The structure of the moduli spaces of toric dynamical systems

Gheorghe Craciun\textsuperscript{1}, Jiaxin Jin\textsuperscript{2}, Miruna-Ştefana Sorea\textsuperscript{3}

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Abstract

We consider complex-balanced mass-action systems, or toric dynamical systems. They are remarkably stable polynomial dynamical systems arising from reaction networks seen as Euclidean embedded graphs. We study the moduli spaces of toric dynamical systems, called the toric locus: given a reaction network, we are interested in the topological structure of the set of parameters giving rise to toric dynamical systems. First we show that the complex-balanced equilibria depend continuously on the parameter values. Using this result, we prove that the toric locus of any toric dynamical system is connected. In particular, we emphasize its product structure: it is homeomorphic to the product of the set of complex-balanced flux vectors and the affine invariant polyhedron. Finally, we show that the toric locus is invariant with respect to bijective affine transformations of the generating reaction network.

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\textsuperscript{1}University of Wisconsin-Madison, USA
\textsuperscript{2}Ohio State University, USA
\textsuperscript{3}SISSA (Scuola Internazionale Superiore di Studi Avanzati), Trieste, Italy and Lucian Blaga University of Sibiu, Romania
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1 Introduction

Nonlinear dynamical systems are among the most common mathematical models used in the study of population dynamics, epidemiology, biochemistry, just to name a few [40]. However, the long-term dynamical behaviour of nonlinear dynamical systems is sophisticated. Finding explicit, quantitative answers related to the question of how a system evolves in continuous time is usually impossible. Inspired by the work of Poincaré [34], mathematicians started tackling the qualitative aspects of these systems. However, this task is also a difficult one. For instance, consider the second part of Hilbert’s 16th problem, concerning polynomial dynamical systems in the real plane. After more than a century, the problem of finding an upper bound for the number of limit cycles remains open even in the quadratic case; for technical details and historical aspects of Hilbert’s 16th problem, we refer the reader to [26], [31, Chapter 11]. Another example meant to show that nonlinear dynamical systems are challenging is the Lorenz system: a quadratic polynomial dynamical system, in the three-dimensional Euclidean space, which exhibits chaotic dynamics [30].

1.1 Context

We focus on polynomial dynamical systems generated by (bio-chemical) reaction / interaction networks, the latter being represented by directed graphs in the Euclidean space. One of the goals of reaction network theory is to determine information about the qualitative long-term dynamics from the algebro-combinatorial structure of the network. In order to model the evolution in time of the concentrations of interacting species, we use autonomous systems of ordinary differential equations, dictated by the network structure. Under the assumption of mass-action kinetics ([18, Section 2.1.2]), this leads to fruitful interactions between the study of (bio-chemical) reaction networks and applied algebraic geometry (see [16]), because these systems are polynomial systems. The law of mass-action is very commonly used in mathematical modeling, for instance in population dynamics and in biochemistry [5].

In particular, we are interested in complex-balanced mass-action systems (see [18, Chapter 15]). Introduced by Horn and Jackson in [24], these represent a large class of polynomial dynamical systems that are known and in some cases conjectured to have a stable dynamical behaviour that is very desirable in applications. For instance, Horn and Jackson proved that complex-balanced dynamical systems possess exactly one positive equilibrium up to conservation laws (i.e. in each invariant polyhedron) and that this equilibrium is locally asymptotically stable (see [24], [40, Theorem 2.3]). One of the most important lines of research in the field of reaction network theory is the Global Attractor Conjecture, which says
that this equilibrium is actually \emph{globally} asymptotically stable. This has been already proven in several cases, under mild hypotheses. For the state of the art, we refer the reader to [40]. A proof in all generality of the Global Attractor Conjecture has been proposed by Craciun in [11].

Besides their stable dynamical behaviour, another advantage of complex-balanced dynamical systems is the fact that tools from commutative algebra, computational, applied, real algebraic geometry turned out to be useful in deducing qualitative dynamical properties, which are often encoded or hidden in the geometric structure of the associated reaction networks. For instance, in [12] complex-balanced dynamical systems have also been called \emph{toric dynamical systems} by Craciun, Dickenstein, Shiu and Sturmfels, to emphasize their strong combinatorial aspects and the remarkable algebraic properties of their moduli spaces. Let us be more precise. Consider the parameter space of a reaction network. The set of parameters giving rise to complex-balanced dynamical systems is called \emph{the toric locus} because up to a change of coordinates, this set is a variety given by a binomial ideal, intersected with the positive orthant (see [12]). Toric varieties appear in numerous applications [32] and are very appreciated and well understood by algebraic geometers, who use them often in their quest for examples and counterexamples, due to their combinatorial representation and their computational assets. For a presentation of toric varieties from the point of view of Nonlinear Algebra, the reader may refer to [32, Chapter 8]; according to [32, page 126], “the world is toric”. Increasing interest for the moduli spaces of toric dynamical systems has been shown recently. For instance, methods to expand the toric locus from a set of Lebesgue measure zero to a positive measure set called \emph{the disguised toric locus} are proposed in the form of a systematic algorithm in [33], where the authors leverage the notion of dynamical equivalence from [14]. See also [22], where the authors show that the disguised toric locus is invariant under invertible affine transformations of the network.

1.2 Main contribution

The results of this paper concern the topological structure of the toric locus. One of our main contributions is to show that the complex-balanced equilibria depend \emph{continuously} on the parameter values (Theorem 3.5). The latter are also called reaction rate constants and represent positive real numbers. We further use this result to prove that the moduli space, or toric locus, of any toric dynamical system is \emph{connected} (Theorem 3.16). Next, in Theorem 4.8 we show that the moduli space is \emph{homeomorphic to the product} of the set of complex-balanced flux vectors (Definition 4.2) and the affine invariant polyhedron (Definition 2.9).

Being homeomorphic to the product of two path-connected spaces, it follows that the toric locus is path-connected. Hence, given any two points in the toric locus of a toric dynamical system, there will exist a continuous path between them. This might be advantageous in computations, for instance when using numerical methods for constructing the set of equilibria along a path in parameter space. Recall that the main strategy used by homotopy continuation methods is tracking the solutions of systems of polynomial equations which are easier to solve than the given system, or which are already known (see for instance BERTINI [4], Julia HomotopyContinuation [7], [17], [39], [8], [36], [3]).

Furthermore, we recover a result from [12, Theorem 9], which says that the codimension of the toric locus in the parameter space is equal to the deficiency of the network (see Definition
4.13). We also show that the toric locus is invariant under bijective affine transformations of a network.

1.3 Structure of the paper

In Section 2, we introduce standard terminology and notations concerning dynamical systems generated by reaction networks, mostly focusing on mass-action complex-balanced dynamical systems, also called toric. In Section 3, we prove that complex-balanced equilibria depend continuously on the parameter values. Leveraging this result, in Section 3.1 we show that the toric locus is connected. In Section 4, we first prove that the toric locus is homeomorphic to a product space. Using this property, in Section 4.3 we show Proposition 4.14 which gives a precise formula for the dimension of the toric locus of the network. In Section 4.4, we prove Theorem 4.17 showing that any bijective affine transformation preserves the toric locus.

2 Preliminary notions

In this section, mostly following [40], we present standard terminology, concerning a special class of nonlinear dynamical systems, that are generated by (bio-chemical) reaction networks, under the assumption of mass-action kinetics. For an introduction to the general theory of nonlinear dynamical systems, the reader could refer for instance to the textbooks [28, 37].

First, we give some classical definitions and notations relevant to the study of mass-action dynamical systems and to (bio-chemical) reaction networks. Next, we present a special class of these systems: complex-balanced dynamical systems, which are also called toric dynamical systems. More details can be found in the textbooks [18] and [9], the latter one with a view towards Nonlinear Algebra. See also [12, 33, 14, 10].

Notation 2.1. (a) We let $\mathbb{R}^n_{\geq 0}$ and $\mathbb{R}^n_{> 0}$ denote the sets of vectors with non-negative and positive entries respectively. Similarly, $\mathbb{Z}^n_{\geq 0}$ is the set of vectors with non-negative integer components. We denote the cardinality of a set $A$ as $|A|$, and the disjoint union of sets $A$ and $B$ is denoted by $A \sqcup B$.

(b) Let us consider two vectors $x, y \in \mathbb{R}^n$ with $x = (x_1, \ldots, x_n)^T$ and $y = (y_1, \ldots, y_n)^T$. The following are the vector operations that will be used in this paper:

$$x^y := x_1^{y_1} \cdots x_n^{y_n},$$
$$x \circ y := (x_1 y_1, \ldots, x_n y_n)^T,$$
$$\exp(x) := (\exp(x_1), \ldots, \exp(x_n))^T,$$
$$\log(x) := (\log(x_1), \ldots, \log(x_n))^T.$$

(c) We also apply vector operations on a subset of $\mathbb{R}^n$, where they are applied to all elements of the subset. For example, given a vector $x \in \mathbb{R}^n$ and a set $A \subseteq \mathbb{R}^n$,

$$x \circ A := \{x \circ y : y \in A\}.$$
2.1 Dynamics of reaction networks with mass-action kinetics

We work with deterministic, autonomous and continuous dynamical systems, generated by reaction networks. The goal is to model the variation in time of the concentrations of the species involved, under the assumption of mass-action kinetics. Mostly following the terminology and notations from [40], let us give precise standard definitions of these classical notions.

Definition 2.2. (a) We let $X_i$ denote the species, and $n$ denote the number of species involved in the reaction network.

(b) Denote by $x_i$ the concentration of the species $X_i$, for $i = 1, \ldots, n$. We consider $x_i$ as functions of time $t$: $x_i = x_i(t)$. At any time $t \geq 0$, this gives us a vector $\mathbf{x} = (x_1, \ldots, x_n)^t \in \mathbb{R}^n$, also called a state of the system.

(c) A formal linear combination of species $\{X_i\}_{i=1}^n$, with non-negative real coefficients is called a complex. A reaction is a directed edge between two distinct complexes.

Definition 2.3. A reaction network, also called a Euclidean embedded graph, is a finite directed graph $G = (V, E)$ such that the set $V \subset \mathbb{R}^n$ is a finite set of vertices and the set $E \subseteq V \times V$ represents the finite set of edges. We assume that there are neither self-loops nor isolated vertices.

(a) We denote the number of vertices by $m$, and let $V = \{y_1, \ldots, y_m\}$, where each vertex $y_i \in V$ corresponds to a complex. The entries of the vertex are the coefficients of the species in the corresponding formal linear combination.

(b) A directed edge connecting two vertices $y_i \in V$ to $y_j \in V$ is denoted by $y_i \rightarrow y_j \in E$ and represents a reaction in the network. We call the difference vector $y_j - y_i \in \mathbb{R}^n$, the reaction vector. Here $y_i$ and $y_j$ denote the source vertex and target vertex respectively.

