as accounting for the number of times the normal vectors span the interior of our evolute.

For example, the EDD of a parabola is 3. For points above the evolute of the parabola, the number of real solutions is 3. Points below the evolute have exactly one real solution, and points on the evolute have two real solutions where a pair of solutions coincide. Below shows various points $u$ and their solutions.



# 5 Mixed Volumes

The EDD is more difficult to compute over families of reaction networks with higher dimensions and degrees. So, as in [5], it is useful to consider the mixed volume of a network, which provides an upper bound for the number of positive steady-states, assuming this number is finite. To understand when this assumption breaks down, we need an additional pair of definitions:

**Definition 16.** Given an $m \times n$ stiochiometric matrix $N$, the *stoichiometric subspace* is the subspace in $\mathbb{R}^m$ spanned by the columns of $N$. In other words, the stoichiometric subspace is a vector representation of the potential ways in which a dynamical system can evolve over time.

**Definition 17.** Given a chemical reaction network, a *conservation law* is the equation the orthogonal complement to the stoichiometric subspace of a network. As such, it represents all linear combinations of elements that remain unchanged by a dynamical system.

The maximum number of positive steady-states is related to the intersection of the positive steady-state variety and the conservation law. If this intersection is infinite, the mixed volume does not provide a useful upper bound on the number of positive steady-states.

One network with an infinite intersection between the positive steady-state variety and the conservation law is the following:

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

In this case, the conservation law and the positive steady-state variety are both vertical lines in the positive quadrant. They are shown below:

$$x_a = c \text{ where } c \in \mathbb{R}$$
$$x_a = \frac{\kappa_1}{\kappa_2}$$

Thus, if $c$ equals $\frac{\kappa_1}{\kappa_2}$, the conservation law and the positive steady-state variety have infinite overlap. Yet, while this only occurs for a single network within our specified cohort, it necessitates precaution whenever using mixed volume as an upper bound for the number of positive steady-states for a network. This network has mixed volume zero, but a nonempty positive steady-state variety. It is further important that in the cases where the conservation law and the positive steady-state variety cannot overlap, even if they are parallel, the mixed volume would still hold as an upper bound.

# 6 Species Reaction Graphs

As insightful as the database [1] is for the study of chemical reaction networks, the information must be translated to a form which can be readily used for calculations. Specifically, the data is enclosed via files of numerical strings and is organized by the number of species and reactions. The pairs of digits encode the edges of a species-reaction graph. Our interests lie with Table 2, which contains genuine, at-most bimolecular reaction networks. We define these terms as follows:

**Definition 18.** A *genuine* chemical reaction network leaves no species unused. A reaction is *at-most bimolecular* if every complex contains at most two elements.

To illustrate this process more clearly, let us consider the first entry of the 2-species, 2-reaction file.

2203032121

Let the first two entries be $m, n$. They represent the number of reactions and species, respectively. Hence, we know the first two digits will be the same for every entry in the file.

As seen in our example, the string representing the actual network 03032121 is composed of the set $\{0, 1, 2, 3\}$, call this $H$. For the $h_i \in H$, if $0 \leq h_i \leq m-1$, then $h_i$ represents a unique reaction. The set of reactions will be referred to as $R$, and thus for our example $R = \{0, 1\}$ where the reactions are labeled sequentially. Likewise, the numbers corresponding to the species will be composed of all integers $h_i \in H$ such that $m \leq h_i \leq n$. We let the set of species be $S$, so for this string we have $S = \{2, 3\}$ where 2 corresponds to species $A$ and 3 to species $B$.

The strings are constructed such that after the initial entries of $m$ and $n$, the integers are paired to create indices. Each index is composed of one element of $R$ and one from $S$, providing a species and reaction. From here, the ordering of the pair indicates if the species is in the product or reactant complex of the reaction. If the species integer is listed first it will reside in the reactant complex, and if the species number is listed second then it resides in the product complex.

We can then create diagrams for each ordered pair, pointing from the product complex to the reactant complex, with the arrow being marked by its designated reaction number from the set $R$. Either the reactant or product complex will contain the species indicated by its element from $S$, but that doesn't necessarily mean the "empty" complex is zero, as explained later.

Returning to the example above, all of our indices can be listed as ordered pairs, shown below. Let $r_0$ correspond to the reaction indexed by 0 in our data, and similarly for $r_1$.

$$(0,3) : \xrightarrow{r_0} B$$

$$(0,3) : \xrightarrow{r_0} B$$

$$(2,1) : A \xrightarrow{r_1}$$

$$(2,1) : A \xrightarrow{r_1}$$

Once the individual indices are transformed into these structures, we can "sum" the product and reactant complexes, respectively, for each individual reaction. Using the example above, we "add" the $r_0$ arrows together to create $0 \xrightarrow{r_0} 2B$. Similarly, we do the same for the $r_1$ arrows, giving $2A \xrightarrow{r_1} 0$. This same process would be used if the product complex of any of these weren't zero, "adding" the non-zero complexes together. This example just happens to be one with trivial complexes.

Finally, to create the chemical reaction network, we combine the unique reactions into one, making sure to append the reaction rates, denoted as $\kappa_i$. For this example, we have

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

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

While running calculations in our software, these were written as a list $\{0 \to 2B, 2A \to 0\}$ rather than a network, for practical reasons. The specific code is included in the appendix.

# 7 Main Results

In this paper, we analyze and classify the positive steady-state varieties of all 210 genuine, at-most bimolecular, 2-species, 2-reaction networks. For the remainder of this section, "chemical reaction network" or "network" will refer to 2-species, 2-reaction networks satisfying these properties. An additional property of reaction networks is useful in their classification:

**Definition 19.** The set of all unique species present in a complex is called the *support* of that complex. In particular, we consider the supports of reactant complexes.

Among all 210 chemical reaction networks, there are eleven possible shapes of the steady-state variety, not accounting for horizontal versus vertical orientation; this orientation corresponds to the arbitrary labeling of the species and the corresponding axes. We give an example of each class.

## 7.1 Empty variety

First, we examine the class of networks with an empty steady-state variety (and therefore and empty positive steady-state variety). For these networks, the system of steady-state equations has no solutions. Consider the network

$$\begin{aligned} A + B &\xrightarrow{\kappa_1} 2A \\ 0 &\xrightarrow{\kappa_2} A \end{aligned}$$

and its steady-state equations

$$\begin{aligned} f_A &= \kappa_1 x_A x_B + \kappa_2 \\ f_B &= -\kappa_1 x_A x_B \end{aligned}$$

We can see that this system has no solutions both geometrically and algebraically. First, the zero set of $f_A$ here is a hyperbola contained entirely in the interiors of the second and fourth quadrants, while the zero set of $f_B$ consists of both axes. These zero sets do not intersect, and so there are no points that solve both equations. Alternatively, setting $f_A$ equal to zero gives $x_A x_B = \frac{-\kappa_2}{\kappa_1}$, while setting $f_B$ equal to zero gives $x_A x_B = 0$, which occurs if and only if one or both values are zero. Since both of the $\kappa_i$ are strictly positive, these equalities cannot be satisfied simultaneously, and there are no solutions.

## 7.2 Origin

There are 44 networks whose steady-state variety is the single point $(x_A, x_B) = (0, 0)$. Consider the network

$$\begin{aligned} 2B &\xrightarrow{\kappa_1} A \\ A &\xrightarrow{\kappa_2} A + B \end{aligned}$$

and its steady-state equations

$$\begin{aligned} f_A &= \kappa_1 x_B^2 \\ f_B &= -2\kappa_1 x_B^2 + \kappa_2 x_A \end{aligned}$$

Geometrically, the zero set of $f_A$ is the line $x_B = 0$, or the $x_A$-axis, while the zero set of $f_B$ is a parabola intersecting the origin and opening in the positive $x_A$ direction. These curves intersect only in the origin. Algebraically, $f_A$ gives that $x_B^2 = 0$ while $f_B$ gives that $x_B^2 = \frac{\kappa_2}{2\kappa_1} x_A$; this system is solved only when $x_A = 0$, which also gives $x_B = 0$. So, the steady-state variety is the origin. These networks all have an empty positive steady-state variety, since the origin does not intersect the interior of the positive orthant.

## 7.3 Single axis

Our first foray into one-dimensional steady-state varieties is with the class of single-axis varieties. These networks, the most numerous class, have an empty positive steady-state variety and a steady-state variety consisting of a single coordinate hyperplane. The identity of this axis depends only on the arbitrary labeling of species, and so the $x_A$ and $x_B$ axes are considered equivalent in this classification. Consider the network

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

and its steady-state equations

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

Written in factored form, the shared factor of $x_A$ is clear. Both equations equal zero when $x_A = 0$, and the other factors are distinct. So, the steady-state variety is the line $x_A = 0$, or the $x_B$-axis.

## 7.4 Both axes

The next class of networks has a steady-state variety consisting of both coordinate hyperplanes. Consider the network

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

and its steady-state equations

$$f_A = -\kappa_1 x_A x_B$$
$$f_B = \kappa_1 x_A x_B - \kappa_2 x_A x_B = x_A x_B(\kappa_1 - \kappa_2)$$

Both equations are constant multiples of $x_A x_B$, and thus their zero set is the union of the lines $x_A = 0$ and $x_B = 0$, or the union of the $x_B$ and $x_A$ axes. While not of much interest due to its empty positive steady-state variety, the classification of these networks is remarkably simple, summarized in the following proposition:

**Proposition 20.** *A network's steady-state variety consists of both coordinate hyperplanes if and only if both reactant complexes are $A + B$.*

*Proof.* First, suppose that the steady-state variety consists of both coordinate hyperplanes. Then, both steady-state equations must have a shared factor of $x_A x_B$. This factor is already degree two, the maximal degree for the steady-state equations of at-most bimolecular networks, so each equation must be some constant (possibly zero) multiple of $x_A x_B$. This means every nontrivial monomial term must have a factor of $x_A x_B$, and therefore both reactant complexes take the form $A + B$.

Now, suppose that both reactant complexes are $A + B$. Then, the corresponding steady-state equations consist of monomials that are constant (possibly zero) multiples of $x_A x_B$. Any sum of these monomials will be a constant multiple of $x_A x_B$, which equals zero if and only if at least one variable is zero. So, the variety consists of the union of the lines $x_A = 0$ and $x_B = 0$, which is precisely the pair of coordinate hyperplanes. □

## 7.5 Line through the origin

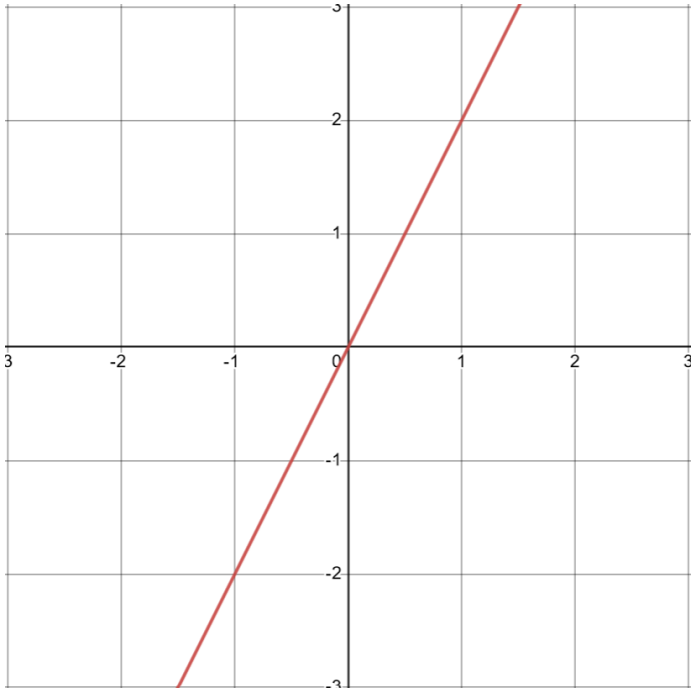
The next class is the first we have seen whose members can, and do, exhibit nonempty positive steady-state varieties. The following network is one such specimen:

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

Its steady-state equations are given by

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

Note that these equations are linear multiples of each other, and so their zero sets define the same curve. In particular, they define the line $x_B = \frac{\kappa_1}{\kappa_2} x_A$, which is a line through the origin with positive slope, the precise value of which depends on the rate constants. The following graph shows the variety when $\kappa_1 = 6$ and $\kappa_2 = 3$:




## 7.6 Parallel lines

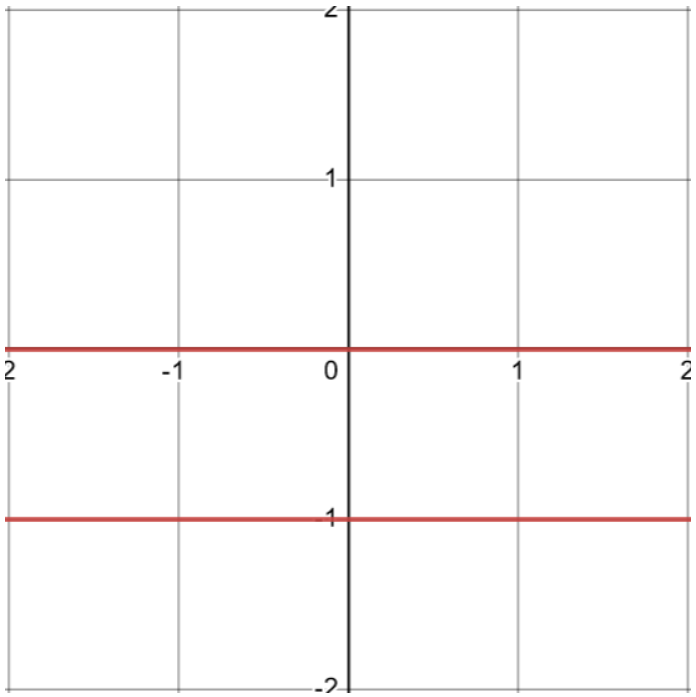
The next—and smallest—class, with only two members, have steady-state varieties consisting of two parallel lines, one of which is a coordinate axis. Consider the network

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

and its steady-state equations

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

As with the previous class, the two equations are linear multiples of each other, and so we need only consider one. The equations equal zero when either $x_B = 0$, or when $x_B = \frac{-\kappa_2}{2\kappa_1}$. So, the variety is the union of these two parallel lines, one of which is the $x_A$-axis. The following graph shows the variety when $\kappa_1 = 1$ and $\kappa_2 = 2$:




## 7.7 Plus sign

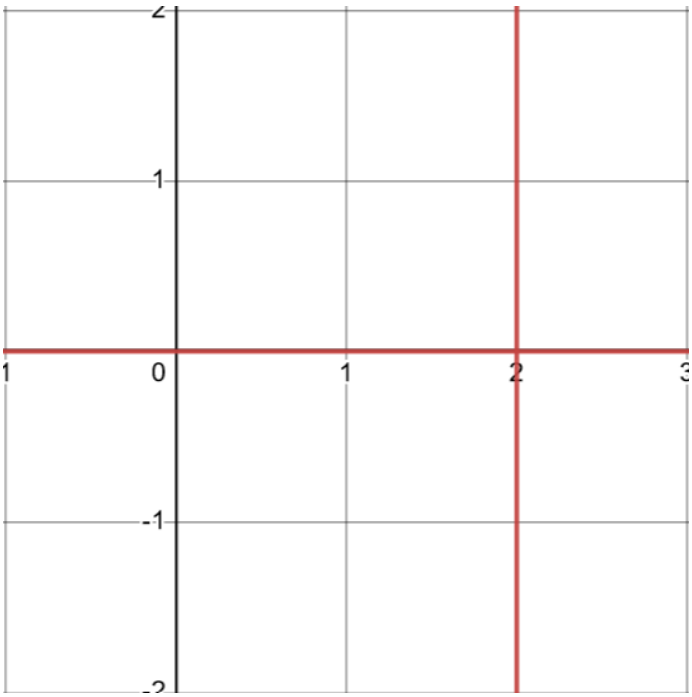
The next class of networks have varieties in a plus-sign shape, where one line is a coordinate axis and the other is a perpendicular non-axis line. Consider the following network:

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

and its steady-state equations

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

In this network, one steady-state equation is the zero polynomial, so its zero set is the entire plane, meaning $f_A$ places no restrictions on the variety. So, the variety is defined entirely by $f_B$, which equals zero when either $x_B = 0$, or when $x_A = \frac{\kappa_1}{\kappa_2}$. So, the variety is the union of these two perpendicular lines, one of which is the $x_A$-axis. When $\kappa_1 = 2$ and $\kappa_2 = 1$, the variety looks as follows:




## 7.8 Rotated X

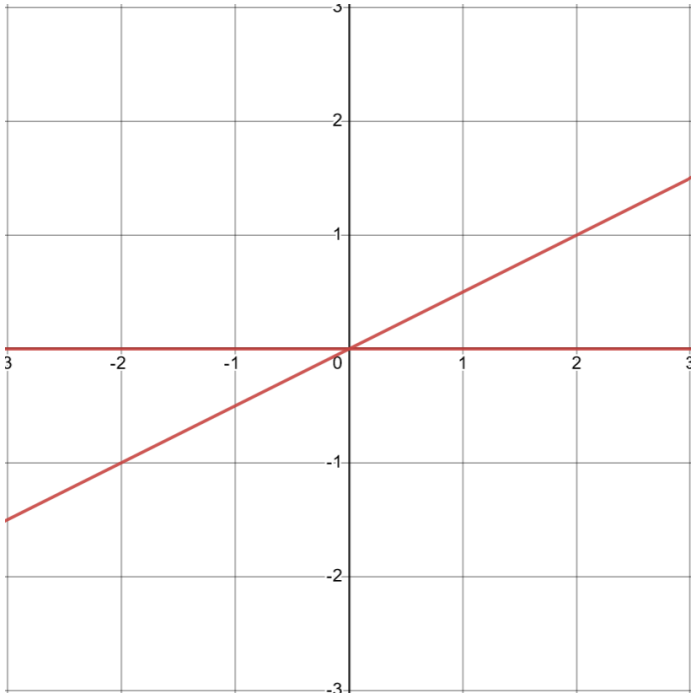
Continuing on to another class whose variety consists of two intersecting straight lines, we next have the shape we call a "rotated X." These varieties look like one coordinate axis and one non-perpendicular line through the origin. The following network is in this class:

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

Its steady-state equations are given by

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

Once again, these equations are linear multiples of each other. After factoring, we see that they both equal zero when either $x_B = 0$, or when $x_B = \frac{\kappa_1}{\kappa_2} x_A$. So, the steady-state variety is the union of these two lines. One is the $x_A$-axis, and the other is a line with positive slope through the origin. Letting $\kappa_1 = 1.5$ and $\kappa_2 = 3$, the variety looks as follows:




## 7.9 X-Shape

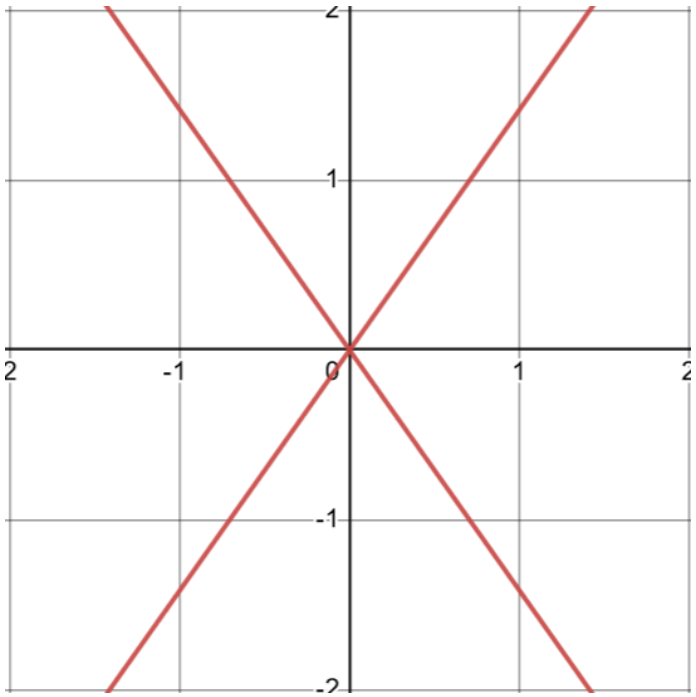
The final class made up only of straight lines consists of an X-shape centered at the origin, where neither line is a coordinate axis. Consider the network

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

and its steady-state equations

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

As in the previous two examples, these equations are linear multiples of each other. They equal zero when $x_B^2 = \frac{2\kappa_1}{\kappa_2} x_A^2$. Taking the square root yields the equation $x_B = \pm\sqrt{\frac{2\kappa_1}{\kappa_2}} x_A$, which defines two lines with opposite slope through the origin. The following graph shows this variety when $\kappa_1 = \kappa_2 = 1$:




## 7.10 Parabola

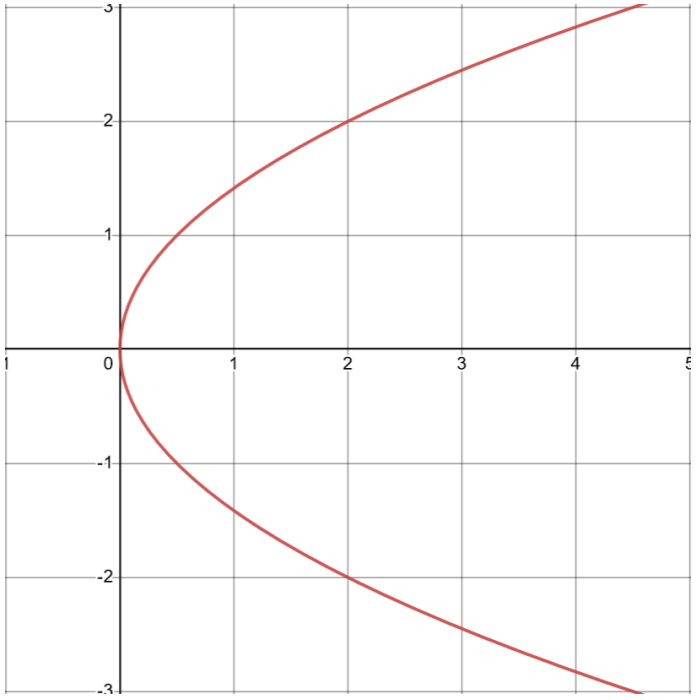
At long last, we depart the world of straight lines for the last two classes of networks, the first of which forms parabolic varieties. All of these networks have nonempty positive steady-state varieties, which equal their steady-state varieties. Similar to the single axes, whether the parabola opens upward or rightward depends only on the arbitrary relabeling of the species, so these two cases are considered equivalent. As an example, consider

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

Its steady-state equations are given by

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

Since these equations are linear multiples of each other, both equations equal zero when $x_A = \frac{\kappa_2}{\kappa_1} x_B^2$. So, the steady-state variety takes the form of a parabola at the origin opening in the positive $x_A$ direction. Letting $k_1 = 2$ and $k_2 = 1$, the variety looks as follows:




## 7.11 Hyperbola

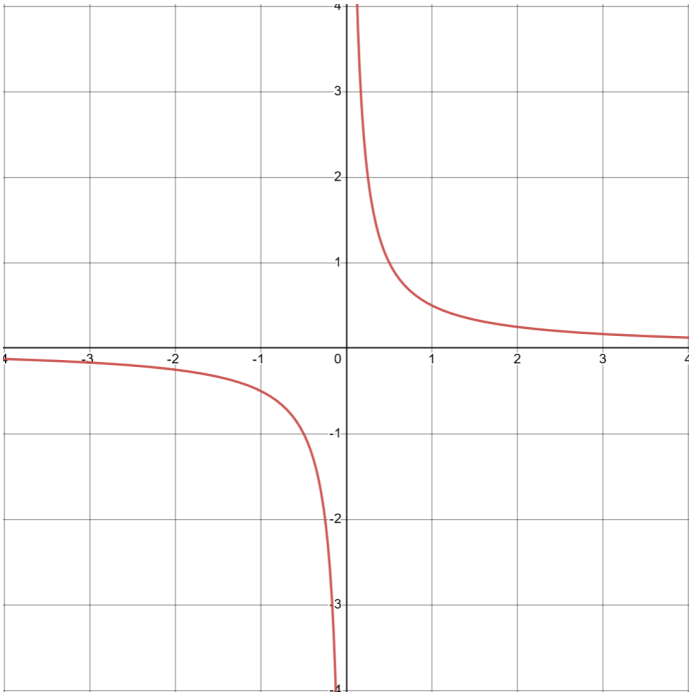
The final class is also a degree two conic, taking the form of a hyperbola contained in the first and third quadrants. As with the parabola, all of these networks have a nonempty positive steady-state variety which equals their steady-state variety. Consider the network

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

and its steady-state equations

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

Since $f_A = f_B$, the variety of one gives the solution to both the equations. Thus, the variety is given by $x_A x_B = \frac{\kappa_2}{\kappa_1}$ which defines a hyperbola. When $k_1 = 2$ and $k_2 = 1$ the variety appears as follows:




## 7.12 Classification Theorems

We have now seen an example of every possible steady-state variety. Considering now only nonempty positive steady-state varieties, there are four classes: horizontal or vertical lines, lines through the origin, parabolas, and hyperbolas. We give classifications of all networks producing these varieties.

**Theorem 7.1.** *Given a chemical reaction network, the positive steady-state 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*

*Remark.* Before proving this theorem, we note that the second criterion, phrased here in terms of the stoichiometric matrix, can also be described with the notion of T-alternating subnetworks described in [5]. Through this lens, we instead require that, when viewing the behavior of each species individually, the network is 1-alternating.

*Proof.* ($\Rightarrow$)
Suppose we have an arbitrary network whose PSSV is a non-axis horizontal or vertical line. Therefore, the network's simplified variety will be $V(bx_a - a)$ where $a, b \in \mathbb{R}\backslash\{0\}$ and $x_a$ is an arbitrary variable representing one of our two species.

Thus, since the positive steady-state variety is a component of the steady-state variety, the positive steady-state equation will be a factor of the steady-state equation. As such, our steady-state equation will a product of $(bx_a - a)$ and a term whose degree is limited by the network's

bimolecularity.

$$(bx_a - a) * (\text{Factor of degree 1 or 0}) = (\text{Entire steady-state equation})$$

Should our zero degree factor be equal to zero, our PSSV will be empty, contradicting our assumption that it is a line. Further, should our zero degree factor be a constant other than one, our PSSV will remain unchanged while the equation will be scaled by a constant, contradicting $a$ and $b$ being represented in their simplest form. Therefore, as defined, should our PSS equation be non-trivial factor of the steady-state equation, the degree of the other factor is one. Thus, our variety will be $(bx_a - a) * h_1$ where $h_1$ is degree one. However, note that for all two-reaction networks, the corresponding steady-state equations will have at most two terms. Therefore, our degree one factor is a monomial, leaving us with the following potential steady-state equations:

$$(bx_a - a)$$
$$(bx_a - a) * (x_a)$$
$$(bx_a - a) * (x_b)$$

The logic applied to yield these steady-state equations also applies to our second set of equations. Therefore, we must only determine the potential pairings between this list of equations and itself. Following from the assumption of mass action kinetics, the terms of steady-state equations correspond to the reactant complexes of a network. Since each term has a unique product of variable, these three equations correspond to unique networks. Thus, the only possible steady-state equations are the following:

$$f = (bx_a - a)\ ,\ g = (dx_a - c)$$
$$f = (bx_a - a) * (x_a)\ ,\ g = (dx_a - c) * (x_a)$$
$$f = (bx_a - a) * (x_b)\ ,\ g = (dx_a - c) * (x_b)$$

Having a PSSV necessitates that the factors corresponding to the variety are multiples of one another. Thus, the binomial factors, and therefore each pair of equations, are multiples. This corresponds to the rows of the network's stoichiometric matrix also being multiples. Further, following from our construction of a positive line's simplified equation, the terms of each binomial have opposite parity. This corresponds to the columns of the stoichiometric matrix having opposite parity. In combination, these two principles prove our first criterion. For all pairs of equations above, the columns of the corresponding stoichiometric matrix are negative multiples. This additional restriction necessitates that the first two equations correspond to non-genuine chemical reaction networks: $A \longleftrightarrow 0$ and $2A \longleftrightarrow A$, respectively. Thus, the only form the steady-state equations may take are the following:

$$f = (bx_a - a) * (x_b)\ ,\ g = (dx_a - c) * (x_b)$$

Further, as demonstrated in the above example, these equations are derived from a network with one support of $A + B$ and another uni-molecular support. This proves our second criterion and the forwards direction of the proof.

($\Leftarrow$) Given a chemical reaction network, suppose the columns of the corresponding stoichiometric matrix are negative multiples of one another, and one support is $A + B$ while the other is

unimolecular. Then the PSSV is a non-axis horizontal or vertical line. Take the general form of a network as shown below:

$$\alpha_0 A + \beta_0 B \to \alpha_1 A + \beta_1 B$$
$$\alpha_2 A + \beta_2 B \to \alpha_3 A + \beta_3 B$$

Let us manipulate this equation to align with our second assumption. WLOG, allow our second equation to have a the unimolecular reactant complex $A$.

$$\begin{aligned} A + B &\to \alpha_1 A + \beta_1 B \\ A &\to \alpha_3 A + \beta_3 B \end{aligned}$$

This yields the general steady-state equations shown below. Manipulation according to our first assumption finding the variety yields the following equations of lines for $\kappa_1$, $\kappa_2 \in \mathbb{R}\backslash\{0\}$:

$$\begin{aligned} f_A &= (\alpha_1 - 1)\kappa_1 x_A x_B + (\alpha_3 - 1)\kappa_2 x_A \\ f_B &= (\beta_1 - 1)\kappa_1 x_A x_B + (\beta_3)\kappa_2 x_A \end{aligned}$$

$$\begin{aligned} f_A &= (\alpha_1 - 1)\kappa_1 x_A x_B + (1 - \alpha_1)\kappa_2 x_A \\ \Rightarrow x_A &= 0,\ x_B = \frac{\kappa_2}{\kappa_1} \end{aligned}$$

$$\begin{aligned} f_B &= (-\beta_3)\kappa_1 x_A x_B + (\beta_3)\kappa_2 x_A \\ \Rightarrow x_A &= 0,\ x_B = \frac{\kappa_2}{\kappa_1} \end{aligned}$$

□

**Theorem 7.2.** *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).*

*Proof.* ($\Rightarrow$) Suppose we have a network whose positive steady-state variety is a line through the origin. For this to occur, the line must have positive slope. Since the network is at most bimolecular, its steady-state equations will have degree at most two. Without loss of generality, there are three possible forms of the equation defining a steady-state variety containing the necessary line:

$$x_B = c \cdot x_A \Rightarrow x_B - c \cdot x_A = 0 \tag{1}$$

$$x_B^2 = \cdot x_A^2 \Rightarrow (x_B + \sqrt{c} \cdot x_A)(x_B - \sqrt{c} \cdot x_A) = 0 \tag{2}$$

$$x_A x_B = c \cdot x_A^2 \Rightarrow x_A(x_B - c \cdot x_A) = 0 \tag{3}$$

for some positive constant $c$. The equation defining the steady-state variety must be a shared factor of the two steady-state equations. In the case of (2) and (3), the shared factor is already degree two. By bimolecularity, the steady-state equations are constant multiples of the same equation, and therefore constant multiples of each other. If the steady-state variety is defined by equation (1), then the steady-state equations are either (1) times a constant or (1) times a single variable. The monomial terms are defined by a fixed pair of reactant complexes, so they must be the same for both steady-state equations, giving that any variable factor must be shared. If such a factor exists, we simply have (3). Otherwise, the steady-state equations are linear multiples of each other.

The individual steady-state equations must therefore take on these same three forms. In each case, there is one positive and one negative term; this is necessary for the line's slope to be positive. By definition, the sign of the steady-state coefficients corresponds to the net change of a species. Here, the signs indicate that if a given species is increasing in one reaction, it is decreasing in the other. Therefore, each row of the stoichiometric matrix will have one positive and one negative term if they are nonzero, and the network satisfies (*1*). Note also that in all three equations the degree of every variable term is equal, necessary for defining a line, meaning that the number of reactant molecules is equal in both reactions and the network satisfies (*2*).

Finally, we observe that in all three equations, there is at least one variable that appears in exactly one monomial term. This corresponds to at least one species that appears in exactly one reactant complex, indicating distinct supports of the reactant complexes. Additionally, all three are binomials, so no reactant complex has an empty support, and the corresponding network satisfies (*3*).

($\Leftarrow$) Now, suppose we have a nontrivial network satisfying the above three conditions. As a consequence of (*1*), the rows of the stoichiometric matrix are multiples of each other as well, and so the steady-state equations are linear multiples of each other with at least one being nonzero. So, to understand the variety we need only examine one equation. Without loss of generality, consider a nonzero $f_B$ in general form:

$$f_B = \kappa_1(\beta_1 - \beta_0)x_A^{\alpha_0}x_B^{\beta_0} + \kappa_2(\beta_3 - \beta_2)x_A^{\alpha_2}x_B^{\beta_2}.$$

By (*3*), we know at least one reactant appears in exactly one reactant complex, meaning that at least one of the reactant coefficients $\alpha_0$, $\beta_0$, $\alpha_2$, and $\beta_2$ is 0. Suppose without loss of generality that $\beta_0 = 0$; note that if one of the $\alpha_i$ were zero instead, we could rewrite $f_B$ as a constant multiple of $f_A$ so that the $\alpha_i$ appeared in the coefficients. Then, $\beta_1 - \beta_0 = \beta_1$ is positive, since we assume $f_B \neq 0$ and (*1*) gives that one coefficient being zero forces both to be zero. So, by (*1*) again, we have $\beta_3 - \beta_2$ is negative. We can then rewrite the equation as

$$\kappa_1\beta_1 x_A^{\alpha_0} = \kappa_2(\beta_2 - \beta_3)x_A^{\alpha_2}x_B^{\beta_2},$$

where all the coefficients are positive. Since $\beta_0 = 0$, we must have $\alpha_0 \neq 0$, as we assume there are no empty reactant complex supports. By (*3*), $\beta_2 \neq 0$ as well; if it were zero, the reactant complex's supports would not be distinct. So, the quantity $\beta_2 - \beta_0 = \beta_2$ is positive. Furthermore, (*2*) gives that $\alpha_0 + \beta_0 = \alpha_2 + \beta_2$. We can rearrange this equation to be $\alpha_0 - \alpha_2 = \beta_2 - \beta_0 = \beta_2$, showing that $\alpha_0 - \alpha_2$ is positive. Armed with this knowledge, we return to our equation, and divide:

$$\kappa_1\beta_1 \frac{x_A^{\alpha_0}}{x_A^{\alpha_2}} = \kappa_2(\beta_2 - \beta_3)x_B^{\beta_2}.$$

In general, it is inadvisable to divide by variables, as this results in lost information about solutions to the equation. However, in this case, if we were to cancel a common factor of $x_A$ from both terms, it would correspond to eliminating a coordinate hyperplane from the steady-state variety. These hyperplanes are not a part of the positive steady-state variety and are therefore irrelevant. So, simplifying gives

$$x_B^{\beta_2} = \frac{\kappa_1\beta_1}{\kappa_2(\beta_2-\beta_3)} x_A^{\alpha_0-\alpha_2}.$$

Note that $\beta_2 - \beta_3$ is nonzero, since we assumed $f_B \neq 0$. So, all coefficients and exponents in this equation are positive. We also have that $2 \geq \alpha_0 - \alpha_2 = \beta_2 - \beta_0 > 0$ by (*2*) and by bimolecularity, so the exponents are equal and either 1 or 2. In both cases, the portion of the variety that intersects the interior of the positive orthant is a line through the origin with positive slope, which is the desired positive steady-state variety. □

**Theorem 7.3.** *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.* ($\Rightarrow$) Given the positive steady-state variety is $V(y - kx^2)$, where $k \in \mathbb{R}$ is positive, let $x, y$ represent the variables $x_A, x_B$ under no prescribed choice. Since $V(y-kx^2)$ comes from the 2-species network $G$, then $V(y - kx^2) = V(f_A) \cap V(f_B)$. We know $G$ is at-most-bimolecular, implying both $\deg(f_A)$ and $\deg(f_B)$ cannot be greater than 2. Then, we have

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

where $c_1$ and $c_2$ are constants and not both zero.

