

The Dimension of the \mathbb{R} -Disguised Toric Locus of a Reaction Network

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Online seminar, Formal Reaction Kinetics and Related Questions

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- 3 The \mathbb{R} -Disguised Toric Locus $\mathcal{K}_{\mathbb{R}\text{-disg}}(G)$

History of mass-action kinetics

- In 1972, Horn and Jackson introduced the basic properties and found the complex balancing in mass-action kinetics [1, 2].
- In 2009, Craciun, Dickenstein, Shiu and Sturmfels gave a characterization of the toric locus [3].

[1]: F. Horn. “Necessary and sufficient conditions for complex balancing in chemical kinetics”. In: *Arch. Ration. Mech. Anal.* 49.3 (1972), pp. 172–186

[2]: F. Horn and R. Jackson. “General mass action kinetics”. In: *Arch. Rational Mech. Anal.* 47 (1972), pp. 81–116

[3]: G. Craciun, A. Dickenstein, A. Shiu, and B. Sturmfels. “Toric dynamical systems”. In: *J. Symbolic Comput.* 44.11 (2009), pp. 1551–1565

My work on mass-action kinetics

- In 2022, Craciun, **Jin** and Sorea found a new structural of the toric locus [4, 5].
- In 2023, Craciun, Deshpande and **Jin** discovered more properties on the disguised toric locus [6, 7, 8].

[4]: **J. Jin**, G. Craciun, and M.-S. Sorea. “The structure of the moduli spaces of toric dynamical systems”. In: *Submitted* (2023)

[5]: **J. Jin**, G. Craciun, and M.-S. Sorea. “The toric locus of a reaction network is a smooth manifold”. In: *Submitted* (2023)

[6]: **J. Jin**, G. Craciun, and Deshpande A. “On the connectivity of the Disguised Toric Locus”. In: *Accepted by Journal of Mathematical Chemistry* (2023)

[7]: **J. Jin**, G. Craciun, and A. Deshpande. “A Lower Bound on the Dimension of the Disguised Toric Locus”. In: *In revision by SIAM Journal on Applied Algebra and Geometry* (2023)

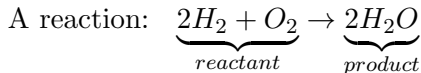
[8]: **J. Jin**, G. Craciun, and A. Deshpande. “On the Dimension of the R-Disguised Toric Locus of Reaction Networks”. In: *Preprint* (2023)

- A **biochemical reaction** can happen in the transformation of one molecule to a different molecule inside a cell. Biochemical reactions are mediated by enzymes, which are biological catalysts that can alter the rate and specificity of chemical reactions inside cells.

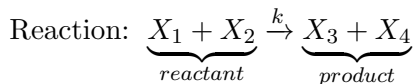
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- The key processes in biological and chemical systems are described by **biochemical reaction networks**.

- A **biochemical reaction** can happen in the transformation of one molecule to a different molecule inside a cell. Biochemical reactions are mediated by enzymes, which are biological catalysts that can alter the rate and specificity of chemical reactions inside cells.
- The key processes in biological and chemical systems are described by **biochemical reaction networks**.
- A biochemical reaction network comprises a set of **complexes** (**reactants** and **products**), and a set of **reactions**.

Complexes: $\{H_2, O_2, H_2O\}$



- **Standard deterministic mass-action kinetics** says that the rate at which a reaction occurs is proportional to the concentrations of the reactant species.

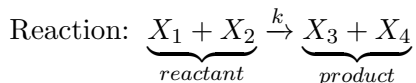


x_i : the concentration of species X_i ,

k : the reaction rate constant,

Reaction rate: kx_1x_2 .

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- A reaction network can be regarded as a **Euclidean embedded graph** $G = (V, E)$, where $V \subset \mathbb{R}_{\geq 0}^n$ is the set of vertices of the graph, and $E \subset V \times V$ is the set of oriented edges of G .

Example: The Lotka-Volterra systems can be considered as a reaction network in XY -plane with 6 complexes and 3 reactions.

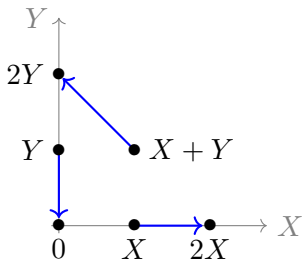


Figure 1: A reaction network of the Lotka-Volterra system.

Species: $\mathcal{S} = \{X, Y\}$,

Complexes: $\mathcal{C} = \{X, X + Y, Y, 2X, 2Y, 0\}$,

Reactions: $\mathcal{R} = \{X \rightarrow 2X, X + Y \rightarrow 2Y, Y \rightarrow 0\}$.

Example: We can translate the Lotka-Volterra systems into a Euclidean embedded graph G in \mathbb{R}^2 with 6 vertices and 3 reactions.

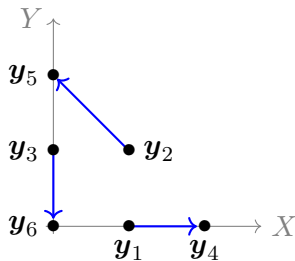
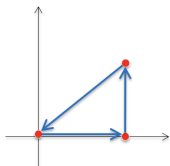
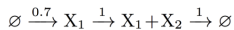
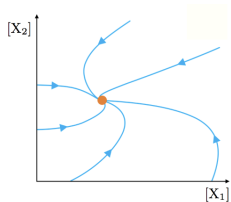


Figure 2: A Euclidean embedded graph $G = (V, E)$ of the Lotka-Volterra system.

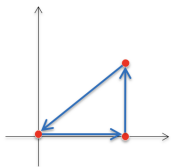
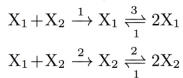
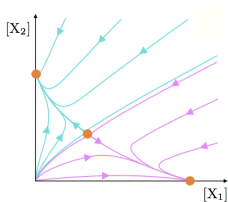
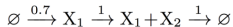
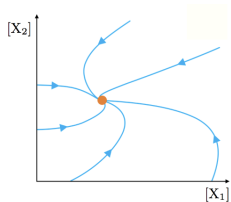
The set of vertices $V = \{y_1, y_2, y_3, y_4, y_5, y_6\},$

The set of edges $E = \{y_1 \rightarrow y_4, y_2 \rightarrow y_5, y_3 \rightarrow y_6\}.$

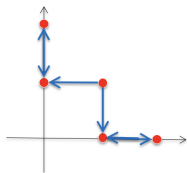


(a)

Figure 3: Reaction networks and Euclidean embedded graphs.

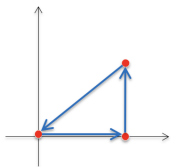
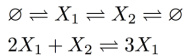
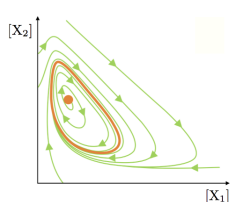
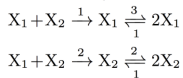
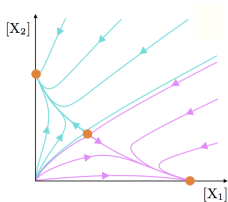
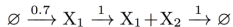
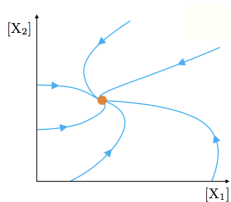


(a)

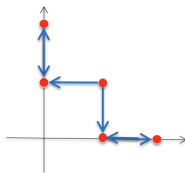


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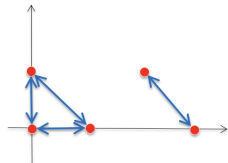
Figure 3: Reaction networks and Euclidean embedded graphs.