Example 2.4. Let us consider the reaction network from Figure 1. There are three interacting species: $X_1$, $X_2$ and $X_3$, and three complexes:

$$2X_1 + 3X_2, \quad 2X_2, \quad X_3,$$

and four reactions (directed edges):

$$2X_1 + 3X_2 \rightarrow 2X_2, \quad 2X_2 \rightarrow 2X_1 + 3X_2, \quad 2X_2 \rightarrow X_3, \quad X_3 \rightarrow 2X_1 + 3X_2.$$
The real coefficients appearing in each formal linear combination of species of the complexes of the reaction network from Figure 1 can be represented by vectors in the three dimensional Euclidean space:

\[ y_1 = \begin{pmatrix} 2 \\ 3 \\ 0 \end{pmatrix}, \quad y_2 = \begin{pmatrix} 0 \\ 2 \\ 0 \end{pmatrix}, \quad y_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \]

This gives rise to a Euclidean embedded graph (see Figure 2), whose edges become actual vectors \( y_i - y_j \in \mathbb{R}^3 \).

**Definition 2.5.** Let \( G = (V, E) \) be a Euclidean embedded graph.

(a) The set of vertices \( V \) is partitioned by its connected components, also called linkage classes, and we identify them by the subset of vertices that belong to that connected component. We denote the number of connected components by \( \ell \), and let \( V = V_1 \sqcup V_2 \sqcup \cdots \sqcup V_\ell \), where each \( V_i \) represents a connected component of \( G \).

(b) A connected component is called strongly connected, if every edge is part of an oriented cycle. Furthermore, a strongly connected component is said to be terminal, if no other strongly connected component is reachable from it.
(c) A graph \( G = (V, E) \) is **weakly reversible**, if every connected component is strongly connected.

We work under the assumption of the mass-action kinetics, which says that the rate with which a reaction takes place is directly proportional to the product of the concentrations of the reactant species. See [40] and references therein. Under this assumption, the dynamics can be modeled using the ODE system (1) below. Starting with the work of Gatermann (see [12, 20]), the structure of the polynomial right hand side gives rise to fruitful interactions between the field of reaction networks and computational algebra and combinatorics.

**Definition 2.6.** Given a Euclidean embedded graph \( G = (V, E) \), each edge \( y_i \rightarrow y_j \) is decorated with a positive constant \( k_{ij} \) or \( k_{y_i \rightarrow y_j} \), called a **reaction rate constant**. Further, we denote by \( k := (k_{ij}) \in \mathbb{R}^E \) the **vector of reaction rate constants**. The associated **mass-action system** generated by \( (G, k) \) on \( \mathbb{R}^n_{>0} \) is given by:

\[
\frac{dx}{dt} = \sum_{y_i \rightarrow y_j \in E} k_{y_i \rightarrow y_j} x^{y_i}(y_j - y_i).
\]

**Example 2.7.** Consider the reaction network from Example 2.4. Under the mass-action kinetics, the associated dynamical system is:

\[
\frac{dx}{dt} = k_{12} x_1^2 x_2^3 (y_2 - y_1) + k_{21} x_2^2 (y_1 - y_2) + k_{23} x_2^2 (y_3 - y_2) + k_{31} x_3 (y_1 - y_3)
\]

\[
= k_{12} x_1^2 x_2^3 \begin{pmatrix} -2 \\ 1 \end{pmatrix} + k_{21} x_2^2 \begin{pmatrix} 2 \\ 0 \end{pmatrix} + k_{23} x_2^2 \begin{pmatrix} 0 \\ -2 \end{pmatrix} + k_{31} x_3 \begin{pmatrix} 2 \\ 3 \end{pmatrix}
\]

\[
= \begin{pmatrix} 
-2k_{12}x_1^2 x_2^3 + 2k_{21}x_2^2 + 2k_{31}x_3 \\
-k_{12}x_1^2 x_2^3 + (k_{21} - 2k_{23})x_2^2 + 3k_{31}x_3 \\
k_{23}x_2^2 - k_{31}x_3
\end{pmatrix}.
\]

Before the end of this subsection, let us define the affine invariant polyhedron; it will play an important role in the proof of our main results, starting with Section 3.

**Remark 2.8 ([40]).** Note that we set the domain of (1) to be \( \mathbb{R}^n_{>0} \). In general, systems of ODEs do not allow \( \mathbb{R}^n_{>0} \) to be forward-invariant. But under the assumption that \( V \subset \mathbb{Z}^n_{\geq 0} \), the positive orthant \( \mathbb{R}^n_{>0} \) is forward-invariant under system (1). See also [22, Remark 2.3, page 3]; we could also allow \( V \subset \mathbb{R}^n_{>0} \) or \( V \subset \mathbb{R}^n \).

**Definition 2.9.** Let \( G = (V, E) \) be a Euclidean embedded graph. We denote the **stoichiometric subspace** of \( G \) by \( S \), which is

\[
S = \text{span}\{y_j - y_i : y_i \rightarrow y_j \in E\}.
\]

From Remark 2.8, any solution to (1) with initial condition \( x_0 \in \mathbb{R}^n_{>0} \) and \( V \subset \mathbb{Z}^n_{\geq 0} \), is confined to \( (x_0 + S) \cap \mathbb{R}^n_{>0} \), and \( (x_0 + S) \cap \mathbb{R}^n_{>0} \) is called the **affine invariant polyhedron** of \( x_0 \). For the sake of simplicity, we use the notation: \( S_{x_0} := (x_0 + S) \cap \mathbb{R}^n_{>0} \).
2.2 Complex-balanced dynamical systems and their properties

The importance of complex-balanced dynamical systems is mostly due to their strong stability properties. We advise the reader to consult [24], [40, Theorem 2.3]: using a strictly convex Lyapunov function, Horn and Jackson proved in [24] that if a mass-action system has a complex-balanced steady state, then all its positive steady states are also complex-balanced and that there is a unique and locally asymptotically stable steady state in each affine invariant polyhedron.

Definition 2.10. Consider the associated mass-action system generated by \((G, k)\):

\[
\frac{dx}{dt} = \sum_{y_i \rightarrow y_j \in E} k_{y_i \rightarrow y_j} x^{y_{i}}(y_{j} - y_{i}).
\]

A state \(x^* \in \mathbb{R}^n_0\) is called a positive steady state, if

\[
\frac{dx}{dt} = \sum_{y_i \rightarrow y_j \in E} k_{y_i \rightarrow y_j}(x^*)^{y_{i}}(y_{j} - y_{i}) = 0.
\]

A positive steady state \(x^* \in \mathbb{R}^n_0\) is called a complex-balanced steady state, if at each vertex \(y_0 \in V\), we have

\[
\sum_{y_0 \rightarrow y' \in E} k_{y_0 \rightarrow y'}(x^*)^{y_{0}} = \sum_{y \rightarrow y_0 \in E} k_{y \rightarrow y_0}(x^*)^{y}.
\]

We say that the pair \((G, k)\) satisfies the complex-balanced condition, and the mass-action system generated by \((G, k)\) is called a complex-balanced system or toric dynamical system.

The following classical theorem illustrates some of the most important dynamical properties of complex-balanced dynamical systems.

Theorem 2.11 (Horn and Jackson theorem), [24],[40, Theorem 2.3]

Let us consider a complex-balanced system \((G, k)\), having one steady state \(x^* \in \mathbb{R}^n_0\). Denote its associated stoichiometric subspace by \(S\). Then the following hold:

(a) All positive steady states are complex-balanced. There is exactly one steady state within each invariant polyhedron.

(b) Any complex-balanced steady state \(x\) satisfies the following relation: \(\ln x - \ln x^* \in S^\perp\).

(c) Every complex-balanced steady state is asymptotically stable regarding its invariant polyhedron.

Moreover, the mass-action system (1) admits a matrix decomposition, which helps us in studying complex-balanced steady states. Recall that the number of species is denoted by \(n\), and the number of vertices is denoted by \(m\). Following [12], we set the \(n \times m\) matrix \(Y\), whose columns correspond to vertices:

\[
Y := (y_1, y_2, \ldots, y_m) = (y_{ji}) \in \mathbb{R}^{n \times m},
\]
Next, we build the following vector of monomials:

\[ \Psi(x) := \begin{pmatrix} x^{y_1} \\ \vdots \\ x^{y_m} \end{pmatrix} \in \mathbb{R}^m. \]

Since each directed edge \( y_i \rightarrow y_j \in E \) has a reaction rate constant \( k_{ij} \in \mathbb{R}_{>0} \), we construct the \( m \times m \) Kirchoff matrix \( A_k \), which is the transpose of the negative of the graph Laplacian of \((V,E,k)\):

\[
[A_k]_{ji} := \begin{cases} 
    k_{y_i \rightarrow y_j}, & \text{if } y_i \rightarrow y_j \in E; \\
    -\sum_{y_i \rightarrow y_j \in E} k_{y_i \rightarrow y_j}, & \text{if } i = j; \\
    0, & \text{otherwise}.
\end{cases}
\]  

Then the mass-action dynamical system (1) generated by \((G,k)\) can be written in the following vectorial representation:

\[
\frac{dx}{dt} = Y \cdot A_k \cdot \Psi(x).
\]

**Remark 2.12.** Note that the notation we use in (7) is different from the one in [12, page 2], by transposing.

Under direct computation, the \( i \)th component of \( A_k \cdot \Psi(x) \) is:

\[
[A_k \cdot \Psi(x)]_i = \sum_{y_j \rightarrow y_i \in E} k_{y_j \rightarrow y_i} x^{y_j} - \sum_{y_i \rightarrow y_j \in E} k_{y_i \rightarrow y_j} x^{y_i}.
\]

Therefore, the equality (5) is equivalent to

\[
A_k \cdot \Psi(x^*) = 0
\]

where \( x^* \in \mathbb{R}^n_{>0} \) is a complex-balanced steady state for the mass-action system \((G,k)\).

**Theorem 2.13.** [19, page 94] Consider a mass-action system \((G,k)\) with terminal strongly connected components \( T_1, T_2, \ldots, T_t \) and vertices \( \{ y_1, y_2, \ldots, y_m \} \), then \( \ker(A_k) \) (see equation (6) for the definition of \( A_k \)) has a basis \( \{ e_1, \ldots, e_t \} \), such that

\[
e_p = \begin{cases} 
    [e_p]_i > 0, & \text{if } y_i \in T_p; \\
    [e_p]_i = 0, & \text{otherwise},
\end{cases}
\]

where \( 1 \leq i \leq m \) and \( 1 \leq p \leq t \).

**Example 2.14.** Revisiting Example 2.4, we have:

\[
Y = (y_1, y_2, y_3) = \begin{pmatrix} 2 & 0 & 0 \\ 3 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix},
\]
and
\[
A_k = \begin{pmatrix}
-k_{12} & k_{21} & k_{31} \\
k_{12} & -k_{21} - k_{23} & 0 \\
0 & k_{23} & -k_{31}
\end{pmatrix}, \quad \Psi(x) = \begin{pmatrix} x^y_1 \\ x^y_2 \\ x^y_3 \end{pmatrix} = \begin{pmatrix} x^2_1 x^3_2 \\ x^2_2 \\ x^2_3 \end{pmatrix}.
\]

Following Equations (7), we derive
\[
\frac{dx}{dt} = Y \cdot A_k \cdot \Psi(x) = \begin{pmatrix}
-2k_{12} x^2_1 x^3_2 + 2k_{21} x^2_2 + 2k_{31} x^3_3 \\
-k_{12} x^2_1 x^3_2 + (k_{21} - 2k_{23}) x^2_2 + 3k_{31} x^3_3 \\
-k_{23} x^2_2 - k_{31} x^3_3
\end{pmatrix},
\]
which give the same ODE system as (2).