By definition of the steady-state equations, the monomials in $f_A$ and $f_B$ correspond to the reactant complexes of $G$. Since these are exactly $y$ and $x^2$, it directly implies $G$ must have a bimolecular complex and a monomolecular complex. Further, these complexes necessarily have disjoint supports, proving conditions $(1), (2)$.

To prove condition (3), we'll examine two cases, the first of which being exactly one of $c_1$ or $c_2$ is zero, and the other being neither are zero. If exactly one of $c_1$ or $c_2$ is zero, then the stoichiometric matrix $N$ has a row of zeros and hence has determinant zero. Otherwise, when neither $c_1$ nor $c_2$ is zero, then $f_B = \frac{c_2}{c_1} f_A$. If

$$f_A = ak_1y - bk_2x^2$$
$$f_B = ck_1y - dk_2x^2$$

where $\mathsf{sign}(a) = \mathsf{sign}(b)$ and $\mathsf{sign}(c) = \mathsf{sign}(d)$ then the equation $f_B = \frac{c_2}{c_1} f_A$ implies $c = \frac{c_2}{c_1} a$ and $d = \frac{c_2}{c_1} b$. Thus,

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

Since $\det N = 0$, then the columns of $N$ are multiples of each other. Further, this multiple must be negative because of the sign conditions $\mathsf{sign}(a) = \mathsf{sign}(b)$ and $\mathsf{sign}(c) = \mathsf{sign}(d)$. This proves condition (3).

($\Leftarrow$) Given that the reactant complexes are disjoint, and that there's a term with degree two and another of degree one, we can conclude the PSSV will be of the form $V(y - kx^2)$. We also know that the columns of the stoichiometric matrix are negative linear multiples by some real number $-c$. Thus,

$$\begin{aligned} V(f_A) \cap V(f_B) &= V(y - kx^2) \\ f_A &= k_1 ay - k_2 bx^2 \\ f_A &= -c f_B \\ \Rightarrow f_B &= -c\left(k_1 ay - k_2 bx^2\right) \end{aligned}$$

So, the PSSV must be a parabola, as desired.

□

**Theorem 7.4.** *Given any chemical reaction network, the positive steady-state variety will be a hyperbola if and only if all of the following hold:*

1. *$f_A = f_B$, or one of $f_A, f_B$ equal $0$*
2. *The reactant complexes are $A + B$ and $0$*
3. *The columns of the stoichiometric matrix are negative linear multiples of each other.*

*Proof.* ($\Rightarrow$)

Assume the positive steady-state variety is of the form of a hyperbola. Specifically,

$$V(x_A x_B - c) = V(f_A, f_B) = V(f_A) \cap V(f_B)$$

where $c \in \mathbb{R}^+$. Note that the solved equation $x_A x_B = c$ must be a shared factor of both steady-state equations $f_A$ and $f_B$. Following from this, $x_A x_B - c$ is not a factor of a higher degree reducible polynomial nor a factor of a constant multiple, where the constant is greater than 1, because the chemical reaction network is at most bi-molecular. Furthermore, the equations must take the form:

$$\begin{aligned} f_A &= \kappa_1(\alpha_1 - \alpha_0)x_A x_B + \kappa_2 \alpha_3 \\ f_B &= \kappa_1(\beta_1 - \beta_0)x_A x_B + \kappa_2 \beta_3 \end{aligned}$$

such that the quantities $\alpha_1 - \alpha_0$ and $\beta_1 - \beta_0$ must be 0 or $\pm 1$ proving (2). To prove (1) note that solving this equation when $(\alpha_1 - \alpha_0), (\beta_1 - \beta_0)$ are not equal to 0 gives:

$$\begin{aligned} x_A x_B &= \frac{-\kappa_2 \alpha_3}{\kappa_1(\alpha_1 - \alpha_0)} \\ x_A x_B &= \frac{-\kappa_2 \beta_3}{\kappa_1(\beta_1 - \beta_0)} \end{aligned}$$

where $\frac{-\alpha_3}{(\alpha_1 - \alpha_0)}, \frac{-\beta_3}{(\beta_1 - \beta_0)} > 0$.

If the variety is to be a hyperbola then the intersection of the solution for $f_A$ and $f_B$ must also be a hyperbola which leads to the solution:

$$x_A x_B = \frac{-\kappa_2 \alpha_3}{\kappa_1(\alpha_1 - \alpha_0)} = \frac{-\kappa_2 \beta_3}{\kappa_1(\beta_1 - \beta_0)}$$

$f_A \neq -f_B$ because the reactant complex 0 cannot lose any species from a reaction. Thus $\alpha_1 - \alpha_0 = \beta_1 - \beta_0 = \pm 1$ and $\alpha_3 = \beta_3$ when $f_A$ and $f_B$ are non-zero. Similarly, WOLOG, if $\alpha_1 - \alpha_0 = 0$, then $\alpha_3 = 0$ so that $f_A = 0$. If $\alpha_3$ were not equal to zero, the variety would be empty. Hence, the solution to $f_B$ is the variety.

To prove (3), note the stoichiometric matrix:

$$N = \begin{bmatrix} \alpha_1 - \alpha_0 & \alpha_3 \\ \beta_1 - \beta_0 & \beta_3 \end{bmatrix}$$

WOLOG let $f_A$ be nonzero. As shown previously, $d = \frac{-\alpha_3}{(\alpha_1 - \alpha_0)}$ is positive. Thus $-d(\alpha_1 - \alpha_0) = \alpha_3$ shows that the columns are negative linear multiples of one another. For the case where $f_A = 0$ it is sufficient to show that 0 is a negative linear multiple of itself.
($\Leftarrow$) Suppose $f_A = f_B$ and the reactant complexes are $A + B$ and 0, then the equations are of the form:

$$f_A = \kappa_1(\alpha_1 - \alpha_0)x_A x_B + \kappa_2 \alpha_3$$
$$f_B = \kappa_1(\beta_1 - \beta_0)x_A x_B + \kappa_2 \beta_3$$

where $\alpha_1 - \alpha_0 = \beta_1 - \beta_0$ and $\alpha_3 = \beta_3$, thus the solution to both equations is $x_A x_B = \frac{-\kappa_2 \alpha_3}{\kappa_1(\alpha_1 - \alpha_0)}$ which is the equation of a hyperbola. Similarly, if one of the equations, say for example $f_A = 0$, then the solution to the other equation $f_B$ also takes the form of a hyperbola. □

# 8 Network Classification Tables

The following tables give the number of networks exhibiting each type of steady-state and positive steady-state variety.

## 8.1 2-Species, 2-Reaction Networks

Table 1: Networks with nonempty positive steady-state variety

| PSSV | # networks | # with SSV=PSSV | SSV (when distinct) |
|---|---|---|---|
| Line through origin | 7 | 2 | 3 X, 2 rotated X |
| Horiz./vert. line | 3 | 0 | plus sign |
| Parabola | 5 | 5 | – |
| Hyperbola | 3 | 3 | – |
| Total | 18 | 10 | – |

Table 2: Networks with empty positive steady-state variety

| SSV | # networks |
|---|---|
| Origin | 44 |
| Single-axis | 76 |
| Both axes | 6 |
| Line through origin | 3 |
| Horiz./vert. parallel lines | 2 |
| Plus sign | 1 |
| Rotated X | 5 |
| Empty | 55 |
| Total | 192 |

Our data in full detail is available in the attached spreadsheet.

## 8.2 1-Species Networks

Although not explored earlier in this paper, we also examined all 63 genuine at-most bimolecular one-species networks with at most six reactions. We disregard the one-reaction networks; with only one reaction, the steady-state equation will be a monomial, and so either has an empty steady-state variety or a steady-state variety of the point zero. In either case, the positive steady-state variety is empty, and so we begin with two-reaction networks. When working with one species, the varieties are subsets of the number line $\mathbb{R}$. In all cases, when the positive steady-state variety is nonempty, it consists of a single point. Interestingly, in the three- and four-reaction networks, there are positive steady-state varieties whose existence depends upon the values of the rate constants.

Table 3: 1-species 2-reaction networks

| Property | # networks |
|---|---|
| Empty SSV | 1 |
| One-point SSV | 6 |
| Two-point SSV | 8 |
| Total | 15 |
| Non-empty PSSV | 8 |

Table 4: 1-species 3-reaction networks

| Property | # networks |
|---|---|
| One-point SSV | 4 |
| Two-point SSV | 16 |
| Total | 20 |
| Non-empty PSSV | 18 |
| Rate-dependent PSSV | 4 |

Table 5: 1-species 4-reaction networks

| Property | # networks |
|---|---|
| One-point SSV | 1 |
| Two-point SSV | 14 |
| Total | 15 |
| Non-empty PSSV | 15 |
| Rate-dependent PSSV | 3 |

For the five- and six-reaction cases, all networks have two-point steady-state varieties and nonempty, non-rate-dependent positive steady-state varieties. We now give an example of a rate-dependent positive steady-state variety.

**Example 4.** Consider the network

$$A \xrightarrow{\kappa_1} 2A$$
$$A \xrightarrow{\kappa_2} 0$$
$$2A \xrightarrow{\kappa_3} A$$

and its steady-state equation

$$f_A = \kappa_1 x_A - \kappa_2 x_A - \kappa_3 x_A^2 = x_A(\kappa_1 - \kappa_2 - \kappa_3 x_A)$$

This equals zero when either $x_A = 0$, or when $x_A = \frac{\kappa_1 - \kappa_2}{\kappa_3}$. The point $x_A = 0$ will never be in the positive steady-state variety, and we disregard it; the other point exhibits rate-dependence. All the $\kappa_i$ are positive, so $\frac{\kappa_1 - \kappa_2}{\kappa_3}$ is positive if and only if $\kappa_1 > \kappa_2$; otherwise, the value is zero or negative, and the point is not in the interior of the positive orthant. So, this network has a nonempty positive steady-state variety if and only if $\kappa_1 > \kappa_2$.

---

# References


[1] Murad Banaji. Chemical reaction network enumeration. https://reaction-networks.net/networks/.