(a)



(b)



(c)

Figure 3: Reaction networks and Euclidean embedded graphs.

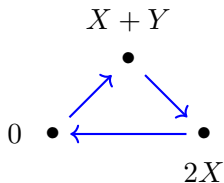
Let $G = (V, E)$ be a Euclidean embedded graph.

- (a) The set of vertices is partitioned by its **connected components**, and we identify them by the subset of vertices that belong to that connected component.

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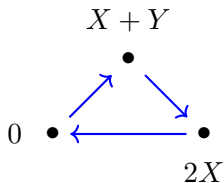
- (a) The set of vertices is partitioned by its **connected components**, and we identify them by the subset of vertices that belong to that connected component.
- (b) A graph $G = (V, E)$ is **weakly reversible**, if every edge in any connected component is part of an oriented cycle.

Example: Two Euclidean embedded graphs G and G' .

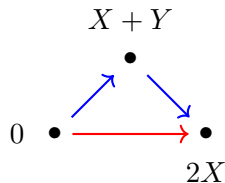


(a) $G = (V, E)$

Example: Two Euclidean embedded graphs G and G' .



(a) $G = (V, E)$



(b) $G' = (V', E')$

Figure 4: G is weakly reversible, but G' isn't weakly reversible

Mass-action system

Let $G = (V, E)$ be a Euclidean embedded graph.

- Let $\mathbf{k} = (k_{\mathbf{y} \rightarrow \mathbf{y}'})_{\mathbf{y} \rightarrow \mathbf{y}' \in G} \in \mathbb{R}_{>0}^E$ be a vector of *rate constants*. We call (G, \mathbf{k}) a *mass-action system*, and its *associated dynamical system* is given by

$$\frac{d\mathbf{x}}{dt} = \sum_{\mathbf{y} \rightarrow \mathbf{y}' \in E} \underbrace{k_{\mathbf{y} \rightarrow \mathbf{y}'} \mathbf{x}^{\mathbf{y}}}_{\text{reaction rate}} \times \underbrace{(\mathbf{y}' - \mathbf{y})}_{\text{change of species}},$$

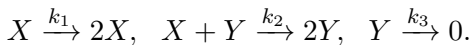
where $\mathbf{x}^{\mathbf{y}} = x_1^{y_1} x_2^{y_2} \cdots x_n^{y_n}$ with $\mathbf{x} \in \mathbb{R}_{>0}^n$ is the vector of *concentrations* of the chemical species in the system.

Given the mass-action system

$$\frac{d\mathbf{x}}{dt} = \sum_{\mathbf{y} \rightarrow \mathbf{y}' \in E} k_{\mathbf{y} \rightarrow \mathbf{y}'} \mathbf{x}^{\mathbf{y}} (\mathbf{y}' - \mathbf{y}).$$

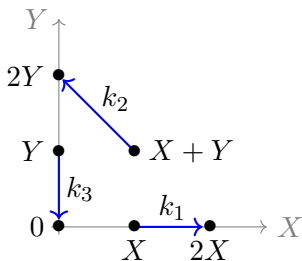
- *The stoichiometric subspace* is the vector space spanned by the reaction vectors with $\mathcal{S} = \text{span}\{\mathbf{y}' - \mathbf{y} : \mathbf{y} \rightarrow \mathbf{y}' \in E\}$.
- For any positive vector $\mathbf{x}_0 \in \mathbb{R}_{>0}^n$, the set $\mathcal{S}_{\mathbf{x}_0} := (\mathbf{x}_0 + \mathcal{S}) \cap \mathbb{R}_{>0}^n$ is known as the (*affine*) *invariant polyhedron* of \mathbf{x}_0 .

Example: Recall a reaction network of the Lotka-Volterra system in XY -plane. Given a rate constants vector $\mathbf{k} = (k_{\mathbf{y} \rightarrow \mathbf{y}'})_{\mathbf{y} \rightarrow \mathbf{y}' \in G} \in \mathbb{R}_{>0}^E$, the mass-action system (G, \mathbf{k}) is given by



Then the associated dynamical system is

$$\frac{d\mathbf{x}}{dt} = k_1 x_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + k_2 x_1 x_2 \begin{pmatrix} -1 \\ 1 \end{pmatrix} + k_3 x_2 \begin{pmatrix} 0 \\ -1 \end{pmatrix} = \begin{pmatrix} k_1 x_1 - k_2 x_1 x_2 \\ k_2 x_1 x_2 - k_3 x_2 \end{pmatrix}.$$



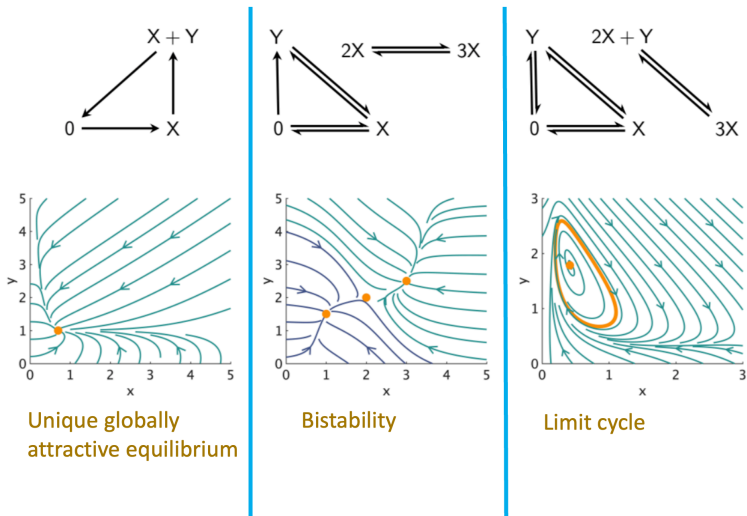


Figure 5: Possible dynamic for mass-action systems in two dimensions.

Complex-balanced system

- Let (G, \mathbf{k}) be a mass-action system, a state $\mathbf{x}_0 \in \mathbb{R}_{>0}^n$ is a **positive steady state** if

$$\mathbf{0} = \sum_{\mathbf{y} \rightarrow \mathbf{y}' \in G} k_{\mathbf{y} \rightarrow \mathbf{y}'} \mathbf{x}_0^{\mathbf{y}} (\mathbf{y}' - \mathbf{y}).$$

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- A positive steady state $\mathbf{x}_0 \in \mathbb{R}_{>0}^n$ is **complex-balanced** if for every vertex $\mathbf{y}_0 \in V_G$, we have

$$\underbrace{\sum_{\mathbf{y}_0 \rightarrow \mathbf{y}' \in G} k_{\mathbf{y}_0 \rightarrow \mathbf{y}'} \mathbf{x}_0^{\mathbf{y}_0}}_{\text{outgoing flux on } \mathbf{y}_0} = \underbrace{\sum_{\mathbf{y} \rightarrow \mathbf{y}_0 \in G} k_{\mathbf{y} \rightarrow \mathbf{y}_0} \mathbf{x}_0^{\mathbf{y}}}_{\text{incoming flux on } \mathbf{y}_0}.$$

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- If (G, \mathbf{k}) has a complex-balanced steady state, then it is called a **complex-balanced system** or **toric dynamical system**.