### 2.3 The toric locus

Next we introduce the notion of *toric locus*, which is a key concept in this paper. See [33, Definition 2.2].

**Definition 2.15.** Consider a Euclidean embedded graph \( G = (V, E) \), we let \( V(G) \subseteq \mathbb{R}^E_{>0} \) denote the set of parameters \( k \in \mathbb{R}^E_{>0} \) for which the dynamical system generated by \((G, k)\) is toric or complex-balanced. We refer to \( V(G) \) as the moduli space or the toric locus of toric dynamical systems given by the Euclidean embedded graph \( G \).

The following theorem is a classical result, which shows that complex-balanced mass action systems share important connections with Euclidean embedded graphs.

**Theorem 2.16 ([25]).** Every Euclidean embedded graph which permits a complex-balanced mass action system is weakly reversible. Moreover, every Euclidean embedded graph which is weakly reversible permits complex-balanced mass action systems.

As a subsequence, given a Euclidean embedded graph \( G = (V, E) \), we conclude that

- If \( G = (V, E) \) is weakly reversible, then \( V(G) \neq \emptyset \).
- If \( G = (V, E) \) isn’t weakly reversible, then \( V(G) = \emptyset \).

Since we are not interested in the case when \( V(G) \) is empty, we always assume that the Euclidean embedded graph \( G = (V, E) \) is weakly reversible when we work on \( V(G) \) in the rest of this paper.

In practice, it is difficult to compute precise values for the parameters \( k_{ij} \in \mathbb{R}_{>0} \), so we usually choose a symbolic approach and consider them as varying parameters, as in [12]. For instance, in Example 2.4, suppose \( x = (x_1, x_2, x_3) \) is a complex-balanced steady state, then the complex-balanced conditions are as follows:

\[
\begin{align*}
k_{21} x^2_2 + k_{31} x^3_3 &= k_{12} x^2_1 x^3_2, \\
k_{12} x^2_1 x^3_2 &= k_{21} x^2_2 + k_{23} x^2_2, \\
k_{23} x^2_2 &= k_{31} x^3_3.
\end{align*}
\]
Surprisingly, the toric locus $\mathcal{V}(G)$ in Example 2.4 is the whole positive orthant $\mathbb{R}^4_{>0}$. This follows from a classical result, known as the \textit{Deficiency Zero Theorem}. We will revisit this example and show the details in Section 4.3.

For small enough Euclidean embedded graphs, one can successfully use Computer Algebra software such as Macaulay2 [21], in order to apply Elimination theory [32, Chapter 4] or Real quantifier elimination [2, Chapter 12.3] for computing the toric locus $\mathcal{V}(G)$.

In general, the toric locus can have quite a complicated algebraic description and it is usually not easy to study. This is reflected by Example 2.17 below, which shows that even for simple Euclidean embedded graphs, the topological structure of the moduli spaces of toric dynamical systems is interesting.

\textbf{Example 2.17.} Consider the mass-action system $(G, k)$ in Figure 3, with four vertices:

\[
y_1 = \begin{pmatrix} 3 \\ 0 \end{pmatrix}, \quad y_2 = \begin{pmatrix} 2 \\ 1 \end{pmatrix}, \quad y_3 = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \quad y_4 = \begin{pmatrix} 0 \\ 3 \end{pmatrix}.
\]

Suppose $x = (x_1, x_2)$ is a complex-balanced steady state, then the complex-balanced conditions follows:

\[
k_{14}x_1^3 = k_{21}x_1x_2^2 = k_{32}x_1x_2^2 = k_{43}x_2^3.
\]

By eliminating $x_1, x_2$ above, the moduli space $\mathcal{V}(G) \subset \mathbb{R}^4_{>0}$ is the following algebraic variety given by equations (9) and (10), intersected with the positive orthant.

(9) \[ (k_{43}k_{32}k_{21})(k_{21}k_{14}k_{43}) = (k_{14}k_{43}k_{32})^2, \]

and

(10) \[ (k_{14}k_{43}k_{32})(k_{32}k_{21}k_{14}) = (k_{21}k_{14}k_{43})^2. \]

After a change of variables, the moduli space becomes a toric variety in the positive orthant. More precisely, equations (9) and (10) become

(11) \[ K_1K_3 - K_2^2 = 0, \]
and

\[ K_2 K_4 - K_3^2 = 0, \]

where we set \( K_1 := k_{43} k_{32} k_{21}, \) \( K_2 := k_{14} k_{31} k_{21}, \) \( K_3 := k_{21} k_{14} k_{43}, \) \( K_4 := k_{32} k_{21} k_{14}. \)

From the algebraic point of view, binomial equations are desirable in computations and toric varieties are the cornerstone of algebraic geometry, since the latter provide many tractable examples due to their combinatorial structure, which is well understood [32, Chapter 8].

### 3 Complex-balanced equilibria depend continuously on the parameter values

In this section, we show the first main result of our paper, namely that complex-balanced equilibria depend continuously on the parameters \( k \) in the toric locus \( V(G) \) (see Definition 2.15).

Now we introduce a map from \( V(G) \) to \( Sx_0 \), which is crucial in the later proofs.

**Definition 3.1.** Let \( G = (V, E) \) be a weakly reversible Euclidean embedded graph with the stoichiometric subspace \( S \). Given a fixed state \( x_0 \in R^n > 0 \), we define the following map:

\[ Q_{x_0} : V(G) \to (x_0 + S) \cap R^n > 0, \]

such that

\[ Q_{x_0}(k) := x_0^k, \]

where \( x_0^k \) is the complex-balanced equilibrium in the invariant polyhedron \( Sx_0 \), under the mass-action system \( (G, k) \).

The map \( Q_{x_0} \) is well-defined for any fixed state \( x_0 \in R^n_{>0} \) and \( k \in V(G) \). This follows from Theorem 2.11: every complex-balanced system admits a unique equilibrium within each invariant polyhedron. Let us show some basic properties of the map \( Q_{x_0} \).

**Lemma 3.2.** For any fixed state \( x_0 \in R^n_{>0} \), the map \( Q_{x_0} \) is surjective.

**Proof.** To prove the surjectivity of \( Q_{x_0} \), we show that for any point \( \hat{x} \in (x_0 + S) \cap R^n > 0 \), there exists \( \hat{k} \in V(G) \), such that \( Q_{x_0} (\hat{k}) = \hat{x} \).

Recall from Theorem 2.11 that, given some parameters \( k \in V(G) \), there exists \( x_0^k \) such that \( Q_{x_0}(k) = x_0^k \) and such that the pair \( (k, x_0^k) \) satisfies the complex-balanced relations (5), namely: for each vertex \( y_i \in V \),

\[ \sum_{y_i \rightarrow y_j \in E} k_{y_i \rightarrow y_j}(x_0^k)_{y_j} = \sum_{y_j \rightarrow y_i \in E} k_{y_j \rightarrow y_i}(x_0^k)_{y_i}. \]

Now we define the set of parameters \( \hat{k} = (\hat{k}_{y_i \rightarrow y_j}) \) as

\[ \hat{k}_{y_i \rightarrow y_j} := \frac{k_{y_i \rightarrow y_j}(x_0^k)_{y_i}}{x_0^k_{y_i}}. \]
From (15) and (16), we derive that for each vertex $y_i \in V$,
\[
\sum_{y_i \to y_j \in E} \hat{k}_{y_i \to y_j} \hat{x}^{y_i} = \sum_{y_i \to y_j \in E} k_{y_i \to y_j} (x_0^k)^{y_i} = \sum_{y_j \to y_i \in E} k_{y_j \to y_i} (x_0^k)^{y_j} = \sum_{y_j \to y_i \in E} \hat{k}_{y_j \to y_i} \hat{x}^{y_j}.
\]

It is clear that $\hat{k} \in \mathbb{R}^E_{\geq 0}$ thus from (17) we get that $\hat{k} \in V(G)$ and the pair $(\hat{k}, \hat{x})$ satisfies the complex-balanced condition (5). Hence, we conclude $Q_{x_0}(\hat{k}) = \hat{x}$.

\[\text{Lemma 3.3.} \text{ Given any fixed state } \hat{x} \in (x_0 + S) \cap \mathbb{R}^n_{>0}, \text{ the preimage } Q_{x_0}^{-1}(\hat{x}) \text{ is connected.}\]

\[\text{Proof.} \text{ From Lemma 3.2, we have that for any } \hat{x} \in (x_0 + S) \cap \mathbb{R}^n_{>0}, \text{ there exist parameters } \hat{k} \in V(G), \text{ such that the complex-balanced conditions hold:}\]
\[
\sum_{y_i \to y_j} \hat{k}_{y_i \to y_j} \hat{x}^{y_i} = \sum_{y_j \to y_i} \hat{k}_{y_j \to y_i} \hat{x}^{y_j}. \tag{18}
\]

Now we claim that the fiber $Q_{x_0}^{-1}(\hat{x})$ is a convex set. Suppose both $k^*, k^{**} \in V(G)$ satisfy (18). We will show that any convex combination of $k^*$ and $k^{**}$ also satisfies (18). Let us consider the following set:
\[
L(k^*, k^{**}) := \{ ak^* + (1 - a)k^{**} : 0 \leq a \leq 1 \}.
\]

Under direct computation, we obtain that for any $0 \leq a \leq 1$,
\[
\sum_{y_i \to y_j} (ak^{*}_{y_i \to y_j} + (1 - a)k^{**}_{y_i \to y_j}) \hat{x}^{y_i} = \sum_{y_j \to y_i} (ak^{*}_{y_j \to y_i} + (1 - a)k^{**}_{y_j \to y_i}) \hat{x}^{y_j}. \tag{20}
\]

Hence, we showed that $L(k^*, k^{**}) \subseteq Q_{x_0}^{-1}(\hat{x})$. Thus the preimage $Q_{x_0}^{-1}(\hat{x})$ is a convex set, and we conclude that $Q_{x_0}^{-1}(\hat{x})$ is connected.

\[\text{Lemma 3.4.} \text{ For any fixed state } x_0 \in \mathbb{R}^n_{>0}, \text{ the map } Q_{x_0} \text{ is open.}\]

\[\text{Proof.} \text{ Pick a point } k \in V(G), \text{ we consider an open neighborhood } U \text{ of } k, \text{ such that } k \in U \subseteq V(G).
\]

Assume $Q_{x_0}(k) = x_0^k$, it suffices for us to prove that $x_0^k$ is in the interior of $Q_{x_0}(U)$. Hence, it is equivalent to show that, for any $0 < \epsilon \ll 1$, there exists $\delta > 0$ such that for all $\hat{x}$ satisfying $\| \hat{x} - x_0^k \| \leq \delta$, there is a point $\hat{k} \in V(G)$, such that $\hat{x} = Q_{x_0}(\hat{k})$ and $\| \hat{k} - k \| \leq \epsilon$.

