Duality in mass-action networks

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Introductory example (phosphorylation of a protein)

[“Stoichiometric” point of view]
Consider the following directed graph:

$$x_1 x_2 \underset{k_2}{\overset{k_1}{\rightleftharpoons}} x_3 \xrightarrow{k_3} x_1 x_4$$

It represents a dynamical system:

$$\dot{x} = (Y_p - Y_e)\mathrm{diag}(k)x^{Y_e}$$

More explicitely:

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \end{pmatrix} = \left[\begin{pmatrix} 0 & 1 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix} \right] \begin{pmatrix} k_1 & 0 & 0 \\ 0 & k_2 & 0 \\ 0 & 0 & k_3 \end{pmatrix} \begin{pmatrix} x_1 x_2 \\ x_3 \\ x_3 \end{pmatrix}$$

Introductory example (phosphorylation of a protein)

["Laplacian" point of view]
Consider the following directed graph:

$$x_1x_2 \underset{k_{21}}{\overset{k_{12}}{\rightleftarrows}} x_3 \xrightarrow{k_{23}} x_1x_4$$

It represents a dynamical system:

$$\dot{x} = x^Y A_k Y$$

More explicitely:

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \dot{x}_4 \end{pmatrix}^T = (x_1x_2, x_3, x_1x_4) \begin{pmatrix} -k_{12} & k_{12} & 0 \\ k_{21} & -k_{21} - k_{23} & k_{23} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

The general object of study

"Stoichiometric" Definition

A mass-action network is a quadruple (k, x, Y_e, Y_p), where $k := (k_1, \ldots, k_r)$ are real positive parameters, $x := (x_1, \ldots, x_n)$ are real positive variables, and $Y_e, Y_p \in \mathbb{Z}_{\geq 0}^{r \times n}$. Such mass-action network can always be represented as a directed graph whose i^{th} arrow is

$$\prod_{j=1}^{n} x_j^{Y_{e,ji}} \xrightarrow{k_i} \prod_{j=1}^{n} x_j^{Y_{p,ji}},$$

and it defines the following dynamical system:

$$\dot{x} = (Y_p - Y_e)\mathrm{diag}(k)x^{Y_e}$$

where x^{Y_e} is a column vector whose i^{th} coordinate is $\prod_{j=1}^{n} x_j^{Y_{e,ji}}$.

The general object of study

"Laplacian" Definition

A mass-action network is a triple (k, x, Y), where $k := \{k_{ij} | i, j \in [m], i \neq j\}$ are real positive parameters, $x := (x_1, \ldots, x_n)$ are real positive variables, and $Y \in \mathbb{Z}_{\geq 0}^{m \times n}$. Such mass-action network can always be represented as a directed graph whose arrows are

$$\prod_{l=1}^{n} x_l^{Y_{il}} \xrightarrow{k_{ij}} \prod_{l=1}^{n} x_l^{Y_{jl}},$$

and it defines the following dynamical system:

$$\dot{x} = \left(x^Y\right)^T A_k Y$$

where x^Y is a column vector whose i^{th} coordinate is $\prod_{j=1}^{n} x_j^{Y_{ji}}$ and A_k is the negative of the Laplacian of the corresponding directed graph.

Toricity in mass-action networks

There are basically two different (but related) notions of toricity:

1. **Toric dynamical systems**: It refers to mass-action networks with the property that, for any complex, the amount produced of that complex at steady state is equal to the amount consumed by reactions. *Equivalently, they are systems for which the equation* $\left(x^Y\right)^T A_k = 0$ *admits a solution* $x^* \in \mathbb{R}^n_{>0}$.
2. **Networks with toric steady states**: They are systems whose steady state variety is a toric variety. They can further be classified into
   1. **Networks with binomial steady state ideal**.
   2. **Systems with the isolation property**.
   3. **Networks with positive toric steady states** (the weakest).

Toric Dynamical Systems $\subset$ Binomial Ideal $\subset$ Positive toric steady states.

Conjecture* : $\qquad\qquad \parallel$

Isolation Property $\subset$ Positive toric steady states.