Example: This system is complex-balanced. For example, at the vertex $(0, 1)$, there is one reaction going into it with flux value 3, and there are two reactions leaving this vertex, with sum of fluxes being $2 + 1 = 3$.

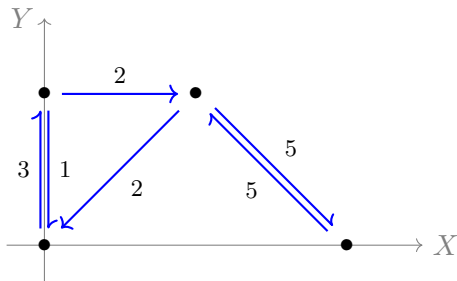


Figure 6: An example of a complex-balanced system. The positive numbers on any edge is the flux of that reaction $\mathbf{y} \rightarrow \mathbf{y}'$.

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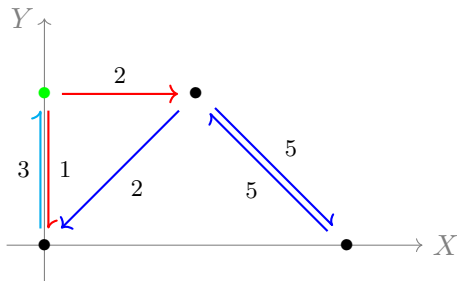


Figure 6: An example of a complex-balanced system. The positive numbers on any edge is the flux of that reaction $\mathbf{y} \rightarrow \mathbf{y}'$.

Dynamical properties of complex-balanced systems

In [2], it shows that given a complex-balanced system (G, \mathbf{k}) with the stoichiometric subspace \mathcal{S} . Let $\mathbf{x}^* \in \mathbb{R}_{>0}^n$ be a complex-balanced steady state, then

- (a) All positive steady states are complex-balanced. There is exactly one steady state within each invariant polyhedron.
- (b) Any complex-balanced steady state \mathbf{x} satisfies the following relation: $\ln(\mathbf{x}) - \ln(\mathbf{x}^*) \in \mathcal{S}^\perp$.
- (c) Every complex-balanced steady state is locally asymptotically stable within its invariant polyhedron.

[2]: F. Horn and R. Jackson. “General mass action kinetics”. In: *Arch. Rational Mech. Anal.* 47 (1972), pp. 81–116

- Consider a E-graph $G = (V, E)$, let $\mathcal{V}(G) \subseteq \mathbb{R}_{>0}^E$ denote the set of parameters $\mathbf{k} \in \mathbb{R}_{>0}^E$, for which the dynamical system generated by (G, \mathbf{k}) is toric (i.e., complex-balanced).

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- $\mathcal{V}(G)$ is called the **toric locus** of toric dynamical systems given by the Euclidean embedded graph G .

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- $\mathcal{V}(G)$ is called the **toric locus** of toric dynamical systems given by the Euclidean embedded graph G .
- In [1], it shows that given an E-graph $G = (V, E)$,
 - (a) If $G = (V, E)$ is weakly reversible, then $\mathcal{V}(G) \neq \emptyset$.
 - (b) If $G = (V, E)$ is not weakly reversible, then $\mathcal{V}(G) = \emptyset$.

[1]: F. Horn. “Necessary and sufficient conditions for complex balancing in chemical kinetics”. In: *Arch. Ration. Mech. Anal.* 49.3 (1972), pp. 172–186

Deficiency and Deficiency Zero Theorem

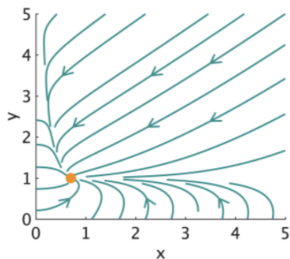
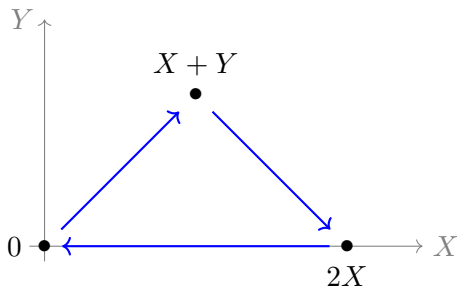
Let $G = (V, E)$ be a reaction network with ℓ connected components and the stoichiometric subspace \mathcal{S} . Suppose that $s = \dim \mathcal{S}$, then the **deficiency** of the network G is given by

$$\delta = |V| - \ell - s \geq 0.$$

Theorem 1.1 ([1], Deficiency Zero Theorem)

A mass-action system is complex-balanced for every set of positive rate constants if and only if it is weakly reversible and deficiency zero.

Example: This system is weakly reversible and deficiency zero.



**Unique globally
attractive equilibrium**

Figure 7: An example of a weakly reversible and deficiency zero system. It is complex-balanced for any positive rate constants

Characterization of the complex-balanced equilibria

The following proposition proved in [3] gives a characterization of the complex-balanced equilibria.

Proposition 1.2

Consider a weakly reversible mass-action system (G, \mathbf{k}) . For any two vertices \mathbf{y}_i and \mathbf{y}_j , let $K_i = \sum_{\mathcal{T} \text{ an } i\text{-tree}} \mathbf{k}^{\mathcal{T}}$ and construct the following equation:

$$K_i \mathbf{x}^{\mathbf{y}_j} - K_j \mathbf{x}^{\mathbf{y}_i} = 0. \quad (1)$$

Then \mathbf{x} is a complex-balanced equilibrium for the reaction rate vector \mathbf{k} if and only if Equations (1) are satisfied for every pair of vertices in the same connected component in G .

[3]: G. Craciun, A. Dickenstein, A. Shiu, and B. Sturmfels. “Toric dynamical systems”. In: *J. Symbolic Comput.* 44.11 (2009), pp. 1551–1565

Example: Consider a strongly connected mass-action system (G, \mathbf{k}) in Figure 8, with three vertices:

$$\mathbf{y}_1 = \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \quad \mathbf{y}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \mathbf{y}_3 = \begin{pmatrix} 0 \\ 2 \end{pmatrix}.$$

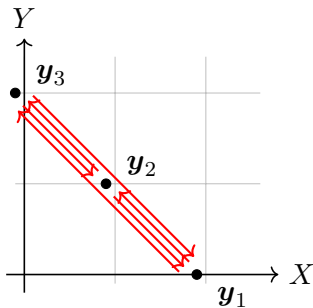


Figure 8: Complete bidirected graph with three vertices.