[2] Jane Ivy Coons, Mark Curiel, and Elizabeth Gross. Mixed volumes of networks with binomial steady-states, 2023.

[3] Jan Draisma, Emil Horobeţ, Giorgio Ottaviani, Bernd Sturmfels, and Rekha R. Thomas. The Euclidean distance degree of an algebraic variety. *Found. Comput. Math.*, 16(1):99–149, 2016.

[4] Lukas Gustafsson. *The Euclidean Distance Degree of Conics*. PhD thesis, KTH Royal Institute of Technology, 2019.

[5] Nida Obatake, Anne Shiu, and Dilruba Sofia. Mixed volume of small reaction networks. *Involve, a Journal of Mathematics*, 13(5):845–860, dec 2020.

**Kernel:** SageMath 10.0

In [0]:
```
#This is a compilation of the functions and procedures used for all
calculations.
#Some of these use the SageMath 10.0 kernel while others used
Macaulay2.
```

In [0]:
```
#How we studied the original 25 networks:

loadPackage "ReactionNetworks"

rxnInfo = G -> (
    RR1=createRing(G,QQ);
    f1= subRandomReactionRates G;
    S1=QQ[G.ConcentrationRates];
    f1=apply(f1,q->sub(q,S1));
    I1=ideal f1;
    print G;
    print(concatenate{"degree: ", toString(degree I1)});
    print(concatenate{"dimension: ", toString(dim I1)});
    print(concatenate{"weakly reversibe? ",toString isWeaklyReversible
G});
    print(concatenate{"deficiency: ", toString isDeficient G}) )

#Created a list of all 25 CRNs called L

for G in L do rxnInfo(G)
```

In [0]:
```
#Our original EDD fucntion

EDD = G -> (
    R=createRing(G,QQ); --creates a ring in the rationals in terms of
the concentrations and rxn rates
    f=subRandomReactionRates G; --inputs rxn rates so we can calculate
    S=QQ[G.ConcentrationRates]; --makes a smaller ring where only the
concentrations are variables
    g=apply(f,p->sub(p,S)); --puts the steady state polynomials into
the smaler ring
    I=ideal g; --steady state ideal of G
    u={random(QQ),random(QQ)}; --random point to let us calculate the
EDD (this is the generic point u)
    sing=I+minors(codim I, jacobian I); --singular ideal, generated by
the steady state functions and the rxr minors of the jacobian. the
singular locus is its variety
    M = (matrix{apply(# gens S, i->(gens S)_i-u_i)})||
(transpose(jacobian I)); --concatenates a new row x-u onto the
jacobian
    J = saturate(I+minors((codim I)+1,M),sing);
    print(G);
    print(concatenate{"dimension and EDD: ", toString(dim J, degree
J)}))

#Another version of this function was

EDDInfo = G -> (
    R=createRing(G,QQ);
```

```
    h=steadyStateEquations G;
    f=subRandomReactionRates G;
    S=QQ[G.ConcentrationRates];
    g=apply(f,p->sub(p,S));
    I=ideal g;
    u={random(QQ),random(QQ)};
    sing=I+minors(codim I, jacobian I);
    M = (matrix{apply(# gens S, i->(gens S)_i-u_i)})||
(transpose(jacobian I));
    J = saturate(I+minors((codim I)+1,M),sing);
    K = saturate(I,sing);
    N = gens gb ideal h;
    print("reaction network:");
    print(G);
    print("steady-state equations:");
    print(h);
    print(concatenate{"generators of the steady state variety: ",
toString (entries N)});
    print(concatenate{"steady-state ideal with random rates:
",toString ideal f});
    print(concatenate{"dimension and EDD: ", toString(dim J, degree
J)});
    print(concatenate{"singular ideal: ", toString(sing)});
    print(concatenate{"dimension of singular locus: ", toString(dim
sing)}); --if this is -1, the singular locus is empty
    print(concatenate{"generators of the singular ideal: ",
toString(entries gens gb sing)});
    print(concatenate{"saturation of the singular ideal in the steady-
state ideal: ", toString K}); --not sure if this is the right thing
for the saturation
)
```

In [0]:

```
#For the list of 210 2S2R CRNs, created a few functions which provided
information about the reaction networks.
#After downloading the file from the database, we created a function
that would read it and turn it into a CRN that we could pair with a
modified version of the original EDD function.

loadPackage "ReactionNetworks"
loadPackage "ReflexivePolytopesDB" --for matrixFromString();

file = "s2r2G.txt"
directory = "~/PRiME2023/Garcia Puente Research Group/EDD
computations"
fn3 = concatenate(directory,"/",file)
get fn3;

codes = apply(lines get fn3, s-> flatten entries matrixFromString s)
edges = for c in codes list(t = drop(c, 2); while #t > 0 list (t_0,
t_1) do t = drop(t,2))
m = (codes_0)_0
n = (codes_0)_1

R = matrix table(n,m, (i,j) -> number(edges_0, e -> e == (j,i+m)) )
L = matrix table(n,m, (i,j) -> number(edges_0, e -> e == (i+m,j)) )
#Formats the edges list into of text file rows into columns of CRN
coefficients

R2 = apply (edges, f -> matrix table(n,m, (i,j) -> number(f, e -> e ==
(j,i+m)) ));
```

```
L2 = apply (edges, f -> matrix table(n,m, (i,j) -> number(f, e -> e == (i+m,j)) ));
```

In [0]:

```
#Defined a function which turns these left and right hand side matrices into a list of CRNs

crnRing = QQ[A, B]
varMatrix = vars crnRing
makeCRN = (m, LHS, RHS) -> (
    myList = apply (m, i -> concatenate(toString((flatten entries LHS_0)_i), " --> ", toString((flatten entries RHS_0)_i)) ); --concatenates and formats the CRNs
    myList2 = apply (m, i -> concatenate separate("[*]", myList_i)); --removes star
    myCRN = reactionNetwork apply(myList2, s -> replace( "0", "0A", s )) --changes 0 into o times a variable
    )

#Due to the limitations of our software, we had to create 4 lists called "Iteration" (numbered, with about 54 elements in each) to call the function and make lists of CRNs corresponding to the database file.

#An example of that is below:

Iteration = for g from 0 to 52 list makeCRN(m, varMatrix*(L2_{g}), varMatrix*(R2_{g}))
```

In [0]:

```
#Also made an all-encompasing function to use for these lists based off of the original EDD function defined above.

loadPackage "ReactionNetworks"

SuperEDD = G ->(
    R1 = createRing(G,QQ);
    f=subRandomReactionRates G;
    S=QQ[G.ConcentrationRates];
    g=apply(f,p->sub(p,S));
    I=ideal g;
    u={random(QQ),random(QQ)};
    if codim (I) == infinity then return("codimension of I is infinite", G) else
    sing=I+minors(codim I, jacobian I);
    M = (matrix{apply(# gens S, i->(gens S)_i-u_i)})||(transpose(jacobian I));
    J = saturate(I+minors((codim I)+1,M),sing);
    print("network:");
    print G;
    --print("steady-state equations:");
    --print(steadyStateEquations G);
    print(concatenate{"dim(J) and EDD: ", toString(dim J, degree J)});
    print(concatenate{"dim(I): ", toString(dim I)});
    print(concatenate{"degree(I): ", toString(degree I)});
    print(concatenate{"generators of singular locus: ", toString(gens gb sing)});
    print(concatenate{"dimension of singular locus: ", toString(dim sing)});
    print
```

```
)

#Example of calling it

for G in Iteration do SuperEDD(G)

#To deal with the "bad" networks, created the following function to
tell us exactly which ones they were

ProblemNetworks = G -> (                          #function to pick out
and print the problem networks!
    R=createRing(G,QQ);
    f=subRandomReactionRates G;
    S=QQ[G.ConcentrationRates];
    g=apply(f,p->sub(p,S));
    I=ideal g;
    if codim I == infinity then print G;
    if codim I == infinity then print ""

)

#Example call

for G in Iteration do ProblemNetworks G
```