Here we define the set of parameters $\hat{k} = (\hat{k}_{y_i \to y_j})$ as
\[
\hat{k}_{y_i \to y_j} := \frac{k_{y_i \to y_j} (x_0^k)^{y_i}}{\hat{x}^{y_i}}. \tag{21}
\]

Using Lemma 3.2, we get $\hat{k} \in V(G)$ and $Q_{x_0}(\hat{k}) = \hat{x}$. Moreover, we rewrite (21) as follows:
\[
\frac{\hat{k}_{y_i \to y_j}}{k_{y_i \to y_j}} = \frac{(x_0^k)^{y_i}}{\hat{x}^{y_i}}.
\]
For any reaction $y_i \rightarrow y_j \in E$ and $0 < \epsilon \ll 1$, the continuity of the function $x^{y_i}$ guarantees the existence of $\delta_{y_i \rightarrow y_j}$, such that for all $\|\hat{x} - x^k\| \leq \delta_{y_i \rightarrow y_j}$, we have $|\hat{k}_{y_i \rightarrow y_j} - k_{y_i \rightarrow y_j}| \leq \epsilon/|E|$. Then we work on all reactions and set $\delta = \min_{y_i \rightarrow y_j \in E} \{\delta_{y_i \rightarrow y_j}\}$.

Thus suppose any $\hat{x}$ satisfying $\|\hat{x} - x^k\| \leq \delta$, we derive that

$$\|\hat{k} - k\| \leq \sum_{y_i \rightarrow y_j \in E} |\hat{k}_{y_i \rightarrow y_j} - k_{y_i \rightarrow y_j}| \leq \epsilon.$$

Therefore, $x^k_0$ is in the interior of $Q_{x_0}(U)$ and the proof is concluded. \hfill \Box

Now we state the main result of this section, Theorem 3.5. We will use this result in the following sections, for the proof of the connectedness of the toric locus.

**Theorem 3.5.** For any fixed state $x_0 \in \mathbb{R}^n_{>0}$, the map $Q_{x_0}$ is continuous. In other words, the complex balanced equilibria depend continuously on the parameter values.

Before proving Theorem 3.5, we need to address some necessary Notations and Lemmas.

**Definition 3.6.** Let $G = (V, E)$ be a strongly connected Euclidean embedded graph.

(a) We call $T$ a **spanning tree** of $G$, if it is a connected, acyclic subgraph of $G$ that contains all vertices in $V$.

(b) For a spanning tree $T$ of $G$, the vertex $y \in V$ is called a **sink** of $T$, if $y$ is the target vertex for all reactions in $T$ involving $y$.

(c) For a spanning tree $T$ of $G$ and a vertex $y_i \in V$, then we call $T$ a **spanning $y_i$-tree** or $i$-**tree**, if $y_i$ is the only sink of $T$.

**Notation 3.7.** Let $G = (V, E)$ be a strongly connected Euclidean embedded graph.

(a) Consider a spanning tree $T$ of $G$, we denote by $k^T$ the product of all the reaction rate constants associated with reactions in the spanning tree $T$.

(b) Consider every spanning $y_i$-tree of $G$, let $K_i$ denote the sum of all products associated with spanning $y_i$-trees, such that

$$K_i := \sum_{T : \text{an } i\text{-tree}} k^T.$$

**Proposition 3.8 ([12, Proposition 3]).** Consider a mass-action system $(G, k)$ with the Euclidean embedded graph $G = (V, E)$ which is strongly connected. Let $A_k$ be its corresponding Kirchhoff matrix $A_k$ (i.e., the transpose of the negative of the Laplacian matrix of $G$), and $M_i$ be the matrix obtained by removing the $i$-th row and the $i$-th column of $A_k$, then

$$(22) \quad \det(M_i) = (-1)^{m-1} K_i,$$

where $K_i = \sum_{T : \text{an } i\text{-tree}} k^T$ defined in Notation 3.7.
The following Proposition gives a characterization of the complex balanced equilibria. The similar conclusion can be obtained from [12]. For the completeness of the paper, we sketch the proof here.

**Proposition 3.9.** Suppose a weakly reversible mass-action system \((G, k)\) with \(l\) connected components. For any two vertices \(y_i\) and \(y_j\), we construct the following equation:

\[
\begin{align*}
K_i x^{y_j} - K_j x^{y_i} &= 0,
\end{align*}
\]

where \(K_i = \sum_{\text{t, an i-tree}} k^T\) defined in Notation 3.7. Then \(x\) is a complex-balanced equilibrium for the reaction rate vector \(k\) if and only if Equations (23) are satisfied for every pair of vertices in the same connected component in \(G\).

**Proof.** From (6), we get \([A_k]_{ji} \neq 0\), if \(y_i \rightarrow y_j \in E\) or \(i = j\). After we relabel the vertices according to the connected components of \(G\), the Kirchhoff matrix \(A_k\) will be a block diagonal matrix, where each diagonal block corresponds to a connected component of \(G\).

Following Equations (8), \(x\) is a complex-balanced equilibrium if and only if \(A_k \cdot \Psi(x) = 0\) under the reaction rate vector \(k\). Since we consider \(A_k\) as a block diagonal matrix, it suffices to prove the proposition when the system has a single connected component (i.e. \(\ell = 1\)).

Now suppose \(G = (V, E)\) has one connected component, thus it is strongly connected. Applying Theorem 2.13 on the system \((G, k)\), we deduce that

\[
\dim(\ker(A_k)) = 1, \quad \text{and} \quad \det(A_k) = 0.
\]

Note that the minor of matrix \(A_k\) is independent of the choice of rows because the column sums of \(A_k\) are zero. Using Proposition 3.8 and expanding the determinant of \(A_k\) in terms of its minors, we derive that

\[
(25) \quad A_k \cdot K = 0,
\]

where \(K = (K_1, K_2, \ldots, K_m)^T\).

Now we obtain both \(K\) and \(\Psi(x)\) belongs to the null-space of \(A_k\). From \(\dim(\ker(A_k)) = 1\) in Equation (24), we deduce that two vectors \(K\) and \(\Psi(x)\) are proportional. Hence, it is clear that \(A_k \cdot \Psi(x) = 0\) if and only if Equations (23) are satisfied for every pair of vertices of \(G\). Again using Equations (8), we conclude this proposition. \(\square\)

**Example 3.10.** [23, Equation 3.12] Consider a strongly connected mass-action system \((G, k)\) in Figure 4, with three vertices:

\[
y_1 = \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \quad y_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad y_3 = \begin{pmatrix} 0 \\ 2 \end{pmatrix}.
\]
Figure 4: Complete bidirected graph with three vertices, considered in Example 3.10.

For the vertex $y_1$, we list all spanning $y_1$-trees of $G$ as follows:

![Diagram of spanning $y_1$-trees](image)

Figure 5: Spanning $y_1$-trees of $G$.

From Notation 3.7, we obtain that

$$K_1 = k_{21}k_{31} + k_{32}k_{21} + k_{23}k_{31}.$$  

Analogously, we can derive $K_2, K_3$ corresponding to the vertices $y_2, y_3$ in $G$,

$$K_2 = k_{12}k_{32} + k_{13}k_{32} + k_{31}k_{12}$$

$$K_3 = k_{13}k_{23} + k_{21}k_{13} + k_{12}k_{23}.$$  

Suppose $x = (x_1, x_2)$ is a complex-balanced steady state. Using Proposition 3.9, we get that $k \in \mathcal{V}(G)$, if and only if

$$\frac{K_1}{x^{y_1}} = \frac{K_2}{x^{y_2}} = \frac{K_3}{x^{y_3}}.$$  

By eliminating $x_1, x_2$ in equation (26), the moduli space $\mathcal{V}(G) \subset \mathbb{R}^6_{>0}$ must satisfy the following binomial:

$$K_1K_3 - K_2^2 = 0.$$  

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Therefore, we recover the result from [23, Equation 3.12] (see also [12, Example 1], [9, page 195]): the toric locus (moduli space) can be written as

\[ \mathcal{V}(G) = \{ k \in \mathbb{R}^6_{>0} : (k_{21}k_{31} + k_{32}k_{21} + k_{23}k_{31})(k_{13}k_{23} + k_{21}k_{13} + k_{12}k_{23}) - (k_{12}k_{32} + k_{13}k_{32} + k_{31}k_{12})^2 = 0 \} \].

Note that in general one could use elimination ideals and the Computer Algebra software Macaulay2 ([21]) to obtain the binomial equations of the toric locus (see for instance [32, Chapter 4]).

**Definition 3.11** ([35]). Let us consider two manifolds $A$ and $B$ in the Euclidean space $\mathbb{R}^n$. We say that $A$ and $B$ **intersect transversally** if at any intersection point $x \in A \cap B$ we have $T_x(A) + T_x(B) = \mathbb{R}^n$, namely their tangent spaces span $\mathbb{R}^n$.

**Lemma 3.12** ([15, Lemma 5.4]). Let $x_1, x_2 \in \mathbb{R}^n_{>0}$ be positive vectors. Consider a vector subspace $S$ in $\mathbb{R}^n$. Let $x_1 + S$ and $x_2 \circ \exp(S^\perp)$ be two manifolds of $\mathbb{R}^n$. Then the two manifolds intersect transversally, i.e.

\[ T_p(x_1 + S) + T_p(x_2 \circ \exp(S^\perp)) = \mathbb{R}^n, \]

for any point $p \in (x_1 + S) \cap (x_2 \circ \exp(S^\perp))$.

Finally, we are prepared to prove Theorem 3.5.

**Proof of Theorem 3.5.** Here, for the sake of simplicity, we have abused the notation temporarily:

\[ X = (X_1, \ldots, X_n)^\top := \log x = (\log x_1, \ldots, \log x_n)^\top. \]

Recall Notation 3.7, for each vertex $y_i \in V$, we have

\[ K_i = \sum_{\text{Tan } i-\text{tree}} k^T, \]

where $k^T$ is the product of reaction rates $k_{ij}$ associated with reactions in the spanning $y_i$-tree $\mathcal{T}$ of $G$. It is standard to derive that the vector $K = (K_i) \in \mathbb{R}^m_{>0}$ depends continuously on the reaction rate vector $k = (k_{ij}) \in \mathbb{R}^E_{>0}$. Hence, it suffices for us to show that the set of complex balanced equilibria depends continuously on $K$.

From Proposition 3.9, a state $x$ is a complex-balanced equilibrium, if and only if for any two vertices $y_i, y_j$ in the same connected component of $G$,

\[ K_i x^{y_j} = K_j x^{y_i}. \]

Taking the log of both sides in Equation (29), we derive

\[ \log(K_i) + y_j^\top \cdot \log(x) = \log(K_j) + y_i^\top \cdot \log(x). \]

Thus, we can rewrite (30) as

\[ \log(K_i/K_j) = (y_i^\top - y_j^\top) \cdot X, \]
where $y_i$ and $y_j$ are two vertices belonging to the same connected component of $G$.

We show the rest of proof in two steps. First, we prove the theorem under the assumption that the graph $G$ has only one connected component. Next, we explain how to generalize the result into arbitrary number of connected components.