For the vertex \mathbf{y}_1 , we list all spanning \mathbf{y}_1 -trees of G as follows:

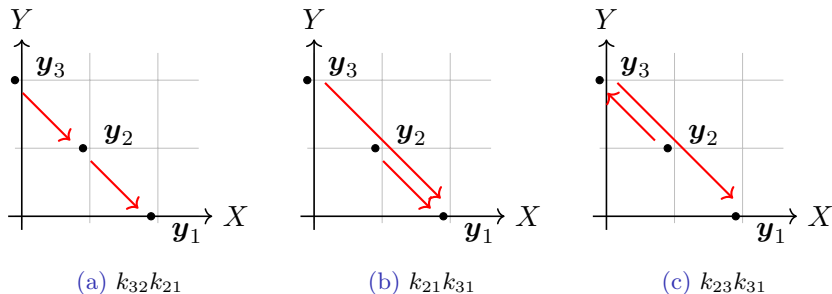


Figure 9: Spanning \mathbf{y}_1 -trees of G and $K_1 = k_{32}k_{21} + k_{21}k_{31} + k_{23}k_{31}$.

The toric locus can be written as

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

Flux vector

Let $G = (V, E)$ be an E-graph.

- Let $\mathbf{J} = (J_{\mathbf{y}_i \rightarrow \mathbf{y}_j})_{\mathbf{y}_i \rightarrow \mathbf{y}_j \in E} \in \mathbb{R}_{>0}^E$ denote a **flux vector**, whose component $J_{\mathbf{y}_i \rightarrow \mathbf{y}_j} > 0$ is called the **flux** of the reaction $\mathbf{y}_i \rightarrow \mathbf{y}_j$.

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- A flux vector \mathbf{J} is called a **complex-balanced flux vector**, if at each vertex $\mathbf{y}_0 \in V$,

$$\sum_{\mathbf{y} \rightarrow \mathbf{y}_0 \in E} J_{\mathbf{y} \rightarrow \mathbf{y}_0} = \sum_{\mathbf{y}_0 \rightarrow \mathbf{y}' \in E} J_{\mathbf{y}_0 \rightarrow \mathbf{y}'}$$

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Let $G = (V, E)$ be an E-graph.

- Let $\mathbf{J} = (J_{\mathbf{y}_i \rightarrow \mathbf{y}_j})_{\mathbf{y}_i \rightarrow \mathbf{y}_j \in E} \in \mathbb{R}_{>0}^E$ denote a **flux vector**, whose component $J_{\mathbf{y}_i \rightarrow \mathbf{y}_j} > 0$ is called the **flux** of the reaction $\mathbf{y}_i \rightarrow \mathbf{y}_j$.
- A flux vector \mathbf{J} is called a **complex-balanced flux vector**, if at each vertex $\mathbf{y}_0 \in V$,

$$\sum_{\mathbf{y} \rightarrow \mathbf{y}_0 \in E} J_{\mathbf{y} \rightarrow \mathbf{y}_0} = \sum_{\mathbf{y}_0 \rightarrow \mathbf{y}' \in E} J_{\mathbf{y}_0 \rightarrow \mathbf{y}'}$$

- Recall that $\mathbf{x}_0 \in \mathbb{R}_{>0}^n$ is a **complex-balanced steady state**, if for every vertex $\mathbf{y}_0 \in V_G$,

$$\sum_{\mathbf{y}_0 \rightarrow \mathbf{y}' \in G} k_{\mathbf{y}_0 \rightarrow \mathbf{y}'} \mathbf{x}_0^{\mathbf{y}_0} = \sum_{\mathbf{y} \rightarrow \mathbf{y}_0 \in G} k_{\mathbf{y} \rightarrow \mathbf{y}_0} \mathbf{x}_0^{\mathbf{y}}$$

$\mathcal{J}(G)$: set of complex-balanced flux vectors

- We define the **set of complex-balanced flux vectors** on G as

$$\mathcal{J}(G) := \{\mathbf{J} \in \mathbb{R}_{>0}^E \mid \mathbf{J} \text{ is a complex-balanced flux vector on } G\}.$$

$\mathcal{J}(G)$: set of complex-balanced flux vectors

- We define the **set of complex-balanced flux vectors** on G as

$$\mathcal{J}(G) := \{\mathbf{J} \in \mathbb{R}_{>0}^E \mid \mathbf{J} \text{ is a complex-balanced flux vector on } G\}.$$

- Analogous to complex-balanced systems, given an E-graph $G = (V, E)$, we conclude that
 - (a) If $G = (V, E)$ is weakly reversible, then $\mathcal{J}(G) \neq \emptyset$.
 - (b) If $G = (V, E)$ isn't weakly reversible, then $\mathcal{J}(G) = \emptyset$.

Example: Revisit the E-graph $G = (V, E)$, the following flux vector is a complex-balanced flux vector in $\mathcal{J}(G) \in \mathbb{R}_{>0}^6$.

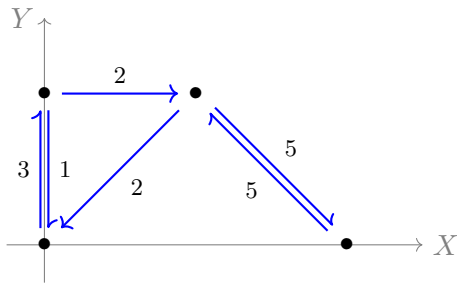


Figure 10: An example of a complex-balanced flux system. The positive numbers on any edge $\mathbf{y} \rightarrow \mathbf{y}'$ is the flux of that reaction.

The product structure of the toric locus

Theorem 1 ([4])

Let $G = (V, E)$ be a weakly reversible E -graph with the stoichiometric subspace \mathcal{S} . For any state $\mathbf{x}_0 \in \mathbb{R}_{>0}^n$, the toric locus $\mathcal{V}(G) \subseteq \mathbb{R}_{>0}^E$ is homeomorphic to the product space $\mathcal{S}_{\mathbf{x}_0} \times \mathcal{J}(G)$, that is,

$$\mathcal{V}(G) \simeq \mathcal{S}_{\mathbf{x}_0} \times \mathcal{J}(G).$$

[4]: **J. Jin**, G. Craciun, and M.-S. Sorea. “The structure of the moduli spaces of toric dynamical systems”. In: *Submitted* (2023)

A map from $\mathcal{S}_{x_0} \times \mathcal{J}(G)$ to $\mathcal{V}(G)$

- Let $G = (V, E)$ be a weakly reversible E-graph. Given a state $\mathbf{x}_0 \in \mathbb{R}_{>0}^n$, we define the following map:

$$\varphi : \mathcal{S}_{x_0} \times \mathcal{J}(G) \rightarrow \mathcal{V}(G),$$

such that for any $\mathbf{x} \in \mathcal{S}_{x_0}$ and $\mathbf{J} = (J_{\mathbf{y}_i \rightarrow \mathbf{y}_j})_{\mathbf{y}_i \rightarrow \mathbf{y}_j \in E} \in \mathcal{J}(G)$,

$$\varphi(\mathbf{x}, \mathbf{J}) := (\varphi_{\mathbf{y}_i \rightarrow \mathbf{y}_j})_{\mathbf{y}_i \rightarrow \mathbf{y}_j \in E}, \text{ with } \varphi_{\mathbf{y}_i \rightarrow \mathbf{y}_j} := \frac{J_{\mathbf{y}_i \rightarrow \mathbf{y}_j}}{x_{\mathbf{y}_i}}.$$

