

Chemical Reaction Sheaf

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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 [2]. 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 [1] 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 Goals for this paper and questions to be answered

- Define a chemical reaction sheaf
- How can this improve a problem?
- What needs to be done?
- Why is this useful?
- What are the implications of this?

3 Chemical Reaction Network

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

4 Sheaf of a Chemical Reaction Network

The sheaf of a chemical reaction network is defined as follows.

Definition 1. Given a chemical reaction network Γ , the *chemical reaction sheaf* associated to a network is the cellular sheaf $\langle \mathcal{F}(v), \mathcal{F}(e), \mathcal{F}_{v \leq e} \rangle$ where (for all $v \in V$ and $e \in E$):

- $\mathcal{F}(v) = \mathbb{R}[x_1, \dots, x_{|V|}]$
- $\mathcal{F}(e) = \mathbb{R}[x_1, \dots, x_{|V|}] / (t(e) - s(e))$
- $\mathcal{F}_{v \leq e}$ is the quotient map by the ideal generated by $t(e) - s(e)$

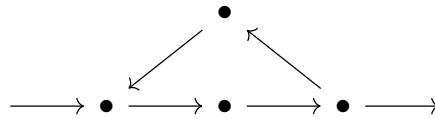
5 Sheaf Cohomology of CRN

We develop a theory of sheaf cohomology for these chemical reaction networks.

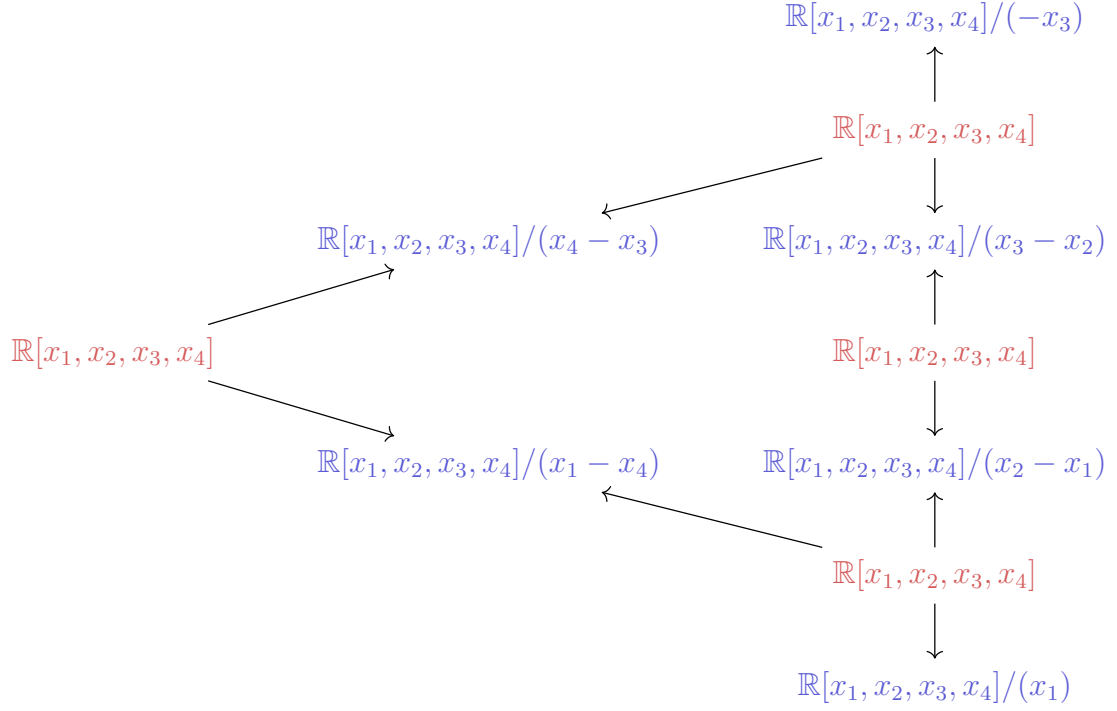
Definition 2. The *kth sheaf cochain group*, is defined to be

$$C^k(X; \mathcal{F}) = \bigoplus_{\dim(\sigma)=k} \mathcal{F}(\sigma)$$

Consider the following directed graph:



This has a corresponding sheaf:



One possible reduction of this graph would be collapsing the cells on the left down to one.

References

- [1] Iulia Duta, Giulia Cassarà, Fabrizio Silvestri, and Pietro Liò. Sheaf hypergraph networks, 2023.
- [2] Yuji Hirono, Takashi Okada, Hiroyasu Miyazaki, and Yoshimasa Hidaka. Structural reduction of chemical reaction networks based on topology. *Phys. Rev. Res.*, 3:043123, Nov 2021.