Now suppose the graph $G$ has a single connected component (i.e. $\ell = 1$), then all vertices $\{y_1, \ldots, y_m\}$ are in the same connected component. It is clear that Equations (31) is equivalent to the following system of linear equations in $X$:

\[
\begin{bmatrix}
\log(K_1/K_2) \\
\log(K_2/K_3) \\
\vdots \\
\log(K_{m-1}/K_m)
\end{bmatrix} = 
\begin{bmatrix}
y_1^\top - y_2^\top \\
y_2^\top - y_3^\top \\
\vdots \\
y_{m-1}^\top - y_m^\top
\end{bmatrix}
\begin{bmatrix}X_1 \\
X_2 \\
\vdots \\
X_n
\end{bmatrix}.
\]

(32)

After we set

$$
\Delta y := \begin{bmatrix}y_1^\top - y_2^\top \\
y_2^\top - y_3^\top \\
\vdots \\
y_{m-1}^\top - y_m^\top \end{bmatrix}, \text{ and } \Delta K := \begin{bmatrix}K_1/K_2 \\
K_2/K_3 \\
\vdots \\
K_{m-1}/K_m \end{bmatrix},
$$

the system (32) can be expressed as

\[
\log(\Delta K) = (\Delta y)X.
\]

(33)

Since $G$ is strongly connected, then its stoichiometric subspace is

$$S = \text{span}\{y_1^\top - y_2^\top, y_2^\top - y_3^\top, \ldots, y_{m-1}^\top - y_m^\top\}.$$

Let $s$ be the dimension of $S$, then we deduce that $s \leq \min\{m-1, n\}$, and the matrix $\Delta y$ has exactly $s$ linearly independent rows. W.l.o.g. we assume the first $s$ rows in $\Delta y$ are linearly independent. Thus, we obtain

\[
S = \text{span}\{y_1^\top - y_2^\top, y_2^\top - y_3^\top, \ldots, y_s^\top - y_{s+1}^\top\}.
\]

(34)

Furthermore, we consider the system of equations as follows:

\[
\log(\Delta_s K) = (\Delta_s y)X,
\]

(35)

where

$$
\Delta_s y := \begin{bmatrix}y_1^\top - y_2^\top \\
y_2^\top - y_3^\top \\
\vdots \\
y_s^\top - y_{s+1}^\top \end{bmatrix}, \text{ and } \Delta_s K := \begin{bmatrix}K_1/K_2 \\
K_2/K_3 \\
\vdots \\
K_{s+1} \\
\end{bmatrix}.
$$

Since $k \in \mathcal{V}(G)$, the complex-balanced system $(G, k)$ must admit one steady state $x^* \in \mathbb{R}_{>0}^n$, i.e. $\ln x^*$ is a solution to (33). From Theorem 2.11, any complex-balanced steady state $x$ satisfies $\ln x - \ln x^* \in S^\perp$. Thus the solutions to (33) can be written as $\ln x^* + S^\perp$, and this shows the dimension of the set of solutions to (33) is $n - s$. Moreover, it is straightforward to check that the solutions of (33) must solve (35). Since the rows in the matrix $\Delta_s y$ are
linearly independent, the set of solutions to (35) is also of dimension \( n - s \). Therefore, we conclude that system (33) is equivalent to system (35) in solving \( X \).

Next, we construct a special solution \( X^* \) to system (35) with \( X^* \in S \). Recall that \( s \leq \min\{m - 1, n\} \), we split the dimension of stoichiometric subspace \( s \) into two cases:

**Case 1:** \( s = n \). Then the stoichiometric subspace \( S = \mathbb{R}^n \), and \( \Delta_y \in \mathbb{R}_{n \times n} \) is a square full rank matrix, i.e. \( \Delta_y \) is invertible. Thus, we derive a solution of (35) as

\[
X^* = (\Delta_y)^{-1} \log(\Delta_y K).
\]

It is clear that \( X^* \in S = \mathbb{R}^n \), and \( \exp(X^*) \) satisfies equations (29) by construction. This ensures that \( \exp(X^*) \) is a complex-balanced equilibrium.

**Case 2:** \( s < n \). Now we let \( S^\perp \) denote the orthogonal complement of \( S \). Since the stoichiometric subspace \( S \subset \mathbb{R}^n \), we obtain that \( S^\perp \neq \emptyset \) and

\[
0 < \dim(S^\perp) = n - \dim(S) = n - s.
\]

Then we consider a basis \( B \) of \( S^\perp \), such that

\[
B = \{v_1, \ldots, v_{n-s}\} \subset \mathbb{R}^n.
\]

Furthermore, we build another matrix and vector below

\[
\tilde{\Delta} y := \begin{bmatrix}
\Delta_y \\
v_1 \\
\vdots \\
v_{n-s}
\end{bmatrix}, \quad \text{and} \quad \tilde{\Delta} K := \begin{bmatrix}
\Delta_y K \\
0 \\
\vdots \\
0
\end{bmatrix},
\]

and consider the following system:

\[
\log(\tilde{\Delta} K) = (\tilde{\Delta} y)X.
\]

It is clear that the solutions of (39) must solve (35). From (34) and \( \{v_1, \ldots, v_{n-s}\} \) forming a basis of \( S^\perp \), we deduce that \( \tilde{\Delta} y \in \mathbb{R}_{n \times n} \) is an invertible matrix. Hence, we obtain a solution of (39) as

\[
X^* = (\tilde{\Delta} y)^{-1} \log(\tilde{\Delta} K).
\]

Moreover, for \( i = 1, \cdots, n - s \), we have

\[
v_i^\top \cdot X^* = 0,
\]

and this shows that \( X^* \in S \). By construction, \( \exp(X^*) \) must solve equations (29), thus it is a complex-balanced equilibrium.

In conclusion, we find a vector \( X^* \in S \), such that \( \exp(X^*) \) is a complex-balanced equilibrium of the system \((G, k)\) in both cases. Further, using the fact that both \( (\Delta_y)^{-1} \) and \( (\tilde{\Delta} y)^{-1} \) are fixed real matrices, we deduce \( X^* \) depends continuously on the vector \( K \).

From Theorem 2.11, given a complex-balanced system \((G, k)\) and one steady state \( X^* \) constructed above, the set of all complex-balanced equilibria of the system can be written as
\[ \exp(X^* + S^\perp) \]. More specifically, for any fixed state \( x_0 \in \mathbb{R}^n_{\geq 0} \), the corresponding complex-balanced equilibrium is the unique intersection between the set of complex-balanced equilibria \( \exp(X^* + S^\perp) \) and the affine invariant polyhedron \( (x_0 + S) \cap \mathbb{R}^n_{\geq 0} \). Using Theorem 3.12, we get that the two manifolds \( (x_0 + S) \) and \( \exp(X^* + S^\perp) \) intersect transversally \textit{at every interaction}. Hence, given a fixed state \( x_0 \), the (unique) intersection point varies continuously as a function of \( X^* \). Together with the fact that \( X^* \) depends continuously on \( K \), which additionally varies continuously on \( k \), we conclude that the map \( Q_{x_0} \) is continuous on \( k \in \mathcal{V}(G) \) when the graph \( G \) has only one connected component.

Finally, we consider the case when the graph \( G \) has multiple connected components, \( V_1, \ldots, V_\ell \) with \( \ell > 1 \). Following the proof in Proposition 3.9, we can relabel the vertices according to the connected components of \( G \), i.e. \( V_p = \{ y_{m_p+1}, \ldots, y_{m_{p+1}} \} \) for \( p = 1, \ldots, \ell \), such that the Kirchoff matrix \( A_k \) will be a block diagonal matrix, where each diagonal block corresponds to a connected component of \( G \).

Recall from Equations (31), a state \( x \) is a complex-balanced equilibrium, if and only if for any two vertices \( y_i, y_j \) in the same connected component of \( G \),

\[
\log(K_i/K_j) = (y_i^\top - y_j^\top) \cdot X,
\]

and it is equivalent to the following system of linear equations in \( X \):

\[
\begin{bmatrix}
\log(K_1/K_2) \\
\vdots \\
\log(K_{m_1-1}/K_{m_1}) \\
\log(K_{m_1+1}/K_{m_1+2}) \\
\vdots \\
\log(K_{m_{\ell-1}}/K_{m_{\ell}}) \\
\log(\Delta K)
\end{bmatrix} = 
\begin{bmatrix}
y_1^\top - y_2^\top \\
\vdots \\
y_{m_1-1}^\top - y_{m_1}^\top \\
y_{m_1+1}^\top - y_{m_1+2}^\top \\
\vdots \\
y_{m_{\ell-1}}^\top - y_{m_{\ell}}^\top \\
\Delta y
\end{bmatrix}
\begin{bmatrix}
X_1 \\
X_2 \\
\vdots \\
X_n
\end{bmatrix},
\]

and we can express it as

\[
\log(\Delta K) = (\Delta y)X.
\]

Since \( G \) has \( \ell \) connected components, its stoichiometric subspace is

\[
S = \text{span}\{y_1^\top - y_2^\top, \ldots, y_{m_1-1}^\top - y_{m_1}^\top, y_{m_1+1}^\top - y_{m_1+2}^\top, \ldots, y_{m_{\ell-1}}^\top - y_{m_{\ell}}^\top\}.
\]

Let \( s \) be the dimension of \( S \). Then we deduce that \( s \leq \min\{m - \ell, n\} \), and the matrix \( \Delta y \) has exactly \( s \) linearly independent rows.

Analogously, we pick \( s \) linear independent rows in \( \Delta y \), and they also span stoichiometric subspace \( S \). Moreover, these rows in \( \Delta y \) formulate a full row rank matrix \( \Delta_s y \), while the corresponding rows in \( \log(\Delta K) \) gives us the vector \( \log(\Delta_s K) \). And it is easy to check that system (42) is equivalent to the following system in \( X \):

\[
\log(\Delta_s K) = (\Delta_s y)X.
\]
Next, we construct a special solution $X^*$ to system (43) with $X^* \in S$. Similarly, we consider the dimension of stoichiometric subspace $s$ in two cases: $s = n$ and $s < n$.

If $s = n$, then $\Delta_s y$ is an invertible matrix. Thus, we derive a solution of (43) as

$$X^* = (\Delta_s y)^{-1} \log(\Delta_s K).$$

It is easy to see that $X^* \in S = \mathbb{R}^n$, and $\exp(X^*)$ is a complex-balanced equilibrium.

If $s < n$, we obtain $\dim(S^\perp) = n - s > 0$, and consider a basis $B = \{v_1, \ldots, v_{n-s}\}$ of $S^\perp$. Similar as in Equations (38)-(40), we first add $v_1^\top, \ldots, v_{n-s}^\top$ on the bottom of the matrix $\Delta_s y$, and adapt $n - s$ zeros to the vector $\log(\Delta_s K)$. Then, we obtain the desired solution $X^* \in S$ of (43), with $\exp(X^*)$ is a complex-balanced equilibrium.