A map from $\mathcal{S}_{x_0} \times \mathcal{J}(G)$ to $\mathcal{V}(G)$

- Let $G = (V, E)$ be a weakly reversible E-graph. Given a state $x_0 \in \mathbb{R}_{>0}^n$, we define the following map:

$$\varphi : \mathcal{S}_{x_0} \times \mathcal{J}(G) \rightarrow \mathcal{V}(G),$$

such that for any $x \in \mathcal{S}_{x_0}$ and $\mathbf{J} = (J_{y_i \rightarrow y_j})_{y_i \rightarrow y_j \in E} \in \mathcal{J}(G)$,

$$\varphi(x, \mathbf{J}) := (\varphi_{y_i \rightarrow y_j})_{y_i \rightarrow y_j \in E}, \text{ with } \varphi_{y_i \rightarrow y_j} := \frac{J_{y_i \rightarrow y_j}}{x^{y_i}}.$$

- In [4], we show the map φ is a homeomorphism, that is, φ is bijective, continuous and the inverse function φ^{-1} is continuous.

The dimension of the toric locus $\mathcal{V}(G)$

Proposition 2.1 ([4])

Consider an E -graph $G = (V, E)$ with ℓ connected components. Let s be the dimension of the stoichiometric subspace \mathcal{S} , then

$$\dim(\mathcal{V}(G)) = |E| - |V| + s + \ell.$$

The dimension of the toric locus $\mathcal{V}(G)$

Proposition 2.1 ([4])

Consider an E -graph $G = (V, E)$ with ℓ connected components. Let s be the dimension of the stoichiometric subspace \mathcal{S} , then

$$\dim(\mathcal{V}(G)) = |E| - |V| + s + \ell.$$

The following corollary is a direct consequence of Proposition 2.1, which was also proved in [3].

Corollary 2.2 ([4])

Let $G = (V, E)$ be a weakly reversible E -graph. Then the codimension of the toric locus $\mathcal{V}(G) \subseteq \mathbb{R}_{>0}^E$ is δ .

The toric locus $\mathcal{V}(G)$ is a smooth manifold

- In [5], we further show that

$$\varphi : \mathcal{S}_{x_0} \times \mathcal{J}(G) \rightarrow \mathcal{V}(G).$$

is a diffeomorphism

- The toric locus $\mathcal{V}(G)$ is the image of an embedding, thus it is a smoothly embedded manifold.
- The complex-balanced equilibrium depends smoothly on the reaction rate constants in $\mathcal{V}(G)$.

[5]: **J. Jin**, G. Craciun, and M.-S. Sorea. “The toric locus of a reaction network is a smooth manifold”. In: *Submitted* (2023)

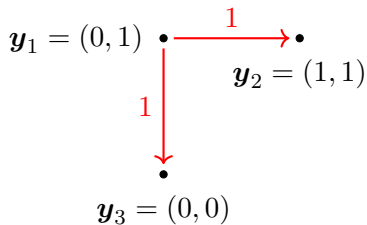
Dynamical Equivalence

Two mass-action systems (G, \mathbf{k}) and (G', \mathbf{k}') are said to be **dynamically equivalent**, if for every vertex $\mathbf{y}_0 \in V \cup V'$,

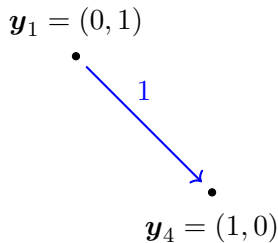
$$\sum_{\mathbf{y}_0 \rightarrow \mathbf{y} \in E} k_{\mathbf{y}_0 \rightarrow \mathbf{y}} (\mathbf{y} - \mathbf{y}_0) = \sum_{\mathbf{y}_0 \rightarrow \mathbf{y}' \in E'} k'_{\mathbf{y}_0 \rightarrow \mathbf{y}'} (\mathbf{y}' - \mathbf{y}_0). \quad (2)$$

We let $(G, \mathbf{k}) \sim (G', \mathbf{k}')$ denote that two systems (G, \mathbf{k}) and (G', \mathbf{k}') are dynamically equivalent.

Example: Figure 11 gives an example of two dynamically equivalent mass-action systems.



(a) $G = (V, E)$



(b) $G' = (V', E')$

Figure 11: The mass-action systems in (a) and (b) are dynamically equivalent.

$\mathcal{D}_0(G)$

- Let $G = (V, E)$ be an E-graph and let $\mathbf{d} = (d_{\mathbf{y} \rightarrow \mathbf{y}'})_{\mathbf{y} \rightarrow \mathbf{y}' \in E} \in \mathbb{R}^{|E|}$. We define the set $\mathcal{D}_0(G)$ as

$$\mathcal{D}_0(G) := \{ \mathbf{d} \in \mathbb{R}^{|E|} \mid \sum_{\mathbf{y}_0 \rightarrow \mathbf{y} \in E} d_{\mathbf{y}_0 \rightarrow \mathbf{y}} (\mathbf{y} - \mathbf{y}_0) = \mathbf{0} \}$$

for every vertex $\mathbf{y}_0 \in V$.

- Let $G = (V, E)$ be an E-graph and let $\mathbf{d} = (d_{\mathbf{y} \rightarrow \mathbf{y}'})_{\mathbf{y} \rightarrow \mathbf{y}' \in E} \in \mathbb{R}^{|E|}$. We define the set $\mathcal{D}_0(G)$ as

$$\mathcal{D}_0(G) := \left\{ \mathbf{d} \in \mathbb{R}^{|E|} \mid \sum_{\mathbf{y}_0 \rightarrow \mathbf{y} \in E} d_{\mathbf{y}_0 \rightarrow \mathbf{y}} (\mathbf{y} - \mathbf{y}_0) = \mathbf{0} \right.$$

for every vertex $\mathbf{y}_0 \in V$ }.

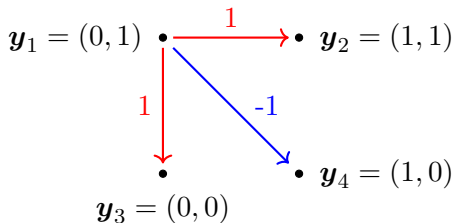


Figure 12: A rate vector $\mathbf{d} \in \mathcal{D}_0(G)$.