| All 2-Species, 2-Reaction Networks | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Number of Reaction Network | networks | degree of l, rad l | dim of l, rad l | EDD wrt l, rad l | dim of sing, sing with rad l | shape of SSV | eqn of SS (xa=x, xb=y) | positive SS variety | EDD of PSSV |
| 183 | A-->0, B-->A+B (Original R22) | 1,1 | 1,1 | 1,1 | -1,-1 | line | y= k1/k2 x | y=k1/k2 x | 1 |
| 184 | A-->B, B-->A (Original R23) | 1,1 | 1,1 | 1,1 | -1,-1 | line | y= k1/k2 x | y=k1/k2 x | 1 |
| 9 | 2A-->2B, 2B-->A+B (Original R1) | 2,2 | 1,1 | 2,2 | 0,0 | X at origin | y^2=2 k1/k2 x^2 | y=sqrt(2 k1/k2)x | 1 |
| 80 | 2A-->2B, 2B-->2A (Original R6) | 2,2 | 1,1 | 2,2 | 0,0 | X at origin | y^2=k1/k2 x^2 | y=sqrt(k1/k2)x | 1 |
| 88 | 2A-->A+B, 2B-->A+B (Original R7) | 2,2 | 1,1 | 2,2 | 0,0 | X at origin | y^2=k1/k2 x^2 | y=sqrt(k1/k2)x | 1 |
| 136 | A+B-->2A, 2A-->2B (Original R19) | 2,2 | 1,1 | 2,2 | 0,0 | rotated X at origin | x(k1 y-2 k2 x)=0 | y=2 k2/k1 x | 1 |
| 144 | A+B-->2B, 2B-->A+B (Original R20) | 2,2 | 1,1 | 2,2 | 0,0 | rotated X at origin | y(k1 x-k2 y)=0 | y=k1/k2 x | 1 |
| 196 | A+B-->A, A-->A+B (Original R25) | 2,2 | 1,1 | 2,2 | 0,0 | plus sign | x(k2-k1 y)=0 | y=k2/k1 | 1 |
| 120 | B-->2B, A+B-->A | 2,2 | 1,1 | 2,2 | 0,0 | plus sign | y(k1 - k2*x) = 0 | x = k1/k2 | 1 |
| 152 | A+B-->2B, B-->A (Original R21) | 2,2 | 1,1 | 2,2 | 0,0 | plus sign | y(k1 x-k2)=0 | x=k2/k1 | 1 |
| 16 | 2A-->2B, B-->A (Original R2) | 2,2 | 1,1 | 3,3 | 0,-1 | parabola | y=2 k1/k2 x^2 | y=2 k1/k2 x^2 | 3 |
| 20 | 2A-->A, B-->A+B (Original R3) | 2,2 | 1,1 | 3,3 | 0,-1 | parabola | y=k1/k2 x^2 | y=k1/k2 x^2 | 3 |
| 69 | B-->A, 2A-->A+B (Original R4) | 2,2 | 1,1 | 3,3 | -1,-1 | parabola | y=k2/k1 x^2 | y=k2/k1 x^2 | 3 |
| 121 | 2B-->0, A-->A+B (Original R10) | 2,2 | 1,1 | 3,3 | -1,-1 | sideways parabola | x=2 k1/k2 y^2 | x=2 k1/k2 y^2 | 3 |
| 127 | A-->2B, 2B-->A (Original R11) | 2,2 | 1,1 | 3,3 | -1,-1 | sideways parabola | x=k2/k1 y^2 | x=k2/k1 y^2 | 3 |
| 112 | 0-->2B, A+B-->A (Original R17) | 2,2 | 1,1 | 4,4 | -1,-1 | hyperbola | xy=2 k1/k2 | xy=2 k1/k2 | 4 |
| 188 | A+B-->0, 0-->A+B (Original R15) | 2,2 | 1,1 | 4,4 | -1,-1 | hyperbola | xy=k2/k1 | xy=k2/k1 | 4 |
| 190 | A+B-->A, 0-->B (Original R24) | 2,2 | 1,1 | 4,4 | -1,-1 | hyperbola | xy=k2/k1 | xy=k2/k1 | 4 |
| 2 | 2A-->2B, 2B-->0 | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 4 | 2B-->0, 2A-->A | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 5 | 2A--> 0, 2B-->A | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 6 | 2A-->2B, 2B-->A | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 11 | 2B-->A, 2A-->A+B | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 12 | 2A-->A, 2B-->A+B | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 79 | 2A-->0, 2B-->0 | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 82 | 2B-->2A, 2A-->A | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 83 | 2B-->0, 2A-->A+B | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 85 | 2A-->B, 2B-->A | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 86 | 2A-->A, 2B-->B | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 87 | 2A-->A, 2B-->A | 4,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 18 | 2A-->2B, B-->A+B | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 22 | B-->0, 2A-->0 | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 23 | B-->2A, 2A-->0 | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 15 | 2A-->0, B-->A | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 54 | B-->2B, 2A-->2B | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 59 | B-->0, 2A-->A | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 60 | B-->2B, 2A-->A | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 63 | B-->2B, 2A-->A+B | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 65 | B-->A, 2A-->B | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 67 | B-->A, 2A-->A | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 71 | B-->A+B , 2A-->A+B | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 91 | B-->2A, 2A-->A | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 110 | 2B-->A, A-->A+B | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 126 | A-->0, 2B-->A | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 129 | A-->2B, 2B-->A+B | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 175 | A-->2A, 2B-->A | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 176 | A-->0, 2B-->A+B | 2,1 | 0,0 | 0,1 | 0,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 24 | B-->2B, 2A-->0 | 2,1 | 0,0 | 0,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 25 | B-->0, 2A-->2B | 2,1 | 0,0 | 0,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 26 | B-->2A, 2A-->2B | 2,1 | 0,0 | 0,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 116 | B-->2B, A-->0 | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 118 | B-->A, A-->A+B | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 130 | A-->2B, B-->0 | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 131 | A-->0, B-->A | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 132 | A-->2B, B-->A | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 133 | A-->2B, B-->A+B | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 178 | A-->0, B-->0 | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 179 | A-->2A, B-->2B | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 180 | A-->2B, B-->2A | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 181 | A-->2A, B-->2A | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 182 | A-->2A, B-->A | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 185 | A-->A+B, B-->A+B | 1,1 | 0,0 | 1,1 | -1,-1 | origin | (x,y)=(0,0) | empty | 0 |
| 7 | 2B-->0, 2B-->A | 2,1 | 1,1 | 0,1 | 1,-1 | x-axis | y=0 | empty | 0 |
| 13 | 2B-->A, 2B-->A+B | 2,1 | 1,1 | 0,1 | 1,-1 | x-axis | y=0 | empty | 0 |
| 81 | 2B-->2A, 2B-->A | 2,1 | 1,1 | 0,1 | 1,-1 | x-axis | y=0 | empty | 0 |
| 21 | 2B-->A, B-->A+B | 1,1 | 1,1 | 1,1 | 0,-1 | x-axis | y=0 | empty | 0 |
| 123 | 2B-->2A, A+B-->A | 1,1 | 1,1 | 1,1 | 0,-1 | x-axis | y = 0 | empty | 0 |
| 138 | A+B-->2B, 2B-->0 | 1,1 | 1,1 | 1,1 | 0,-1 | x-axis | y = 0 | empty | 0 |
| 141 | A+B-->0, 2B-->A | 1,1 | 1,1 | 1,1 | 0,-1 | x-axis | y = 0 | empty | 0 |
| 142 | A+B-->2B, 2B-->A | 1,1 | 1,1 | 1,1 | 0,-1 | x-axis | y = 0 | empty | 0 |
| 150 | A+B-->A, 2B-->A+B | 1,1 | 1,1 | 1,1 | 0,-1 | x-axis | y = 0 | empty | 0 |
| 186 | A+B-->2A, 2B-->A | 1,1 | 1,1 | 1,1 | 0,-1 | x-axis | y=0 | empty | 0 |
| 17 | 2B-->0, B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 55 | B-->2A, 2B-->0 | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 56 | B-->0, 2B-->2A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 57 | B-->2A, 2B-->2A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 58 | B-->2B, 2B-->2A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 61 | B-->0, 2B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 62 | B-->2B, 2B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 64 | B-->2B, 2B-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 66 | B-->A, 2B-->B | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 68 | B-->A, 2B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 72 | B-->A+B, 2B-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 73 | B-->0, B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 74 | B-->2B, B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 75 | B-->2B, B-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 76 | B-->2A, B-->0 | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 77 | B-->2B, B-->2A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 78 | B-->A, B-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 90 | B-->2A, 2B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 92 | B-->2A, B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 124 | B-->2A, A+B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y = 0 | empty | 0 |
| 151 | A+B-->0, B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y = 0 | empty | 0 |
| 162 | A+B-->2B, B-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 163 | A+B-->0, B-->0 | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 164 | A+B-->0, B-->2A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 165 | A+B-->0, B-->2B | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 166 | A+B-->2A, B-->0 | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |

| All 2-Species, 2-Reaction Networks | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| Number of Reaction Network | networks | degree of l, rad l | dim of l, rad l | EDD wrt l, rad l | dim of sing, sing with rad l | shape of SSV | eqn of SS (xa=x, xb=y) | positive SS variety | EDD of PSSV |
| 167 | A+B-->2A, B-->2A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 168 | A+B-->2A, B-->2B | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 169 | A+B-->2B, B-->0 | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 170 | A+B-->2B, B-->2A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 171 | A+B-->2B, B-->2B | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 172 | A+B-->B, B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 173 | A+B-->A, B-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 174 | A+B-->A, B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | x-axis | y=0 | empty | 0 |
| 1 | 2A-->2B, 2A-->0 | 2,1 | 1,1 | 0,1 | 1,-1 | y-axis | x=0 | empty | 0 |
| 3 | 2A-->2B, 2A-->A | 2,1 | 1,1 | 0,1 | 1,-1 | y-axis | x=0 | empty | 0 |
| 8 | 2A-->2B, 2A-->A+B | 2,1 | 1,1 | 0,1 | 1,-1 | y-axis | x=0 | empty | 0 |
| 10 | 2A-->A, 2A-->A+B | 2,1 | 1,1 | 0,1 | 1,-1 | y-axis | x=0 | empty | 0 |
| 14 | 2A-->A, 2A-->B | 2,1 | 1,1 | 0,1 | 1,-1 | y-axis | x=0 | empty | 0 |
| 84 | 2A-->0, 2A-->A+B | 2,1 | 1,1 | 0,1 | 1,-1 | y-axis | x=0 | empty | 0 |
| 111 | 2A-->2B, A+B-->0 | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 113 | 2A-->0, A+B-->A | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 114 | 2A-->2B, A+B-->A | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 134 | A+B-->0, 2A-->0 | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 135 | A+B-->2B, 2A-->0 | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 139 | A+B-->0, 2A-->A | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 140 | A+B-->2B, 2A-->A | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 145 | A+B-->B, 2A-->B | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 147 | A+B-->A, 2A-->B | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 148 | A+B-->A, 2A-->A | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 149 | A+B-->A, 2A-->A+B | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x = 0 | empty | 0 |
| 187 | A+B-->2A, 2A-->A | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x=0 | empty | 0 |
| 189 | A+B-->0, 2A-->A+B | 1,1 | 1,1 | 1,1 | 0,-1 | y-axis | x=0 | empty | 0 |
| 108 | 2A-->2B, A-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x = 0 | empty | 0 |
| 109 | 2A-->A, A-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x = 0 | empty | 0 |
| 122 | 2A-->0, A-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x = 0 | empty | 0 |
| 125 | A-->2B, 2A-->A | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x = 0 | empty | 0 |
| 128 | A-->2B, 2A-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x = 0 | empty | 0 |
| 177 | A-->0, 2A-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x=0 | empty | 0 |
| 192 | A-->2B, A-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x=0 | empty | 0 |
| 193 | A-->0, A+B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x=0 | empty | 0 |
| 194 | A-->2B, A+B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x=0 | empty | 0 |
| 195 | A+B-->2B, A-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x=0 | empty | 0 |
| 200 | A-->0, A-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x=0 | empty | 0 |
| 201 | A-->2A, A+B-->A | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x=0 | empty | 0 |
| 202 | A+B-->0, A-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | y-axis | x=0 | empty | 0 |
| 197 | A+B-->2B, A+B-->0 | 2,2 | 1,1 | 2,2 | 0,0 | both axes | x=0, y=0 | empty | 0 |
| 198 | A+B-->0, A+B-->A | 2,2 | 1,1 | 2,2 | 0,0 | both axes | x=0, y=0 | empty | 0 |
| 199 | A+B-->2B, A+B-->A | 2,2 | 1,1 | 2,2 | 0,0 | both axes | x=0, y=0 | empty | 0 |
| 203 | A+B-->2A, A+B-->A | 2,2 | 1,1 | 2,2 | 0,0 | both axes | x=0, y=0 | empty | 0 |
| 204 | A+B-->2A, A+B-->2B | 2,2 | 1,1 | 2,2 | 0,0 | both axes | x=0, y=0 | empty | 0 |
| 205 | A+B-->A, A+B-->B | 2,2 | 1,1 | 2,2 | 0,0 | both axes | x=0, y=0 | empty | 0 |
| 19 | 0-->A, B-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | line | y=-k1/k2 | empty | 0 |
| 93 | 0-->2B, A-->A+B | 1,1 | 1,1 | 1,1 | -1,-1 | line | x=-2k1/k2 | empty | 0 |
| 117 | B-->2B, A-->A+B (Original R9) | 1,1 | 1,1 | 1,1 | -1,-1 | line | y= -k2/k1 x | empty | 0 |
| 70 | B-->A, 2B-->A+B (Original R5) | 2,2 | 1,1 | 2,2 | 0,-1 | horizontal parallel lines | y(k1+k2 y)=0 | empty | 0 |
| 89 | 2B-->2A, B-->A (Original R8) | 2,2 | 1,1 | 2,2 | -1,-1 | horizontal parallel lines | y(k1+2 k2 y)=0 | empty | 0 |
| 191 | A+B-->2A, B-->A (Original R16) | 2,2 | 1,1 | 2,2 | 0,0 | plus sign | y(k1+k2 x)=0 | empty | 0 |
| 115 | 2B-->0, A+B-->A (Original R18) | 2,2 | 1,1 | 2,2 | 0,0 | rotated X at origin | y(2 k1 y+k2 x)=0 | empty | 0 |
| 119 | B-->0, A+B-->A | 2,2 | 1,1 | 2,2 | 0,0 | rotated X at origin | y=0, x = -k1/k2 | empty | 0 |
| 137 | A+B-->2B, 2A-->2B (Original R12) | 2,2 | 1,1 | 2,2 | 0,0 | rotated X at origin | x(k1 y+2 k2 x)=0 | empty | 0 |
| 143 | A+B-->2B, 2A-->A+B (Original R13) | 2,2 | 1,1 | 2,2 | 0,0 | rotated X at origin | x(k1 x+k2 y)=0 | empty | 0 |
| 146 | A+B-->B, 2A-->A (Original R14) | 2,2 | 1,1 | 2,2 | 0,0 | rotated X at origin | x(k1 x+k2 y)=0 | empty | 0 |
| 27 | 0-->2B, 2A-->0 | | | | | empty | | empty | 0 |
| 28 | 0-->2A, 2A-->2B | | | | | empty | | empty | 0 |
| 29 | 0-->2B, 2A-->2B | | | | | empty | | empty | 0 |
| 30 | 0-->2B, 0-->A | | | | | empty | | empty | 0 |
| 31 | 2A-->2B, 0-->A | | | | | empty | | empty | 0 |
| 32 | 0-->2B, 2A-->A | | | | | empty | | empty | 0 |
| 33 | 2B-->0, 0-->A | | | | | empty | | empty | 0 |
| 34 | 0-->2B, 2B-->A | | | | | empty | | empty | 0 |
| 35 | 0-->2B, 0-->A+B | | | | | empty | | empty | 0 |
| 36 | 2A-->2B, 0-->A+B | | | | | empty | | empty | 0 |
| 37 | 0-->2B, 2A-->A+B | | | | | empty | | empty | 0 |
| 38 | 0-->2B, 2B-->A+B | | | | | empty | | empty | 0 |
| 39 | 0-->B, 2A-->B | | | | | empty | | empty | 0 |
| 40 | 0-->B, 2A-->A | | | | | empty | | empty | 0 |
| 41 | 0-->A, 2A-->B | | | | | empty | | empty | 0 |
| 42 | 0-->A, 0-->A+B | | | | | empty | | empty | 0 |
| 43 | 2A-->A, 0-->A+B | | | | | empty | | empty | 0 |
| 44 | 0-->A, 2A-->A+B | | | | | empty | | empty | 0 |
| 45 | 2B-->A, 0-->A+B | | | | | empty | | empty | 0 |
| 46 | 0-->A, 2B-->A+B | | | | | empty | | empty | 0 |
| 47 | 0-->A+B, 2A-->A+B | | | | | empty | | empty | 0 |
| 48 | 0-->2B, B-->A | | | | | empty | | empty | 0 |
| 49 | 0-->2B, B-->A+B | | | | | empty | | empty | 0 |
| 50 | B-->0, 0-->2A | | | | | empty | | empty | 0 |
| 51 | B-->2A, 0-->2A | | | | | empty | | empty | 0 |
| 52 | B-->2B, 0-->2A | | | | | empty | | empty | 0 |
| 53 | B-->2A, 0-->2B | | | | | empty | | empty | 0 |
| 94 | B-->0, 0-->A | | | | | empty | | empty | 0 |
| 95 | B-->2B, 0-->A | | | | | empty | | empty | 0 |
| 96 | B-->2B, 0-->A+B | | | | | empty | | empty | 0 |
| 97 | B-->A, 0-->B | | | | | empty | | empty | 0 |
| 98 | B-->A, 0-->A | | | | | empty | | empty | 0 |
| 99 | B-->A, 0-->A+B | | | | | empty | | empty | 0 |
| 100 | B-->A+B, 0-->A+B | | | | | empty | | empty | 0 |
| 101 | 2B-->2A, 0-->A | | | | | empty | | empty | 0 |
| 102 | 0-->2A, 2B-->A | | | | | empty | | empty | 0 |
| 103 | 2A-->0, 0-->A+B | | | | | empty | | empty | 0 |
| 104 | 0-->2A, 0-->2B | | | | | empty | | empty | 0 |
| 105 | 0-->A, 0-->B | | | | | empty | | empty | 0 |
| 106 | 0-->2A, B-->A | | | | | empty | | empty | 0 |
| 107 | B-->2A, 0-->A | | | | | empty | | empty | 0 |