*This conjecture was informally proposed to me by Carsten Conradi and Thomas Kahle during my PhD (2016-2019). Now I might have a proof of it.

Two algebro-combinatorial objects

1. Siphons: subsets of the variables having the potential of being absent in a steady state. They are related to the cone $\ker(A_p - A_e)^T \cap \mathbb{R}^n_{\geq 0}$.
2. Clusters*: partition of the arrow set collecting relations between the coordinates of the cone $\ker(A_p - A_e) \cap \mathbb{R}^r_{\geq 0}$.

Conjecture:

Siphons and clusters are related through some duality relation.

Evidence for the conjecture

The set of *preclusters* is dual[a] to the set of *maximal invariant polyhedral supports* (MIPS).

[a] We will make precise the duality in the next slides.

*Clusters were introduced in 2011 by Conradi and Flockerzi. In this talk we use the term in a slightly more general sense.

The state of art in a ("non-commutative") diagram

$$
\begin{tikzcd}
\ker(A_p - A_e) \arrow[rr, leftrightarrow, "\text{dual}"] & & \ker\left((A_p - A_e)^T\right) \\
\text{Clustering graph} \arrow[u] & & \text{Chamber decomposition} \arrow[u] \\
& & \text{Decorations of invariant polyhedra} \arrow[u, phantom, "\wr"] \\
\{P \mid P \text{ is a precluster}\} \arrow[uu, phantom, "\wr"] \arrow[d, "\text{Refine}"] \arrow[rr, leftrightarrow, "\text{dual}"] & & \{M \mid M \text{ is a MIPS}\} \arrow[u] \arrow[d, "\text{"Refine"}"] \\
\{C \mid C \text{ is a cluster}\} \arrow[rr, leftrightarrow, "\text{¿duality relation?}"] & & \{S \mid S \text{ is a siphon}\}
\end{tikzcd}
$$

The dual network

Definition (Stoichiometric version)

The dual of the network (k, x, Y_e, Y_p) is the network (x, k, Y_e^T, Y_p^T).

Definition (Laplacian version)

The dual of the network (k, x, Y) is ...[a].

[a] While we do not have yet a good duality definition in this formalism, finding one is quite desirable, for all the work of Craciun et al. on the Global Atractor Conjecture is done in this formalism.

Two Examples

Why should we care? Part I

The following appear in Anne Shiu's Thesis:

1. "Relevant siphons determine which faces of an invariant polyhedron contain steady states".
2. "To prove the conjecture it is sufficient to verify that no positive trajectory approaches such a steady state".

Theorem (Craciun, Dickenstein, Shiu, Sturmfels; 2007)

Consider a conservative toric dynamical system whose stoichiometric subspace[a] is two-dimensional. Then the Birch point is a global attractor of its invariant polyhedron.

[a] that is, the span of the columns of the matrix $Y_e - Y_p$

Question

Is it possible to use duality in order to prove the theorem in codimension 2?

Why should we care? Part II

Definition

$\Sigma = \{x_i | i \in I \subseteq [n]\}$ is a *maximal invariant polyhedral supports* (MIPS) if all combinatorial types of decorated invariant abstract polyhedra are invariant under $x_i \mapsto x_j \ \forall \ x_i, x_j \in \Sigma$ (related to $\ker(A_p - A_e)^T \cap \mathbb{R}^n_{\geq 0}$).

Definition

Consider the graph G over $[r]$ wich has an edge $\{i, j\}$ whenever the i^{th} and the j^{th} arrow have the same source and let $n_1, \ldots, n_r$ denote the rows of a matrix with columns the rays $\ker(A_p - A_e) \cap \mathbb{Z}^r_{\geq 0}$. If to the graph G we add the edges $\{i, s\}$ and $\{j, s\}$ whenever n_s is in the span of $\{n_i, n_j\}$ for each edge $\{i, j\}$ of G, we obtain the preclustering graph. A precluster is a connected component of the preclustering graph.

Theorem (I.)

For conservative mass-action networks that do not have two species with exactly the same rates the set of preclusters is dual to the set of MIPS.

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