Flux Equivalence and $\mathcal{J}_0(G)$

- Two flux systems $(G, \mathbf{J}) = (V, E, \mathbf{J})$ and $(G', \mathbf{J}') = (V', E', \mathbf{J}')$ are said to be **flux equivalent**, denoted by $(G, \mathbf{J}) \sim (G', \mathbf{J}')$, if for every vertex $\mathbf{y}_0 \in V \cup V'$

$$\sum_{\mathbf{y}_0 \rightarrow \mathbf{y} \in E} J_{\mathbf{y}_0 \rightarrow \mathbf{y}}(\mathbf{y} - \mathbf{y}_0) = \sum_{\mathbf{y}_0 \rightarrow \mathbf{y}' \in E'} J'_{\mathbf{y}_0 \rightarrow \mathbf{y}'}(\mathbf{y}' - \mathbf{y}_0).$$

Flux Equivalence and $\mathcal{J}_0(G)$

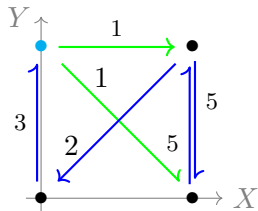
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$$\sum_{\mathbf{y}_0 \rightarrow \mathbf{y} \in E} J_{\mathbf{y}_0 \rightarrow \mathbf{y}}(\mathbf{y} - \mathbf{y}_0) = \sum_{\mathbf{y}_0 \rightarrow \mathbf{y}' \in E'} J'_{\mathbf{y}_0 \rightarrow \mathbf{y}'}(\mathbf{y}' - \mathbf{y}_0).$$

- Let $G = (V, E)$ be an E-graph and let $\mathbf{J} = (J_{\mathbf{y}_i \rightarrow \mathbf{y}_j})_{\mathbf{y}_i \rightarrow \mathbf{y}_j \in E} \in \mathbb{R}^E$. We define the set $\mathcal{J}_0(G)$ as

$$\mathcal{J}_0(G) := \left\{ \mathbf{J} \in \mathcal{D}_0(G) \mid \sum_{\mathbf{y} \rightarrow \mathbf{y}_0 \in E} J_{\mathbf{y} \rightarrow \mathbf{y}_0} = \sum_{\mathbf{y}_0 \rightarrow \mathbf{y}' \in E} J_{\mathbf{y}_0 \rightarrow \mathbf{y}'} \right. \\ \left. \text{for every vertex } \mathbf{y}_0 \in V \right\}.$$

Example: The following two flux systems are flux equivalent.



(a)

Example: The following two flux systems are flux equivalent.

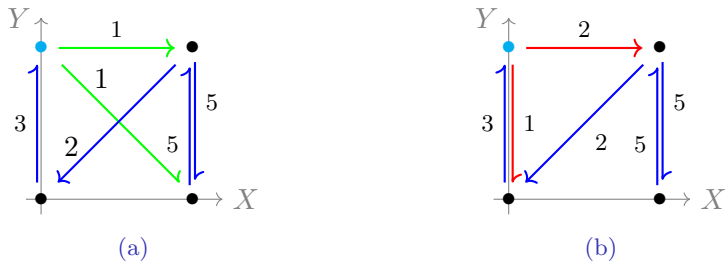


Figure 13: The flux systems in (a) and (b) are flux equivalent. The flux system in (b) is a complex-balanced flux system.

Proposition 3.1 ([9])

Let (G, \mathbf{k}) and (G', \mathbf{k}') be two mass-action systems and let $\mathbf{x} \in \mathbb{R}_{>0}^n$. Define the flux vector $\mathbf{J}(\mathbf{x}) = (J_{\mathbf{y} \rightarrow \mathbf{y}'})_{\mathbf{y} \rightarrow \mathbf{y}' \in E}$ on G , such that for every $\mathbf{y} \rightarrow \mathbf{y}' \in E$

$$J_{\mathbf{y} \rightarrow \mathbf{y}'} = k_{\mathbf{y} \rightarrow \mathbf{y}'} \mathbf{x}^{\mathbf{y}}.$$

Further, define the flux vector $\mathbf{J}'(\mathbf{x}) = (J'_{\mathbf{y} \rightarrow \mathbf{y}'})_{\mathbf{y} \rightarrow \mathbf{y}' \in E'}$ on G' , such that for every $\mathbf{y} \rightarrow \mathbf{y}' \in E'$

$$J'_{\mathbf{y} \rightarrow \mathbf{y}'} = k'_{\mathbf{y} \rightarrow \mathbf{y}'} \mathbf{x}^{\mathbf{y}}.$$

Then the following are equivalent:

- (a) $(G, \mathbf{k}) \sim (G', \mathbf{k}')$.
- (b) $(G, \mathbf{J}(\mathbf{x})) \sim (G', \mathbf{J}'(\mathbf{x}))$ for some $\mathbf{x} \in \mathbb{R}_{>0}^n$.

[9]: **J. Jin, G. Craciun, and P. Yu.** “An efficient characterization of complex-balanced, detailed-balanced, and weakly reversible systems”. In: *SIAM J. Appl. Math.* 80.1 (2020), pp. 183–205

- Recall that the **toric locus** on an E-graph G is

$$\mathcal{K}(G) := \{\mathbf{k} \in \mathbb{R}_{>0}^E \mid \text{the mass-action system generated by } (G, \mathbf{k}) \text{ is toric}\}.$$

- In [7], a dynamical system of the form

$$\frac{dx}{dt} = \mathbf{f}(x),$$

is called **disguised toric** on G , if it is realizable on G for some $\mathbf{k} \in \mathcal{K}(G) \subseteq \mathbb{R}_{>0}^E$, i.e., it has a **complex-balanced realization** on $G = (V, E)$.

[7]: **J. Jin, G. Craciun, and A. Deshpande.** “A Lower Bound on the Dimension of the Disguised Toric Locus”. In: *In revision by SIAM Journal on Applied Algebra and Geometry* (2023)

Let $G = (V, E)$ and $G' = (V', E')$ be two E-graphs.

(a) Define the set $\mathcal{K}_{\mathbb{R}\text{-disg}}(G, G')$ as

$$\mathcal{K}_{\mathbb{R}\text{-disg}}(G, G') := \{\mathbf{k} \in \mathbb{R}^E \mid \text{the dynamical system } (G, \mathbf{k}) \text{ is disguised toric on } G'\}.$$

Let $G = (V, E)$ and $G' = (V', E')$ be two E-graphs.

(a) Define the set $\mathcal{K}_{\mathbb{R}\text{-disg}}(G, G')$ as

$$\mathcal{K}_{\mathbb{R}\text{-disg}}(G, G') := \{\mathbf{k} \in \mathbb{R}^E \mid \begin{array}{l} \text{the dynamical system } (G, \mathbf{k}) \\ \text{is disguised toric on } G' \end{array}\}.$$

(b) From [9], we define the **\mathbb{R} -disguised toric locus** of G as

$$\mathcal{K}_{\mathbb{R}\text{-disg}}(G) = \bigcup_{G' \sqsubseteq G_c} \mathcal{K}_{\mathbb{R}\text{-disg}}(G, G'),$$

where G_c represents the complete graph of G .

Theorem 3.2 ([6])

Let $G = (V, E)$ and $G' = (V', E')$ be two E -graphs. Then

- (a) The set $\mathcal{K}_{\mathbb{R}\text{-disg}}(G, G')$ is connected.
- (b) The \mathbb{R} -disguised toric locus of G is also connected.

