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# DUALITY IN MASS-ACTION NETWORKS

ALEXANDRU IOSIF

ABSTRACT. We introduce a duality theory for mass-action networks and we show that preclusters and maximal invariant polyhedral supports are dual objects.

## 1. INTRODUCTION

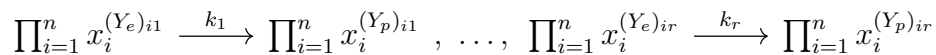
A *chemical reaction* is a transformation between two sets of chemical species; a set of chemical reactions is called *chemical reaction network*. Often chemical reaction networks are regarded as dynamical systems in which the concentrations of the chemical species are described by partial differential equations depending on position and time. When the chemical system is spatially homogeneous one can use ordinary differential equations instead. This rough approximation is often made in Biochemistry where the rate at which a concentration  $x_i$  changes is

$$\dot{x}_i = \sum_j \phi_{ij}(x_1, \dots, x_n).$$

Here  $j$  runs over all chemical reactions involving  $x_i$  and  $\phi_{ij}$  is the rate at which  $x_i$  is consumed or produced by the  $j^{\text{th}}$  reaction. A special case of this dynamics can be derived from the *Law of Mass-Action*: “*The rate at which a unit of a chemical species is consumed or produced by a chemical reaction is proportional to the product of the concentrations of the reactants.*” This law was first introduced by Guldberg and Waage in a series of papers during the second part of XIX century. Interestingly enough, this principle has been successfully applied to biochemical reaction networks (see, for example, [5]).

## 2. COMBINATORIAL VIEW OF MASS-ACTION NETWORKS

Mathematically, a mass-action network is a finite directed graph whose vertices are labelled by monomials and whose edges are labelled by *rate constants*:



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If we use the notation  $x = (x_1, \dots, x_n)^T$  and  $k = (k_1, \dots, k_r)^T$ , any mass-action network can be uniquely expressed as a quadruple  $(Y_e, Y_p, k, x)$ . The dynamics of a mass-action network is given by

$$(1) \quad \dot{x} = (Y_p - Y_e)\text{diag}(k)x^{Y_e},$$

where  $x^{Y_e}$  is a column vector of length  $r$  such that  $(x^{Y_e})_j = \prod_{i=1}^n x_i^{(Y_e)_{ij}}$ .

Realistic models tend to be large; hence often one does not intend to solve them, but rather study their asymptotic behaviour, like their steady states. Steady states are defined as the non-negative solutions of

$$(2) \quad (Y_p - Y_e)\text{diag}(k)x^{Y_e} = 0.$$

Note that, when one replaces the dynamical system (1) with the static system (2), information about the conserved quantities is lost. Therefore one has to regard the solutions of system (2) with respect to such conserved quantities. In biochemical reaction networks one usually restricts conservation laws to linear ones, that is, those which are of the form  $z_1x_1 + \dots + z_nx_n = c$ , where  $z$  is an element of the conservation space  $\text{left-ker}(Y_p - Y_e)$  and  $c$  is the value of the conserved quantity. As  $x$  are nonnegative, it only makes sense to consider those solutions to the conservation equations contained in  $\mathbb{R}_{\geq 0}^n$ . The set of such solutions gives rise to a polyhedron called *invariant polyhedron*. As the values of the conserved quantities change, the shape of the invariant polyhedron also changes. However it is known that there is only a finite number of combinatorial changes of such polyhedra [3]. The relevance of these polyhedra lays in the fact that they are related to siphons, which are combinatorial objects that indicate which concentrations are allowed to vanish at steady states. It is usual that one decorates the vertices of the abstract shapes of such polyhedra by the product of the variables whose supports coincide with these vertices (see [4] for a method to compute all combinatorial types of invariant polyhedra and their decorations). We call such representation a *decorated abstract invariant polyhedron*. Siphons have also proved to be useful in finding partial solutions for the Global Attractor Conjecture [2].

Note that when the trajectories of (1) are bounded (i.e., when the system is *conserved*), it is enough to restrict  $z$  to the *conservation cone*  $\ker(Y_p - Y_e)^T \cap \mathbb{R}_{\geq 0}^n$ , and invariant polyhedra become polytopes.

A strategy towards solving (2) is by first linearizing the vector  $\text{diag}(k)x^{Y_e}$ , and then by imposing binomial relations between its coordinates. For the linearization step, note that  $x$  is non-negative, so information about the *stoichiometric cone*  $\ker(Y_p - Y_e) \cap \mathbb{R}_{\geq 0}^r$  is enough. For the second step, the authors of [1] introduced a key concept, namely

*clusters*. *Clusters* and special unions of them, *preclusters*<sup>1</sup>, were used in author’s thesis to show that mass-action networks with the *isolation property* have toric steady states.

A set of species  $\Sigma = \{x_i \mid i \in I \subseteq [n]\}$  is called a *maximal invariant polyhedral supports* if all combinatorial types of decorated invariant abstract polyhedra are invariant under the map  $x_i \mapsto x_j$  for all  $x_i, x_j \in \Sigma$ . In order to compute the maximal invariant polyhedral supports, one needs to compute the chamber decomposition in the space of linear conserved quantities, and decorate each ray with the corresponding variables. The set of all variables decorating an individual ray is a maximal invariant polyhedral support. A *maximal symmetric chamber support* is a maximal set of concentration indices such that, when the supports are changed within these sets, the vertices of the invariant polyhedra do not change supports.

### 3. THE DUAL OF A MASS-ACTION NETWORK

There is a clear duality between the stoichiometric and the conservation space. This duality can be interpreted as a duality between chemical species and rate constants. Consequently, we define the dual of a chemical reaction network to be

$$\left( x^{Y_e} \xrightarrow{k} x^{Y_p} \right)^* = k^{Y_e^T} \xrightarrow{x} k^{Y_p^T} .$$

For conservative systems the duality between the conservation and the stoichiometric space can be interpreted in terms of a duality between the corresponding nonnegative cones. As there is a one to one correspondence between the extreme rays of the stoichiometric cone and the minimal cycles of the mass-action network, one can conclude that conserved quantities are dual to minimal cycles. Consequently we get the following result:

**Theorem.** *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 maximal invariant polyhedral supports.*

The condition  $\dot{x}_i = \dot{x}_j$  is necessary because we need to make sure that no further clustering on the left kernel is done.

We conclude with the following question:

**Question.** *Is there a duality relation between clusters and siphons?*

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<sup>1</sup>Clusters and preclusters are defined in Chapter 4 of Author’s Thesis:  
<https://www.opendata.uni-halle.de/handle/1981185920/14078>

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