Furthermore, $X^*$ depends continuously on the vector $K$ in both cases. We omit the rest of proof, since it straightly follows from the single connected component case, and therefore conclude this theorem.

\begin{definition}[29] A surjective, continuous and open map is called a \textit{quotient map}. \end{definition}

\begin{corollary} For any fixed state $x_0 \in \mathbb{R}^n_{>0}$, the map $Q_{x_0}$ is a quotient map. \end{corollary}

\begin{proof} From Lemma 3.2 and Lemma 3.4, we proved the map $Q_{x_0}$ is surjective and open. Together with Theorem 3.5, we conclude the map $Q_{x_0}$ is a quotient map. \end{proof}

\section{The toric locus $V(G)$ is connected}

We first recall a fundamental result in general topology as follows:

\begin{theorem}[38, Theorem 9.4] Consider three topological spaces $A, B, C$ and a surjective map $f : A \rightarrow B$. Let $B$ be endowed with the quotient topology induced by $f$. Given an arbitrary map $g : B \rightarrow C$, then $g$ is continuous if and only if the map $g \circ f : A \rightarrow C$ is continuous. \end{theorem}

Now we are ready to show the connectedness on $V(G)$.

\begin{theorem} If the Euclidean embedded graph $G$ is weakly reversible, then the variety $V(G)$ is connected. \end{theorem}

\begin{proof} We will argue by contradiction. Given a fixed state $x_0 \in \mathbb{R}^n_{>0}$, suppose the set $V(G)$ is not connected. Then there exists a \textit{surjective continuous} map $\mu$, such that

$$\mu : V(G) \rightarrow \{0, 1\}.$$ 

Next we consider the following commutative diagram:

$$
\begin{array}{ccc}
V(G) & \xrightarrow{\mu} & \{0, 1\} \\
\downarrow{Q_{x_0}} & & \\
(x_0 + S) \cap \mathbb{R}^n_{>0} & \xleftarrow{\nu} & \\
\end{array}
$$
The map \( \nu : (x_0 + S) \cap \mathbb{R}^n_{>0} \rightarrow \{0, 1\} \) in the diagram satisfies
\[
\mu = \nu \circ Q_{x_0}.
\]
It is well-defined since \( Q_{x_0} \) is surjective by Lemma 3.2.

By Corollary 3.14, the map \( Q_{x_0} \) is a quotient map. Hence, we derive that \( \nu \) is continuous if and only if \( \mu \) is continuous. Since \( \mu \) is continuous, we conclude that \( \nu \) is a continuous map. We also derive that \( \nu \) is surjective from \( \mu \) being a subjective map.

Note that the invariant polyhedron \( (x_0 + S) \cap \mathbb{R}^n_{>0} \) is connected, while the set \( \{0, 1\} \) is clearly disconnected. This leads to a contradiction since every continuous function maps a connected set to a connected set. Thus the initial supposition is false, and we conclude that \( \mathcal{V}(G) \) is connected. \( \square \)

4 The toric locus \( \mathcal{V}(G) \) is a product space

In this section, we consider a weakly reversible graph \( G = (V, E) \) and show, in Theorem 4.8, that the toric locus \( \mathcal{V}(G) \) is a product space.

4.1 The set of complex-balanced flux vectors \( \mathcal{B}(G) \)

Definition 4.1. Given a Euclidean embedded graph \( G = (V, E) \), we denote the flux vector by \( \beta = (\beta_{y_i \rightarrow y_j})_{y_i \rightarrow y_j \in E} \in \mathbb{R}^E_{>0} \), and the component \( \beta_{y_i \rightarrow y_j} > 0 \) is called the flux of the reaction \( y_i \rightarrow y_j \). Moreover, the pair \( (G, \beta) \) is called a flux system.

Definition 4.2. Consider a Euclidean embedded graph \( G = (V, E) \), a flux vector \( \beta \in \mathbb{R}^E_{>0} \) is called a steady flux vector on \( G \), if it satisfies
\[
\sum_{y_i \rightarrow y_j \in E} \beta_{y_i \rightarrow y_j} (y_j - y_i) = 0.
\]
A steady flux vector \( \beta \) is called a complex-balanced flux vector, if at each vertex \( y_0 \in V \),
\[
\sum_{y \rightarrow y_0 \in E} \beta_{y \rightarrow y_0} = \sum_{y_0 \rightarrow y' \in E} \beta_{y_0 \rightarrow y'}.
\]
We say that the pair \( (G, \beta) \) is a complex-balanced flux system.

Definition 4.3. Given a Euclidean embedded graph \( G = (V, E) \), we define the set of complex-balanced flux vectors on \( G \) as follows:
\[
\mathcal{B}(G) := \{ \beta \in \mathbb{R}^E_{>0} \mid \beta \text{ is a complex-balanced flux vector on } G \}.
\]

Analogous to complex-balanced mass action systems, complex-balanced flux systems also have connections with Euclidean embedded graphs.

Lemma 4.4. Every Euclidean embedded graph which permits a complex-balanced flux system is weakly reversible. Moreover, every Euclidean embedded graph which is weakly reversible permits complex-balanced flux systems.
Proof. First, suppose the Euclidean embedded graph $G = (V, E)$ allows a complex-balanced flux system $\beta = (\beta_{y_i \to y_j})_{y_i, y_j \in E} \in \mathbb{R}_E^>$. We define a mass-action system $(G, k)$ with reaction rate constants

$$k_{y \to y'} = \beta_{y \to y'}, \text{ for every } y \to y' \in E.$$ 

Then, it is clear that $x^* = (1, \ldots, 1)^T$ is a complex-balanced steady state. Applying Theorem 2.16, we deduce that $G = (V, E)$ is weakly reversible.

Next, assume that the Euclidean embedded graph $G = (V, E)$ is weakly reversible. Using Theorem 2.16, there exists a complex-balanced mass action system $(G, k)$ with a steady state $x^*$. We define a flux system $(G, \beta)$ with fluxes

$$\beta_{y \to y'} := k_{y \to y'}(x^*)^y, \text{ for every } y \to y' \in E.$$ 

Inputting $\beta$ into (45), we derive that $(G, \beta)$ is a complex-balanced flux system. \hfill \Box

Subsequently, given a Euclidean embedded graph $G = (V, E)$, we conclude that

- If $G = (V, E)$ is weakly reversible, then $B(G) \neq \emptyset$.
- If $G = (V, E)$ isn’t weakly reversible, then $B(G) = \emptyset$.

We are not interested in the case when $B(G)$ is empty, thus we always assume that the Euclidean embedded graph $G = (V, E)$ is weakly reversible when working on $B(G)$.

**Lemma 4.5.** Let $G = (V, E)$ be a weakly reversible Euclidean embedded graph. Then the set of complex-balanced flux vectors $B(G)$ is a convex cone in $\mathbb{R}_E^>$. 

**Proof.** Suppose both $\beta^*, \beta^{**} \in B(G)$, then we get

$$(47) \quad \sum_{y \to y_0 \in E} \beta^*_{y \to y_0} = \sum_{y' \to y \in E} \beta^*_{y' \to y}, \text{ and } \sum_{y \to y_0 \in E} \beta^{**}_{y \to y_0} = \sum_{y' \to y \in E} \beta^{**}_{y' \to y}.$$ 

Now we consider the following set:

$$(48) \quad L(\beta^*, \beta^{**}) := \{a\beta^* + (1-a)\beta^{**} : 0 \leq a \leq 1\}.$$ 

Under direct computation, we obtain for any number $0 \leq a \leq 1$,

$$(49) \quad \sum_{y_i \to y_j} (a\beta^*_{y_i \to y_j} + (1-a)\beta^{**}_{y_i \to y_j}) = \sum_{y_j \to y_i} (a\beta^*_{y_j \to y_i} + (1-a)\beta^{**}_{y_j \to y_i}).$$ 

Therefore, $L(\beta^*, \beta^{**}) \subset B(G)$, and we prove this Lemma. \hfill \Box

The following remark is a direct consequence of Lemma 4.5.

**Remark 4.6.** Consider a Euclidean embedded graph $G = (V, E)$, the set of complex-balanced flux vectors $B(G)$ is connected.
4.2 The toric locus $V(G)$ is a product space

The goal of this section is to establish the product structure of the moduli spaces of toric dynamical systems via an explicitly constructed homeomorphism.

Let us recall the well-known properties of a homeomorphism (see for instance [29]):

**Definition 4.7.** A function $f : X \to Y$ between two topological spaces is a homeomorphism, if it has the following properties: $f$ is bijective, continuous and the inverse function $f^{-1}$ is continuous. If such a function $f$ exists, we say two topological spaces $X$ and $Y$ are homeomorphic, and write this as $X \simeq Y$.

Now we present the main result in this paper.

**Theorem 4.8.** Let $G = (V, E)$ be a weakly reversible Euclidean embedded graph. For any fixed state $x_0 \in \mathbb{R}^n_{>0}$, the toric locus $V(G) \subseteq \mathbb{R}^E_{>0}$ is homeomorphic to the product space $S_{x_0} \times B(G)$, that is,

$$V(G) \simeq S_{x_0} \times B(G),$$

where $S_{x_0}$ is the invariant polyhedron, and $B(G)$ is the set of complex-balanced flux vectors.

To prove Theorem 4.8, we start by constructing a function $\varphi$ between the product space $S_{x_0} \times B(G)$ and the toric locus $V(G)$. Then we show that $\varphi$ is a homeomorphism.

**Definition 4.9.** Let $G = (V, E)$ be a weakly reversible Euclidean embedded graph. Given a fixed state $x_0 \in \mathbb{R}^n_{>0}$, we define the following map:

$$\varphi : S_{x_0} \times B(G) \to V(G),$$

such that for any $x \in S_{x_0}$ and $\beta = (\beta_{y_i \to y_j})_{y_i \to y_j \in E} \in B(G)$,

$$\varphi(x, \beta) := (\varphi_{y_i \to y_j})_{y_i \to y_j \in E}, \text{ with } \varphi_{y_i \to y_j} := \frac{\beta_{y_i \to y_j}}{x_{y_i}}.$$

**Lemma 4.10.** For any fixed state $x_0 \in \mathbb{R}^n_{>0}$, the map $\varphi$ is well-defined, and continuous.

*Proof.* For any $\beta \in B(G) \subseteq \mathbb{R}^E_{>0}$ and $x \in S_{x_0} \subseteq \mathbb{R}^n_{>0}$, we get

$$\varphi(x, \beta) = (\frac{\beta_{y_i \to y_j}}{x_{y_i}})_{y_i \to y_j \in E} \subseteq \mathbb{R}^E_{>0}.$$

Since $\beta$ is a complex-balanced flux vector, we get

$$\sum_{y_i \to y_j} \varphi_{y_i \to y_j} x_{y_i} = \sum_{y_j \to y_i} \varphi_{y_i \to y_j} x_{y_j}.$$

Hence, $\varphi(x, \beta)$ is a complex-balanced rate vector with the complex-balanced steady state $x \in S_{x_0}$ on $G$. Therefore, we conclude that $\varphi(x, \beta) \in V(G)$, and $\varphi$ is well-defined. Furthermore, it is easy to see that $\varphi$ is continuous from definition.

**Lemma 4.11.** For any fixed state $x_0 \in \mathbb{R}^n_{>0}$, the map $\varphi$ is bijective.
Proof. First, we show $\varphi$ is surjective. By Theorem 2.11, for any reaction rate vector $k \in V(G)$, there exists a (unique) complex-balanced steady state $x \in S_{x_0}$. Then we define a flux vector $\beta = (\beta_{y_i \rightarrow y_j})_{y_i \rightarrow y_j \in E}$ as follows:

$$\beta_{y_i \rightarrow y_j} := k_{y_i \rightarrow y_j} x^{y_i}.$$ 

Using Lemma 4.4, we derive that $\beta \in B(G)$, and $\varphi(x, \beta) = k$.