[6]: **J. Jin**, G. Craciun, and Deshpande A. “On the connectivity of the Disguised Toric Locus”. In: *Accepted by Journal of Mathematical Chemistry* (2023)

- Let (G', J') be a flux system. We say it is **\mathbb{R} -realizable** on G if there exists some $J \in \mathbb{R}^E$, such that for every vertex $y_0 \in V \cup V'$,

$$\sum_{y_0 \rightarrow y_j \in E} J_{y_0 \rightarrow y_j} (y_j - y_0) = \sum_{y_0 \rightarrow y'_j \in E'} J'_{y_0 \rightarrow y'_j} (y'_j - y_0).$$

- Let (G', \mathbf{J}') be a flux system. We say it is **\mathbb{R} -realizable** on G if there exists some $\mathbf{J} \in \mathbb{R}^E$, such that for every vertex $\mathbf{y}_0 \in V \cup V'$,

$$\sum_{\mathbf{y}_0 \rightarrow \mathbf{y}_j \in E} J_{\mathbf{y}_0 \rightarrow \mathbf{y}_j} (\mathbf{y}_j - \mathbf{y}_0) = \sum_{\mathbf{y}_0 \rightarrow \mathbf{y}'_j \in E'} J'_{\mathbf{y}_0 \rightarrow \mathbf{y}'_j} (\mathbf{y}'_j - \mathbf{y}_0).$$

- Further, we define the set $\mathcal{J}_{\mathbb{R}}(G', G)$ as

$$\mathcal{J}_{\mathbb{R}}(G', G) := \{ \mathbf{J}' \in \mathcal{J}(G') \mid \text{the flux system } (G', \mathbf{J}') \\ \text{is } \mathbb{R}\text{-realizable on } G \}.$$

Let $G_1 = (V_1, E_1)$ be a weakly reversible E-graph and let $G = (V, E)$ be an E-graph.

- There exists a set of vectors $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\} \subset \mathbb{R}^{|E_1|}$, such that

$$\mathcal{J}_{\mathbb{R}}(G_1, G) = \{a_1 \mathbf{v}_1 + \dots + a_k \mathbf{v}_k \mid a_i \in \mathbb{R}_{>0}, \mathbf{v}_i \in \mathbb{R}^{|E_1|}\},$$

and

$$\dim(\mathcal{J}_{\mathbb{R}}(G_1, G)) = \dim(\text{span}\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\}).$$

Let $G_1 = (V_1, E_1)$ be a weakly reversible E-graph and let $G = (V, E)$ be an E-graph.

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$$\mathcal{J}_{\mathbb{R}}(G_1, G) = \{a_1 \mathbf{v}_1 + \dots + a_k \mathbf{v}_k \mid a_i \in \mathbb{R}_{>0}, \mathbf{v}_i \in \mathbb{R}^{|E_1|}\},$$

and

$$\dim(\mathcal{J}_{\mathbb{R}}(G_1, G)) = \dim(\text{span}\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\}).$$

- Moreover, if $\mathcal{J}_{\mathbb{R}}(G_1, G) \neq \emptyset$, then

$$\mathcal{J}_0(G_1) \subseteq \text{span}\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\}.$$

Orthonormal basis of $\mathcal{D}_0(G)$ and $\mathcal{J}_0(G_1)$

Let $G_1 = (V_1, E_1)$ be a weakly reversible E-graph and let $G = (V, E)$ be an E-graph.

- (a) Let b denote the dimension of the linear subspace $\mathcal{D}_0(G)$, and denote an orthonormal basis of $\mathcal{D}_0(G)$ by

$$\{\mathbf{B}_1, \mathbf{B}_2, \dots, \mathbf{B}_b\}.$$

- (b) Let a denote the dimension of the subspace $\mathcal{J}_0(G_1)$, and denote an orthonormal basis of $\mathcal{J}_0(G_1)$ by

$$\{\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_a\}.$$

A map from $\mathcal{J}_{\mathbb{R}}(G_1, G)$ to \mathbb{R}^a

- Define the map

$$\psi : \mathcal{J}_{\mathbb{R}}(G_1, G) \rightarrow \mathbb{R}^a,$$

such that for $\mathbf{J} \in \mathcal{J}_{\mathbb{R}}(G_1, G)$,

$$\psi(\mathbf{J}) = (\mathbf{J}\mathbf{A}_1, \mathbf{J}\mathbf{A}_2, \dots, \mathbf{J}\mathbf{A}_a).$$

Moreover, we define the set Q as

$$Q := \psi(\mathcal{J}_{\mathbb{R}}(G_1, G)) = \{\psi(\mathbf{J}) \mid \mathbf{J} \in \mathcal{J}_{\mathbb{R}}(G_1, G)\}.$$

A map from $\mathcal{J}_{\mathbb{R}}(G_1, G)$ to \mathbb{R}^a

- Define the map

$$\psi : \mathcal{J}_{\mathbb{R}}(G_1, G) \rightarrow \mathbb{R}^a,$$

such that for $\mathbf{J} \in \mathcal{J}_{\mathbb{R}}(G_1, G)$,

$$\psi(\mathbf{J}) = (\mathbf{J}\mathbf{A}_1, \mathbf{J}\mathbf{A}_2, \dots, \mathbf{J}\mathbf{A}_a).$$

Moreover, we define the set Q as

$$Q := \psi(\mathcal{J}_{\mathbb{R}}(G_1, G)) = \{\psi(\mathbf{J}) \mid \mathbf{J} \in \mathcal{J}_{\mathbb{R}}(G_1, G)\}.$$

- Suppose $\mathcal{J}_{\mathbb{R}}(G_1, G) \neq \emptyset$, then Q is an open set in \mathbb{R}^a .

A map from $\mathcal{J}_{\mathbb{R}}(G_1, G)$ to $\mathcal{K}_{\mathbb{R}\text{-disg}}(G, G_1)$

- Given an E-graph $G = (V, E)$ and $\mathbf{x}_0 \in \mathbb{R}_{>0}^n$.

A map from $\mathcal{J}_{\mathbb{R}}(G_1, G)$ to $\mathcal{K}_{\mathbb{R}\text{-disg}}(G, G_1)$

- Given an E-graph $G = (V, E)$ and $\mathbf{x}_0 \in \mathbb{R}_{>0}^n$.
- Given a weakly reversible E-graph $G_1 = (V_1, E_1)$ with its stoichiometric subspace \mathcal{S}_{G_1} .