**All 2-Species, 2-Reaction Networks**

| Number of Reaction Network | networks | degree of l, rad l | dim of l, rad l | EDD wrt l, rad l | dim of sing, sing with rad l | shape of SSV | eqn of SS (xa=x, xb=y) | positive SS variety | EDD of PSSV |
|---|---|---|---|---|---|---|---|---|---|
| 153 | 0-->A, A-->A+B | | | | | empty | | empty | 0 |
| 154 | 0-->2B, A+B-->0 | | | | | empty | | empty | 0 |
| 155 | 0-->2A, A+B-->A | | | | | empty | | empty | 0 |
| 156 | A-->2B, 0-->A | | | | | empty | | empty | 0 |
| 157 | A-->2B, 0-->A+B | | | | | empty | | empty | 0 |
| 158 | A+B-->0, 0-->A | | | | | empty | | empty | 0 |
| 159 | A+B-->2B, 0-->A | | | | | empty | | empty | 0 |
| 160 | A+B-->2B, 0-->A+B | | | | | empty | | empty | 0 |
| 161 | A+B-->A, 0-->A+B | | | | | empty | | empty | 0 |
| 206 | A-->0, 0-->A+B | | | | | empty | | empty | 0 |
| 207 | A+B-->2B, 0-->2A | | | | | empty | | empty | 0 |
| 208 | A+B-->2A, 0-->2A | | | | | empty | | empty | 0 |
| 209 | A+B-->2A, 0-->A | | | | | empty | | empty | 0 |
| 210 | A+B-->A, 0-->A | | | | | empty | | empty | 0 |

| SSV color coding | pssv color coding | ssv vs pssv color coding |
|---|---|---|
| empty | empty | same, nonempty |
| point(s) | point(s) | same, empty |
| axis/axes | slanted line | different, nonempty pssv |
| plus sign | horizontal line | different, empty pssv |
| rotated X at origin | vertical line | |
| line | parabola | |
| horizontal parallel lines | hyperbola | |
| X at origin | | |
| parabola | | |
| sideways parabola | | |
| hyperbola | | |

| classifications | | | |
|---|---|---|---|
| **nonempty pssv** | # networks | #with pssv=ssv | ssv when distinct |
| line through origin | 7 | 2 | 3 X at origin, 2 rotated X at origin |
| horizontal line | 1 | 0 | plus sign |
| vertical line | 2 | 0 | plus sign |
| parabola | 5 | 5 | |
| hyperbola | 3 | 3 | |
| total | 18 | 10 | |

| **ssv for empty pssv** | # networks |
|---|---|
| origin | 44 |
| x-axis | 44 |
| y-axis | 32 |
| both axes | 6 |
| line | 3 |
| horizontal parallel lines | 2 |
| plus sign | 1 |
| rotated X at origin | 5 |
| empty | 55 |
| total | 192 |

| All 1-Species, 2-Reaction Networks | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **networks** | **mixed volume** | **shape of variety** | **equation wrt rxn rates** | **EDD** | **pos ssv** | **shape of pssv** | **EDD of PSSV** | **weakly reversible?** | **deficiency** | |
| R5: 0-->A, 0--> 2A | 0 | empty* | N/A | 0 | empty | | 0 | F | 1 | |
| R6: 2A-->A, 2A-->0 | 0 | one point | x=0 | 0** | empty | | 0 | F | 1 | |
| R15: A-->2A, A-->0 | 0 | one point | x=0 | 1 | empty | | 0 | F | 1 | |
| R8: A-->2A, 0-->2A | 1 | one point | x=-2 k2/k1 | 1 | empty | | 0 | F | 1 | |
| R12: A-->2A, 0-->A | 1 | one point | x=-k2/k1 | 1 | empty | | 0 | F | 1 | |
| R7: A-->0, 0-->2A | 1 | one point | x=2 k2/k1 | 1 | x=2 k2/k1 | one point | 1 | F | 0 | |
| R11: A-->0, 0-->A | 1 | one point | x=k2/k1 | 1 | x=k2/k1 | one point | 1 | T | 1 | |
| R9: A-->0, 2A-->0 | 1 | two points | x=0, x=-k1/2 k2 | 2 | empty | | 0 | F | 1 | |
| R13: A-->0, 2A-->A | 1 | two points | x=0, x=-k1/k2 | 2 | empty | | 0 | F | 1 | |
| R10: A-->2A, 2A-->0 | 1 | two points | x=0, x=k1/2 k2 | 2 | x=k1/2 k2 | one point | 1 | F | 1 | |
| R14: A-->2A, 2A-->A | 1 | two points | x=0, x=k1/k2 | 2 | x=k1/k2 | one point | 1 | T | 0 | |
| R1: 0-->2A, 2A-->0 | 2 | two points | x=pm sqrt(k1/k2) | 2 | x=sqrt(k1/k2) | one point | 1 | T | 0 | |
| R2: 0-->2A, 2A-->A | 2 | two points | x=pm sqrt(2 k1/k2) | 2 | x=sqrt(2 k1/k2) | one point | 1 | F | 1 | |
| R3: 0-->A, 2A-->0 | 2 | two points | x=pm sqrt(k1/2 k2) | 2 | x=sqrt(k1/2 k2) | one point | 1 | F | 1 | |
| R4: 0-->A, 2A-->A | 2 | two points | x=pm sqrt(k1/k2) | 2 | x=sqrt(k1/k2) | one point | 1 | F | 1 | |
| | | *gives error message when running function because the steady state variety is empty | | | | | | | | |
| | | | | **x=0 is a singularity because it has multiplicity 2, so we throw it out when calculating the EDD. the EDD using the radical ideal is 1. | | | | | | |

| All 1-Species, 3-Reaction Networks | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| networks | mixed volume | shape of variety | equation wrt rxn rates | EDD | pssv depends on rxn rates? | pos ssv | shape of pssv | EDD of pssv | weakly reversible? | deficiency |
| R17: A-->2A, A-->0, 0-->2A | 1 | one point | x=(-2 k3) / (k1-k2) | 1 | yes | x=(-2 k3) / (k1-k2)  [WHEN k1<k2] | one point | 1 | F | 1 |
| R19: A-->2A, A-->0, 0-->A | 1 | one point | x= k3 / (k2-k1) | 1 | yes | x=k3 / (k2-k1)  [WHEN k1<k2] | one point | 1 | F | 1 |
| R13: A-->0, 0-->A, 0-->2A | 1 | one point | x=(k2+2 k3) / k1 | 1 | no | x=(k2+2 k3) / k1 | one point | 1 | F | 1 |
| R14: A-->2A, 0-->A, 0-->2A | 1 | one point | x=-(k2+2 k3) / k1 | 1 | no | empty | | 0 | F | 1 |
| R18: A-->2A, A-->0, 2A-->0 | 1 | two points | x=0, (k1-k2) / (2 k3) | 2 | yes | x=(k1-k2) / (2 k3)  [WHEN k1>k2] | one point | 1 | F | 1 |
| R20: A-->2A, A-->0, 2A-->A | 1 | two points | x=0, (k1-k2) / k3 | 2 | yes | x=(k1-k2) / k3  [WHEN k1>k2] | one point | 1 | F | 1 |
| R15: A-->0, 2A-->A, 2A-->0 | 1 | two points | x=0, -k1 / (k2+2 k3) | 2 | no | empty | | 0 | F | 1 |
| R16: A-->2A, 2A-->A, 2A-->0 | 1 | two points | x=0, k1 / (k2+2 k3) | 2 | no | x=k1 / (k2+2 k3) | one point | 1 | F | 1 |
| R1: 0-->2A, 2A-->A, 2A-->0 | 2 | two points | x=pm sqrt((2 k1) / (k2+2 k3)) | 2 | no | x=sqrt((2 k1) / (k2+2 k3)) | one point | 1 | F | 1 |
| R2: 2A-->0, 0-->A, 0-->2A | 2 | two points | x=pm sqrt((k2+2 k3) / (2 k1)) | 2 | no | x=sqrt((k2+2 k3) / (2 k1)) | one point | 1 | F | 1 |
| R3: 0-->A, 2A-->A, 2A-->0 | 2 | two points | x=pm sqrt((k1) / (k2+2 k3)) | 2 | no | x=sqrt((k1) / (k2+2 k3)) | one point | 1 | F | 1 |
| R4: 2A-->A, 0-->A, 0-->2A | 2 | two points | x=pm sqrt((k2+2 k3) / k1) | 2 | no | x=sqrt((k2+2 k3) / k1) | one point | 1 | F | 1 |
| R5: A-->0, 0-->2A, 2A-->0 | 2 | two points | x=(-k1 pm sqrt(k1^2+16 k2 k3)) / (4 k3) | 2 | no | x=(-k1 + sqrt(k1^2+16 k2 k3)) / (4 k3) | one point | 1 | F | 1 |
| R6: A-->2A, 0-->2A, 2A-->0 | 2 | two points | x=(k1 pm sqrt(k1^2+16 k2 k3)) / (4 k3) | 2 | no | x=(k1 + sqrt(k1^2+16 k2 k3)) / (4 k3) | one point | 1 | F | 1 |
| R7: A-->0, 0-->2A, 2A-->A | 2 | two points | x=(-k1 pm sqrt(k1^2+8 k2 k3)) / (2 k3) | 2 | no | x=(-k1 + sqrt(k1^2+8 k2 k3)) / (2 k3) | one point | 1 | T | 1 |
| R8: A-->2A, 0-->2A, 2A-->A | 2 | two points | x=(k1 pm sqrt(k1^2+8 k2 k3)) / (2 k3) | 2 | no | x=(k1 + sqrt(k1^2+8 k2 k3)) / (2 k3) | one point | 1 | F | 1 |
| R9: A-->0, 0-->A, 2A-->0 | 2 | two points | x=(-k1 pm sqrt(k1^2+8 k2 k3)) / (4 k3) | 2 | no | x=(-k1 + sqrt(k1^2+8 k2 k3)) / (4 k3) | one point | 1 | F | 1 |
| R10: A-->2A, 0-->A, 2A-->0 | 2 | two points | x=(k1 pm sqrt(k1^2+8 k2 k3)) / (4 k3) | 2 | no | x=(k1 + sqrt(k1^2+8 k2 k3)) / (4 k3) | one point | 1 | T | 1 |
| R11: A-->0, 0-->A, 2A-->0 | 2 | two points | x=(-k1 pm sqrt(k1^2+4 k2 k3)) / (2 k3) | 2 | no | x=(-k1 + sqrt(k1^2+4 k2 k3)) / (2 k3) | one point | 1 | F | 1 |
| R12: A-->2A, 0-->A, 2A-->A | 2 | two points | x=(k1 pm sqrt(k1^2+4 k2 k3)) / (2 k3) | 2 | no | x=(k1 + sqrt(k1^2+4 k2 k3)) / (2 k3) | one point | 1 | F | 1 |