Next, we show $\varphi$ is injective. Assume that $(\hat{x}, \hat{\beta}), (\tilde{x}, \tilde{\beta}) \in S_{x_0} \times B(G)$, such that $\varphi(\hat{x}, \hat{\beta}) = \varphi(\tilde{x}, \tilde{\beta})$. Following (52), we derive two reaction rate vectors $\hat{\varphi}$ and $\tilde{\varphi}$ as follows:

\begin{equation}
(54) \varphi(\hat{x}, \hat{\beta}) := \left(\frac{\hat{\beta}_{y_i \rightarrow y_j}}{\hat{x}^{y_i}}\right)_{y_i \rightarrow y_j \in E}, \quad \text{and} \quad \varphi(\tilde{x}, \tilde{\beta}) := \left(\frac{\tilde{\beta}_{y_i \rightarrow y_j}}{\tilde{x}^{y_i}}\right)_{y_i \rightarrow y_j \in E}
\end{equation}

From $\varphi(\hat{x}, \hat{\beta}) = \varphi(\tilde{x}, \tilde{\beta})$ and Lemma 4.10, the uniqueness on the complex-balanced steady state within each affine invariant polyhedron, we obtain $\hat{x} = \tilde{x}$. On the other hand, it is clear that $\hat{\beta} = \tilde{\beta}$ from Equation (54), and we conclude the injectivity.

Lemma 4.12. For any fixed state $x_0 \in \mathbb{R}_{>0}^n$, the map $\varphi^{-1}$ is well-defined, and continuous.

Proof. We have proved that the map $\varphi$ is bijective in Lemma 4.11, thus it is standard that $\varphi^{-1}$ is well-defined.

Now we show that $\varphi^{-1}$ is continuous. From Lemma 4.10, given any $(x, \beta) \in S_{x_0} \times B(G)$, $\varphi(x, \beta)$ forms a complex-balanced rate vector with $x$ being the complex-balanced steady state. Since $\varphi$ is bijective and the complex-balanced steady state is unique in $S_{x_0}$, for any complex-balanced rate vector $k = (k_{y_i \rightarrow y_j})_{y_i \rightarrow y_j \in E} \in V(G)$, we have

\begin{equation}
(55) \varphi^{-1}(k) = (x, \beta),
\end{equation}

such that

\begin{equation}
(56) \quad x = Q_{x_0}(k) \quad \text{and} \quad \beta_{y_i \rightarrow y_j} := k_{y_i \rightarrow y_j} x^{y_i}, \quad \text{with} \quad \beta = (\beta_{y_i \rightarrow y_j})_{y_i \rightarrow y_j \in E}.
\end{equation}

Applying Theorem 3.5, we get the map $Q_{x_0}$ is continuous, which indicates that $x$ depends continuously on $k$. Moreover, every component in $\beta$ can be written as a polynomial of $k$ and $x$. This reveals that $\beta$ also depends continuously on $k$.

After showing both components in the product space $S_{x_0} \times B(G)$ vary continuously on $k$, we conclude the continuity on the map $\varphi^{-1}$.

Finally, we are able to prove Theorem 4.8.

Proof of Theorem 4.8. From Definition 4.7, it suffices to show that the map $\varphi$ is a homeomorphism. Applying Lemma 4.11, we derive $\varphi$ is a bijective function. From Lemma 4.10 and Lemma 4.12, we show that both $\varphi$ and $\varphi^{-1}$ are continuous functions. Therefore, we conclude $\varphi$ is a homeomorphism, and prove this theorem.
4.3 Connection to deficiency theory

The notion of deficiency of a reaction network or Euclidean embedded graph was introduced by Feinberg and Horn [19, 25]. It is an invariant of the network and plays a key role in the study of complex-balanced steady states of a network [18, 24].

**Definition 4.13** ([18, 40]). Consider a Euclidean embedded graph \(G = (V, E)\) with \(l\) connected components. Let \(s\) be the dimension of the stoichiometric subspace \(S\). The **deficiency** of a Euclidean embedded graph \(G\) is the non-negative integer

\[
\delta := |V| - l - s.
\]

Under mass-action kinetics, networks with low deficiency have special dynamical properties. For example, the deficiency zero theorem shows that weakly reversible deficiency zero networks are complex-balanced for any choices of rate constants [19, 25]. In [12], it was shown that given a weakly reversible Euclidean embedded graph \(G\), the set \(\mathcal{V}(G)\) is an algebraic variety of codimension \(\delta\) in \(\mathbb{R}^E_{>0}\). In the following, we will recover this result by using the product structure of the moduli space \(\mathcal{V}(G)\) from Theorem 3.16.

**Proposition 4.14.** Consider a Euclidean embedded graph \(G = (V, E)\) with \(l\) connected components and \(m\) vertices. Let \(s\) be the dimension of the stoichiometric subspace \(S\), then

\[
\dim(\mathcal{V}(G)) = |E| - m + s + l.
\]

*Proof.* Recall that the dimension of a product of topological spaces is a topological invariant and it is given by the sum of the dimensions of the factors [29]. In addition, the dimension of a variety at a regular point is the dimension of its tangent vector space at that point, thus it is the same dimension as seen as a manifold as well as seen as a variety [27].

Now using Theorem 4.8, we have for any fixed state \(x_0 \in \mathbb{R}^n_{>0}\),

\[
\dim(\mathcal{V}(G)) = \dim((x_0 + S) \cap \mathbb{R}^n_{>0}) + \dim(B(G)),
\]

and it is clear that \(\dim((x_0 + S) \cap \mathbb{R}^n_{>0}) = \dim(S) = s\).

Recall that \(B(G) \subseteq \mathbb{R}^E_{>0}\) represents the set of complex-balanced flux vectors that satisfy (45). Following Kirchhoff junction rules, for each connected component of \(G\) with \(m_i\) vertices, there are \(m_i - 1\) independent conditions among the linear conditions defining \(B(G)\) in (45). Further, we can check that linear conditions are independent when working on different connected components of \(G\). Hence, we get

\[
\dim(B(G)) = |E| - \sum_{i=1}^l (m_i - 1) = |E| - m + l.
\]

Together with (58), we conclude the proposition. \(\square\)

The following corollary is a direct consequence of Proposition 4.14. It was first proved in [12] using a different method.

**Corollary 4.15.** Let \(G = (V, E)\) be a weakly reversible Euclidean embedded graph. Then the codimension of the moduli space \(\mathcal{V}(G) \subseteq \mathbb{R}^E_{>0}\) is \(\delta\).

*Proof.* The codimension on \(\mathcal{V}(G)\) follows

\[
\text{Codim}(\mathcal{V}(G)) = |E| - \dim(\mathcal{V}(G)) = |E| - (|E| - m + s + l) = \delta.
\]

\(\square\)
4.4 Bijective affine transformations preserve the toric locus

In this section, we prove that the toric locus is preserved by bijective affine transformations of the network.

**Definition 4.16.** Let us consider a network $G = (V, E)$ in $\mathbb{R}^n$. Suppose $T : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a bijective affine transformation. Denote by

$$ T(V) := \{ T(y) \mid y \in V \}, \text{ and } T(E) := \{ T(y_i) \rightarrow T(y_j) \mid y_i \rightarrow y_j \in E \}. $$

Then we call the graph $T(G) := (T(V), T(E))$ the **bijective affine image of $G$ by $T$.**

**Theorem 4.17.** Let us consider a weakly reversible Euclidean embedded graph $G_1$. If $G_2$ is a bijective affine image of the graph $G_1$, then $G_1$ and $G_2$ have the same toric locus. Namely,

$$ V(G_1) = V(G_2). $$

**Proof.** The result follows from [12, Theorem 9] and from the Matrix-Tree theorem. In particular see [12, Section 2, page 5]: the change of coordinates given by the spanning trees in the two graphs are the same.

5 Discussion and future work

Researchers have become increasingly interested in the study of the **toric locus** of complex-balanced dynamical systems, that is, the set of parameters giving rise to complex-balanced dynamical systems. This is due to the very stable dynamical behaviour of these systems; for instance, the complex balanced steady states are known to be locally asymptotically stable.

Since complex balanced dynamical systems can be studied using Nonlinear Algebra tools (see for example [6, Chapter 6]), the authors of [12] called these systems **toric dynamical systems** (see also [9, Chapter 5]). Not only the moduli spaces of toric dynamical systems are toric, but also the steady-state locus (i.e. the fixed points) of toric dynamical systems can be described by binomial equations; this was proven by Gatermann, see [20]. Another computational advantage of this fact is that one may describe the steady states of such a system in terms of monomial parametrizations ([1]). The fruitful combinatorial and computational properties of binomial ideals are well-known and they are desirable in applications, since toric algebraic varieties are well-understood.

In this paper we prove that, given a complex balanced mass-action system and positive initial data, the positive complex balanced equilibria vary continuously in function of the parameters. Next, using this result, we show that the toric locus is connected and we emphasize the product structure of the toric locus. Namely, we prove that there exists a homeomorphism between the toric locus and the product of the set of complex balanced flux vectors and the affine invariant polyhedron. We provide an explicit parametrization in terms of the parameters (i.e., the reaction rate constants), as shown in (52).

In future work [13], we will use some of the approaches developed here to show that the positive complex balanced equilibria of a complex balanced mass-action system actually depend smoothly on the reaction rate constants and on the initial data. Furthermore, the approach used on showing the homeomorphism may allow us to derive regularity properties of the toric variety $\mathcal{V}(G)$. 

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References

[1] Michael F. Adamer and Martin Helmer. “Families of toric chemical reaction networks”. In: J. Math. Chem. 58.9 (2020), pp. 2061–2093. ISSN: 0259-9791. DOI: 10.1007/s10910-020-01162-x. URL: https://doi.org/10.1007/s10910-020-01162-x (cit. on p. 27).

[2] Saugata Basu, Richard Pollack, and Marie-Françoise Roy. Algorithms in real algebraic geometry. Second. Vol. 10. Algorithms and Computation in Mathematics. Springer-Verlag, Berlin, 2006, pp. x+662 (cit. on p. 11).

[3] Daniel J. Bates, Paul Breiding, Tianran Chen, Jonathan D. Hauenstein, Anton Leykin, and Frank Sottile. Numerical Nonlinear Algebra. 2023. URL: https://arxiv.org/abs/2302.08585 (cit. on p. 3).

[4] Daniel J. Bates, Jonathan D. Hauenstein., Andrew J. Sommese, and Charles W. Wampler. Bertini: Software for Numerical Algebraic Geometry. 2013. DOI: 10.7274/R0H41PB5. URL: https://bertini.nd.edu (cit. on p. 3).

[5] Balázs Boros. “Existence of positive steady states for weakly reversible mass-action systems”. In: SIAM J. Math. Anal. 51.1 (2019), pp. 435–449. ISSN: 0036-1410. DOI: 10.1137/17M115534X. URL: https://doi.org/10.1137/17M115534X (cit. on p. 2).