A map from $\mathcal{J}_{\mathbb{R}}(G_1, G)$ to $\mathcal{K}_{\mathbb{R}\text{-disg}}(G, G_1)$

- Given an E-graph $G = (V, E)$ and $\mathbf{x}_0 \in \mathbb{R}_{>0}^n$.
- Given a weakly reversible E-graph $G_1 = (V_1, E_1)$ with its stoichiometric subspace \mathcal{S}_{G_1} .
- We consider the following map:

$$\Psi : \mathcal{J}_{\mathbb{R}}(G_1, G) \times [(\mathbf{x}_0 + \mathcal{S}_{G_1}) \cap \mathbb{R}_{>0}^n] \times \mathbb{R}^b \rightarrow \mathcal{K}_{\mathbb{R}\text{-disg}}(G, G_1) \times Q$$

The map Ψ

The map

$$\Psi : \mathcal{J}_{\mathbb{R}}(G_1, G) \times [(\mathbf{x}_0 + \mathcal{S}_{G_1}) \cap \mathbb{R}_{>0}^n] \times \mathbb{R}^b \rightarrow \mathcal{K}_{\mathbb{R}\text{-disg}}(G, G_1) \times Q$$

satisfies that for $(\mathbf{J}, \mathbf{x}, \mathbf{p}) \in \mathcal{J}_{\mathbb{R}}(G_1, G) \times [(\mathbf{x}_0 + \mathcal{S}_{G_1}) \cap \mathbb{R}_{>0}^n] \times \mathbb{R}^b$,

$$\Psi(\mathbf{J}, \mathbf{x}, \mathbf{p}) := (\mathbf{k}, \mathbf{q}),$$

The map Ψ

The map

$$\Psi : \mathcal{J}_{\mathbb{R}}(G_1, G) \times [(\mathbf{x}_0 + \mathcal{S}_{G_1}) \cap \mathbb{R}_{>0}^n] \times \mathbb{R}^b \rightarrow \mathcal{K}_{\mathbb{R}\text{-disg}}(G, G_1) \times Q$$

satisfies that for $(\mathbf{J}, \mathbf{x}, \mathbf{p}) \in \mathcal{J}_{\mathbb{R}}(G_1, G) \times [(\mathbf{x}_0 + \mathcal{S}_{G_1}) \cap \mathbb{R}_{>0}^n] \times \mathbb{R}^b$,

$$\Psi(\mathbf{J}, \mathbf{x}, \mathbf{p}) := (\mathbf{k}, \mathbf{q}),$$

where

$$(G, \mathbf{k}) \sim (G_1, \mathbf{k}_1) \quad \text{with} \quad k_{1, \mathbf{y} \rightarrow \mathbf{y}'} = \frac{J_{\mathbf{y} \rightarrow \mathbf{y}'}}{\mathbf{x}^{\mathbf{y}}}.$$

and

$$\mathbf{p} = (\mathbf{k}B_1, \mathbf{k}B_2, \dots, \mathbf{k}B_b), \quad \mathbf{q} = (\mathbf{J}A_1, \mathbf{J}A_2, \dots, \mathbf{J}A_a).$$

Properties of the map Ψ

- The map Ψ is well-defined and injective.
- The map Ψ is continuous.
- There exists a set of vectors $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\} \subset \mathbb{R}^{|E_1|}$, such that

$$\mathcal{J}_{\mathbb{R}}(G_1, G) = \{a_1 \mathbf{v}_1 + \dots + a_k \mathbf{v}_k \mid a_i \in \mathbb{R}_{>0}, \mathbf{v}_i \in \mathbb{R}^{|E_1|}\},$$

and $\dim(\mathcal{J}_{\mathbb{R}}(G_1, G)) = \dim(\text{span}\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k\})$.

- $\mathcal{K}_{\mathbb{R}\text{-disg}}(G, G_1)$ is a *semialgebraic* set, that is, it can be represented as a finite union of sets defined by polynomial equalities and polynomial inequalities.

The dimension of $\mathcal{K}_{\mathbb{R}\text{-disg}}(G)$

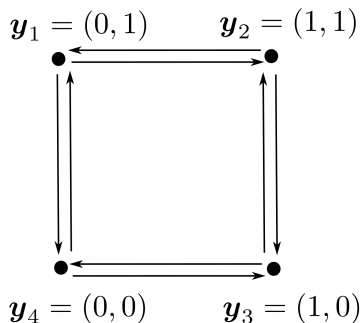
Theorem 3.3 ([8])

Let $G_1 = (V_1, E_1)$ be a weakly reversible E -graph with its stoichiometric subspace \mathcal{S}_{G_1} . Consider an E -graph $G = (V, E)$ and $\mathbf{x}_0 \in \mathbb{R}_{>0}^n$, then

$$\dim(\mathcal{K}_{\mathbb{R}\text{-disg}}(G)) = \max_{G_1 \sqsubseteq G_c} \{ \dim(\mathcal{J}_{\mathbb{R}}(G_1, G)) + \dim(\mathcal{S}_{G_1}) \\ + \dim(\mathcal{D}_O(G)) - \dim(\mathcal{J}_O(G_1)) \}.$$

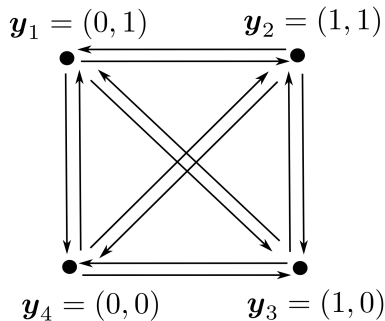
[8]: **J. Jin**, G. Craciun, and A. Deshpande. “On the Dimension of the R-Disguised Toric Locus of Reaction Networks”. In: *Preprint* (2023)

Example. We consider the \mathbb{R} -disguised toric locus on the pair of E-graphs in Figure 14. Specifically, we show how Theorem 3.3 leads to the lower bound of the \mathbb{R} -disguised toric locus.



$$G_1 = (V_1, E_1)$$

(a)



$$G_2 = (V_2, E_2)$$

(b)

Figure 14: Two E-graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$.

Step 1. We start with computing $\dim(\mathcal{J}_{\mathbb{R}}(G_2, G_1)) \subset \mathbb{R}^{12}$.

- First, being a complex-balanced vector in G_2 gives $4 - 1 = 3$ constraints on \mathbf{J} .
- Second, being \mathbb{R} -realizable in G_1 gives no constraints on \mathbf{J} since every flux vector can be transformed into G_1 . Thus we obtain

$$\dim(\mathcal{J}_{\mathbb{R}}(G_2, G_1)) \geq 12 - 3 - 0 = 9.$$

Step 2. Recall from previous example, we get

$$\mathcal{D}_0(G_1) = \{\mathbf{0}\} \quad \text{and} \quad \dim(\mathcal{J}_0(G_2)) = 3.$$

Step 3. By Theorem 3.3, we derive that

$$\begin{aligned} & \dim(\mathcal{K}_{\mathbb{R}\text{-disg}}(\mathbf{G}_1, \mathbf{G}_2)) \\ &= \dim(\mathcal{J}_{\mathbb{R}}(G_2, G_1)) + \dim(\mathcal{S}_{G_2}) + \dim(\mathcal{D}_0(G_1)) - \dim(\mathcal{J}_0(G_2)) \\ &= 8. \end{aligned}$$

Therefore we conclude that $\dim(\mathcal{K}_{\mathbb{R}\text{-disg}}(\mathbf{G}_1)) = 8$.

- The structure of the disguised toric locus
- Elucidate when does the disguised toric locus have full dimension
- Generalization for reaction networks with toric steady states

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