Chemical Reaction Sheaf

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April 13, 2024

1 Introduction

The purpose of this document is to track and monitor the development of
the concept of a sheaf of a chemical reaction network. This follows from the
work of Hirono et al. in [5]. The authors mention of the interpretation of
a chemical reaction network as a hypergraph. This offers a new perspective
of viewing chemical reaction networks, as [2] shows that hypergraphs admit
a sheaf structure. The goal of this document is to develop the concept of a
sheaf of a chemical reaction network. Then, show that the sheaf associated
to a chemical reaction network can be used to study the dynamics of the
chemical reaction network.

2 Sheaf of a Chemical Reaction Network

A chemical reaction network is defined as a quadruple, (V, E, s, t), where V
is a set of species (vertices), E is a set of reactions (edges), $s : E \to V$ is
the source map, and $t : E \to V$ is the target map. The sheaf of a chemical
reaction network is defined as follows.

The cellular sheaf $\mathcal{F}$ of a chemical reaction network is defined as a triple
$\langle \mathcal{F}(v), \mathcal{F}(e), \mathcal{F}_{v \trianglelefteq e} \rangle$, where

- $\mathcal{F}(v)$ is the stalk at $v \in V$,

- $\mathcal{F}(e)$ is the stalk at $e \in E$,

- $\mathcal{F}_{v \trianglelefteq e}$ is the restriction map.

We define the stalk for all $v \in V$, to be $\mathcal{F}(v) = \mathbb{R}^{|V|}$ and the stalk at $e \in E$ to be $\mathcal{F}(e_i) = \mathbb{R}/\mathrm{Span}\{s(e_i), t(e_i)\}$, where e_i is the i-th edge in E. The restriction maps between sections of vertices and edges are exactly the quotient map. This map is also relatively nice, $s(e_i)$ and $t(e_i)$ are linearly independent (pretty sure), so the quotient map will always yield us a vector space.

3 My Thoughts

Nobody seems to talk about the global sections of these sheaves for hypergraphs? From the definition, the global sections of the hypergraph will need to be defined. It seems like the global sections of the hypergraph will be a choice of $x_v \in \mathcal{F}(v)$ for all $v \in V$, such that $\mathcal{F}_{v \trianglelefteq e}(x_v) = \mathcal{F}_{u \trianglelefteq e}(x_u)$ for all $e \in E$ such that $e = v - u$.

In [4], the author mentions that if a graph G is connected with at least one cycle and all the stalks have the same dimension, then almost any choice of restrictions will yield a sheaf with no global sections. This is bad news for us if we want to use sheaf cohomology for these chemical reaction networks. This is because sheaf cohomology is concerned with the global sections of a sheaf.

However, in [3] the authors do mention that that sheaves can encode linear transformations at nodes, which would accommodate reaction balancing! This all seems great and promising.

Need to make use of the hypergraph laplacian. In [6], the authors define a hypergraph laplacian for the vertices and the hyperedges of a hypergraph.

In [5], the authors define a morphism between CRN's and also define a reduction morphism. This all seems to suggest that there would be an isomorphic relationship between the sheaves defined over the CRN's. This is something that needs to be explored.

Also interesting: the author of [1] define a reactant morphism and a stoichiomorphism. This is all to say that if there exists a reactant morphism and a stochiomorphism from one chemical reaction network to another, then there is an *emulation* between the two chemical reaction networks. This actually relates the differential systems of two chemical reaction networks. This is a bit too much at this point.

References

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