| All 1-Species, 4-Reaction Networks | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **networks** | **mixed volume** | **shape of variety** | **equation wrt rxn rates** | **EDD** | **pssv depends on rates?** | **pos ssv** | **shape of pssv** | **EDD of pssv** | **weakly reversible?** | **deficiency** |
| R14: A-->2A, A-->0, 0-->A, 0-->2A | 1 | one point | x=(k3+2k4) / (k2-k1) | 1 | yes | x=(k3+2k4) / (k2-k1)  [WHEN k1<k2] | one point | 1 | F | 1 |
| R10: A-->2A, A-->0, 0-->2A, 2A-->0 | 1 | two points | x=((k1-k2) pm sqrt((k1-k2)^2+16 k3 k4)) / (4 k4) | 2 | no | x=((k1-k2) + sqrt((k1-k2)^2+16 k3 k4)) / (4 k4) | one point | 1 | F | 1 |
| R15: A-->2A, A-->0, 2A-->A, 2A-->0 | 1 | two points | x=0, (k1-k2) / (k3+2 k4) | 2 | yes | x=(k1-k2) / (k3+2 k4)  [WHEN k1>k2] | one point | 1 | F | 1 |
| R2: A-->0, 0-->2A, 2A-->A, 2A-->0 | 2 | two points | x=pm sqrt((2 k2-k1) / (k3+2 k4)) | 2 | yes* | x=sqrt((2 k2-k1) / (k3+2 k4))  [WHEN k1<2k2] | one point | 1 | T | 1 |
| R1: 0-->A, 0-->2A, 2A-->A, 2A-->0 | 2 | two points | x=pm sqrt((k1+2 k2) / (k3+2 k4)) | 2 | no | x= sqrt((k1+2 k2) / (k3+2 k4)) | one point | 1 | F | 1 |
| R3: A-->2A, 0-->2A, 2A-->A, 2A-->0 | 2 | two points | x=(k1 pm sqrt(k1^2+8 k2 k3+16 k2 k4)) / 2(k3+2 k4) | 2 | no | x=(k1 + sqrt(k1^2+8 k2 k3+16 k2 k4)) / 2(k3+2 k4) | one point | 1 | T | 1 |
| R4: A-->0, 2A-->0, 0-->A, 0-->2A | 2 | two points | x=(-k1 pm sqrt(k1^2+8 k2 k3+16 k2 k4)) / (4 k2) | 2 | no | x=(-k1 + sqrt(k1^2+8 k2 k3+16 k2 k4)) / (4 k2) | one point | 1 | T | 1 |
| R5: A-->2A, 2A-->0, 0-->A, 0-->2A | 2 | two points | x=(k1 pm sqrt(k1^2+8 k2 k3+16 k2 k4)) / (4 k2) | 2 | no | x=(k1 + sqrt(k1^2+8 k2 k3+16 k2 k4)) / (4 k2) | one point | 1 | T | 1 |
| R6: A-->0, 0-->A, 2A-->A, 2A-->0 | 2 | two points | x=(-k1 pm sqrt(k1^2+4 k2 k3+8 k2 k4)) / 2(k3+2 k4) | 2 | no | x=(-k1 + sqrt(k1^2+4 k2 k3+8 k2 k4)) / 2(k3+2 k4) | one point | 1 | F | 1 |
| R7: A-->2A, 0-->A, 2A-->A, 2A-->0 | 2 | two points | x=(k1 pm sqrt(k1^2+4 k2 k3+8 k2 k4)) / 2(k3+2 k4) | 2 | no | x=(k1 + sqrt(k1^2+4 k2 k3+8 k2 k4)) / 2(k3+2 k4) | one point | 1 | T | 1 |
| R8: A-->0, 2A-->A, 0-->A, 0-->2A | 2 | two points | x=(-k1 pm sqrt(k1^2+4 k2 k3+8 k2 k4)) / (2 k2) | 2 | no | x=(-k1 + sqrt(k1^2+4 k2 k3+8 k2 k4)) / (2 k2) | one point | 1 | T | 1 |
| R9: A-->2A, 2A-->A, 0-->A, 0-->2A | 2 | two points | x=(k1 pm sqrt(k1^2+4 k2 k3+8 k2 k4)) / (2 k2) | 2 | no | x=(k1 + sqrt(k1^2+4 k2 k3+8 k2 k4)) / (2 k2) | one point | 1 | F | 1 |
| R11: A-->2A, A-->0, 0-->2A, 2A-->A | 2 | two points | x=((k1-k2) pm sqrt((k1-k2)^2+8 k3 k4)) / (2 k4) | 2 | no | x=((k1-k2) + sqrt((k1-k2)^2+8 k3 k4)) / (2 k4) | one point | 1 | T | 1 |
| R12: A-->2A, A-->0, 0-->A, 2A-->0 | 2 | two points | x=((k1-k2) pm sqrt((k1-k2)^2+8 k3 k4)) / (4 k4) | 2 | no | x=((k1-k2) + sqrt((k1-k2)^2+8 k3 k4)) / (4 k4) | one point | 1 | T | 1 |
| R13: A-->2A, A-->0, 0-->A, 2A-->A | 2 | two points | x=((k1-k2) pm sqrt((k1-k2)^2+4 k3 k4)) / (2 k4) | 2 | no | x=((k1-k2) + sqrt((k1-k2)^2+4 k3 k4)) / (2 k4) | one point | 1 | T | 1 |
| | | | | | *real points in variety depend on rxn rates. if k1>2 k2, we have two complex points in the variety (and NO real points) | | | | | |

| All 1-Species, 5-Reaction Networks | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| network | mv | shape of variety | equation wrt rxn rates | EDD | pos ssv | shape of pssv | EDD of pssv | weakly reversible? | deficiency |
| R1: A-->0, 0-->A, 0-->2A, 2A-->A, 2A-->0 | 2 | two points | x=(-k1 pm sqrt(k1^2+4 k2 k4+8 k3 k4+8 k2 k5+16 k3 k5)) / 2(k4+2 k5) | 2 | x=(-k1 + sqrt(k1^2+4 k2 k4+8 k3 k4+8 k2 k5+16 k3 k5)) / 2(k4+2 k5) | one point | 1 | T | 1 |
| R2: A-->2A, 0-->A, 0-->2A, 2A-->A, 2A-->0 | 2 | two points | x=(k1 pm sqrt(k1^2+4 k2 k4+8 k3 k4+8 k2 k5+16 k3 k5)) / 2(k4+2 k5) | 2 | x=(k1 + sqrt(k1^2+4 k2 k4+8 k3 k4+8 k2 k5+16 k3 k5)) / 2(k4+2 k5) | one point | 1 | T | 1 |
| R3: A-->2A, A-->0, 0-->2A, 2A-->A, 2A-->0 | 2 | two points | x=((k1-k2) pm sqrt((k1-k2)^2+8 k3 k4+16 k3 k5)) / 2(k4+2 k5) | 2 | x=((k1-k2) + sqrt((k1-k2)^2+8 k3 k4+16 k3 k5)) / 2(k4+2 k5) | one point | 1 | T | 1 |
| R4: A-->2A, A-->0, 2A-->0, 0-->A, 0-->2A | 2 | two points | x=((k1-k2) pm sqrt((k1-k2)^2+8 k3 k4+16 k3 k5)) / (4 k3) | 2 | x=((k1-k2) + sqrt((k1-k2)^2+8 k3 k4+16 k3 k5)) / (4 k3) | one point | 1 | T | 1 |
| R5: A-->2A, A-->0, 0-->A, 2A-->A, 2A-->0 | 2 | two points | x=((k1-k2) pm sqrt((k1-k2)^2+4 k3 k4+8 k3 k5)) / 2(k4+2 k5) | 2 | x=((k1-k2) + sqrt((k1-k2)^2+4 k3 k4+8 k3 k5)) / 2(k4+2 k5) | one point | 1 | T | 1 |
| R6: A-->2A, A-->0, 2A-->A, 0-->A, 0-->2A | 2 | two points | x=((k1-k2) pm sqrt((k1-k2)^2+4 k3 k4+8 k3 k5)) / (2 k3) | 2 | x=((k1-k2) + sqrt((k1-k2)^2+4 k3 k4+8 k3 k5)) / (2 k3) | one point | 1 | T | 1 |

| All 1-Species, 6-Reaction Networks | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| networks | mv | shape of variety | equation wrt rxn rates | EDD | pos ssv | shape of pssv | EDD of pssv | weakly reversible? | deficiency |
| R1: A-->2A, A-->0, 0-->A, 0-->2A, 2A-->A, 2A-->0 | 2 | two points | x=((k1-k2) pm sqrt((k1-k2)^2+4(k3+2 k4)(k5+2 k6))) / 2(k5+2 k6) | 2 | x=((k1-k2) + sqrt((k1-k2)^2+4(k3+2 k4)(k5+2 k6))) / 2(k5+2 k6) | one point | 1 | T | 1 |

| Original 25 2-Species, 2-Reaction Networks | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 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 |
| 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 |
| R23: A-->B, B-->A | 1 | 1 | 1 | T | 0 | -1 | line | slope k1/k2 | y= k1/k2 x | y=k1/k2 x | 1 |
| R9: B-->2B, A-->B+A | 1 | 1 | 1 | F | 1 | -1 | line | slope -k2/k1 | y= -k2/k1 x | empty | 0 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |
| 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 |