[6] Paul Breiding, Türklü Özlüm Çelik, Timothy Duff, Alexander Heaton, Aida Maraj, Anna-Laura Sattelberger, Lorenzo Venturello, and Oğuzhan Yürük. “Nonlinear algebra and applications”. In: Numer. Algebra Control Optim. 13.1 (2023), pp. 81–116. ISSN: 2155-3289. DOI: 10.3934/naco.2021045. URL: https://doi.org/10.3934/naco.2021045 (cit. on p. 27).

[7] Paul Breiding and Sascha Timme. “HomotopyContinuation. jl: A package for homotopy continuation in Julia”. In: International Congress on Mathematical Software. Springer. 2018, pp. 458–465 (cit. on p. 3).

[8] J. B. Collins and Jonathan D. Hauenstein. “A singular value homotopy for finding critical parameter values”. In: Appl. Numer. Math. 161 (2021), pp. 233–243. ISSN: 0168-9274. DOI: 10.1016/j.apnum.2020.11.009. URL: https://doi.org/10.1016/j.apnum.2020.11.009 (cit. on p. 3).

[9] David A. Cox. Applications of polynomial systems. Vol. 134. CBMS Regional Conference Series in Mathematics. With contributions by Carlos D’Andrea, Alicia Dickenstein, Jonathan Hauenstein, Hal Schenck and Jessica Sidman. American Mathematical Society, Providence, RI, [2020] ©2020, pp. ix+250. ISBN: 978-1-4704-5137-0 (cit. on pp. 4, 17, 27).
[10] Gheorghe Craciun. “Polynomial dynamical systems, reaction networks, and toric differential inclusions”. In: SIAM J. Appl. Algebra Geom. 3.1 (2019), pp. 87–106. DOI: 10.1137/17M1129076. URL: https://doi.org/10.1137/17M1129076 (cit. on p. 4).

[11] Gheorghe Craciun. “Toric Differential Inclusions and a Proof of the Global Attractor Conjecture”. In: (). URL: https://arxiv.org/abs/1501.02860 (cit. on p. 3).

[12] Gheorghe Craciun, Alicia Dickenstein, Anne Shiu, and Bernd Sturmfels. “Toric dynamical systems”. In: J. Symbolic Comput. 44.11 (2009), pp. 1551–1565. URL: https://doi.org/10.1016/j.jsc.2008.08.006 (cit. on pp. 3, 4, 7–10, 14, 15, 17, 26, 27).

[13] Gheorghe Craciun, Jiaxin Jin, and Miruna-Ştefana Sorea. “Smoothness of the toric locus”. In: in preparation () (cit. on p. 27).

[14] Gheorghe Craciun, Jiaxin Jin, and Polly Y. Yu. “An efficient characterization of complex-balanced, detailed-balanced, and weakly reversible systems”. In: SIAM J. Appl. Math. 80.1 (2020), pp. 183–205. URL: https://doi.org/10.1137/19M1244494 (cit. on pp. 3, 4).

[15] Gheorghe Craciun, Stefan Müller, Casian Pantea, and Polly Y. Yu. “A generalization of Birch’s theorem and vertex-balanced steady states for generalized mass-action systems”. In: Math. Biosci. Eng. 16.6 (2019), pp. 8243–8267. URL: https://doi.org/10.3934/mbe.2019417 (cit. on p. 17).

[16] Alicia Dickenstein. “Algebraic geometry tools in systems biology”. In: Notices Amer. Math. Soc. 67.11 (2020), pp. 1706–1715. ISSN: 0002-9920. DOI: 10.1090/noti. URL: https://doi.org/10.1090/noti (cit. on p. 2).

[17] Timothy Duff, Cvetelina Hill, Anders Jensen, Kisun Lee, Anton Leykin, and Jeff Sommars. “Solving polynomial systems via homotopy continuation and monodromy”. In: IMA J. Numer. Anal. 39.3 (2019), pp. 1421–1446. ISSN: 0272-4979. DOI: 10.1093/imaman/dry017. URL: https://doi.org/10.1093/imaman/dry017 (cit. on p. 3).

[18] Martin Feinberg. Foundations of chemical reaction network theory. Vol. 202. Applied Mathematical Sciences. Springer, Cham, 2019, pp. xxix+454 (cit. on pp. 2, 4, 26).

[19] Martin Feinberg and F.J.M. Horn. “Chemical mechanism structure and the coincidence of the stoichiometric and kinetic subspaces”. In: Arch. Rational Mech. Anal. 66 (1977), pp. 83–97. URL: https://doi.org/10.1007/BF00250853 (cit. on pp. 9, 26).

[20] Karin Gatermann. “Counting stable solutions of sparse polynomial systems in chemistry”. In: Symbolic computation: solving equations in algebra, geometry, and engineering (South Hadley, MA, 2000). Vol. 286. Contemp. Math. Amer. Math. Soc., Providence, RI, 2001, pp. 53–69. URL: https://doi.org/10.1090/conm/286/04754 (cit. on pp. 7, 27).

[21] Daniel R. Grayson and Michael E. Stillman. Macaulay2, a software system for research in algebraic geometry. Available at http://www.math.uiuc.edu/Macaulay2/ (cit. on pp. 11, 17).
[22] Sabina J Haque, Matthew Satriano, Miruna-Ştefana Sorea, and Polly Y Yu. “The disguised toric locus and affine equivalence of reaction networks”. In: Accepted for publication in SIADS (SIAM Journal on Applied Dynamical Systems) (2022). URL: https://arxiv.org/abs/2205.06629 (cit. on pp. 3, 7).

[23] F. Horn. “Stability and complex balancing in mass-action systems with three short complexes”. In: Proc. Roy. Soc. London Ser. A 334 (1973), pp. 331–342. ISSN: 0962-8444. DOI: 10.1098/rspa.1973.0095. URL: https://doi.org/10.1098/rspa.1973.0095 (cit. on pp. 15, 17).

[24] F. Horn and R. Jackson. “General mass action kinetics”. In: Arch. Rational Mech. Anal. 47 (1972), pp. 81–116. URL: https://doi.org/10.1007/BF00251225 (cit. on pp. 2, 8, 26).

[25] Fritz Horn. “Necessary and sufficient conditions for complex balancing in chemical kinetics”. In: Archive for Rational Mechanics and Analysis 49.3 (1972), pp. 172–186 (cit. on pp. 10, 26).

[26] Yulij Ilyashenko. “Centennial history of Hilbert’s 16th problem”. In: Bull. Amer. Math. Soc. (N.S.) 39.3 (2002), pp. 301–354. URL: https://doi.org/10.1090/S0273-0979-02-00946-1 (cit. on p. 2).

[27] Keith Kendig. Elementary algebraic geometry. Graduate Texts in Mathematics, No. 44. Springer-Verlag, New York-Berlin, 1977, pp. viii+309 (cit. on p. 26).

[28] Yuri Kuznetsov. Elements of applied bifurcation theory. Vol. 112. Springer, 1998 (cit. on p. 4).

[29] John M. Lee. Introduction to topological manifolds. Second. Vol. 202. Graduate Texts in Mathematics. Springer, New York, 2011, pp. xviii+433. URL: https://doi.org/10.1007/978-1-4419-7940-7 (cit. on pp. 21, 24, 26).

[30] Edward N. Lorenz. “Deterministic nonperiodic flow”. In: J. Atmospheric Sci. 20.2 (1963), pp. 130–141. ISSN: 0022-4928. DOI: 10.1175/1520-0469(1963)020<0130:DNF>2.0.CO;2. URL: https://doi.org/10.1175/1520-0469(1963)020<0130:DNF>2.0.CO;2 (cit. on p. 2).

[31] Stephen Lynch. Dynamical systems with applications using MATLAB®. Second. Birkhäuser/Springer, Cham, 2014, pp. xvi+514. ISBN: 978-3-319-06819-0; 978-3-319-06820-6. DOI: 10.1007/978-3-319-06820-6. URL: https://doi.org/10.1007/978-3-319-06820-6 (cit. on p. 2).

[32] Mateusz Michałek and Bernd Sturmfels. Invitation to nonlinear algebra. Vol. 211. Graduate Studies in Mathematics. American Mathematical Society, Providence, RI, [2021] ©2021, pp. xiii+226. ISBN: 978-1-4704-5367-1 (cit. on pp. 3, 11, 12, 17).

[33] Laura Brustenga i Moncusí, Gheorghe Craciun, and Miruna-Ştefana Sorea. “Disguised toric dynamical systems”. In: J. Pure Appl. Algebra 226.8 (2022), Paper No. 107035, 24. ISSN: 0022-4049. DOI: 10.1016/j.jpaa.2022.107035. URL: https://doi.org/10.1016/j.jpaa.2022.107035 (cit. on pp. 3, 4, 10).
[34] Henri Poincaré. *The three-body problem and the equations of dynamics*. Vol. 443. Astrophysics and Space Science Library. Poincaré’s foundational work on dynamical systems theory, Translated from the 1890 French original and with a preface by Bruce D. Popp. Springer, Cham, 2017, pp. xxii+248. URL: https://doi.org/10.1007/978-3-319-52899-1 (cit. on p. 2).

[35] A.R. Shastri. *Basic Algebraic Topology*. Chapman and Hall/CRC., 2013. URL: https://doi.org/10.1201/b15776 (cit. on p. 17).

[36] Andrew J. Sommese and Charles W. Wampler II. *The numerical solution of systems of polynomials*. Arising in engineering and science. World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2005, pp. xxii+401. ISBN: 981-256-184-6. DOI: 10.1142/9789812567727. URL: https://doi.org/10.1142/9789812567727 (cit. on p. 3).

[37] Steven H. Strogatz. *Nonlinear dynamics and chaos*. Second. With applications to physics, biology, chemistry, and engineering. Westview Press, Boulder, CO, 2015, pp. xiii+513 (cit. on p. 4).

[38] S. Willard. *General Topology*. Addison Wesley series in mathematics/Lynn H.Loomis. Addison-Wesley Publishing Company, 1970. ISBN: 9780201087079. URL: https://books.google.com/books?id=e8IPAQAAMAAJ (cit. on p. 21).

[39] Juan Xu, Michael Burr, and Chee Yap. “An approach for certifying homotopy continuation paths: univariate case”. In: *ISSAC’18—Proceedings of the 2018 ACM International Symposium on Symbolic and Algebraic Computation*. ACM, New York, 2018, pp. 399–406. DOI: 10.1145/3208976.3209010. URL: https://doi.org/10.1145/3208976.3209010 (cit. on p. 3).

[40] Polly Y. Yu and Gheorghe Craciun. “Mathematical Analysis of Chemical Reaction Systems”. In: *Israel Journal of Chemistry, 58, 2018* (). URL: https://doi.org/10.1002/ijch.201800003 (cit. on pp. 2–5, 7, 8, 26).

Authors:
Gheorghe Craciun
University of Wisconsin-Madison, USA
craciun@math.wisc.edu

Jiaxin Jin
Ohio State University, USA
jin.1307@osu.edu

Miruna-Ştefana Sorea
SISSA (Scuola Internazionale Superiore di Studi Avanzati), Trieste, Italy and Lucian Blaga University, Sibiu, Romania
msorea@sissa.it, mirunastefana.sorea@ulbsibiu.ro