Chemical Reaction Sheaf

Mauricio Montes

May 16, 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 [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), $s : E \to V$ is the source map, and $t : E \to V$ 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 $\langle \mathcal{F}(v), \mathcal{F}(e), \mathcal{F}_{v \trianglelefteq e} \rangle$ where (for all $v \in V$ and $e \in E$):

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

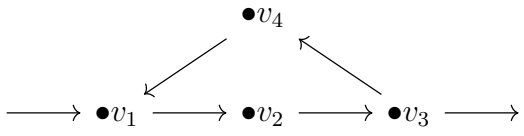
5 Sheaf Cohomology of CRN

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

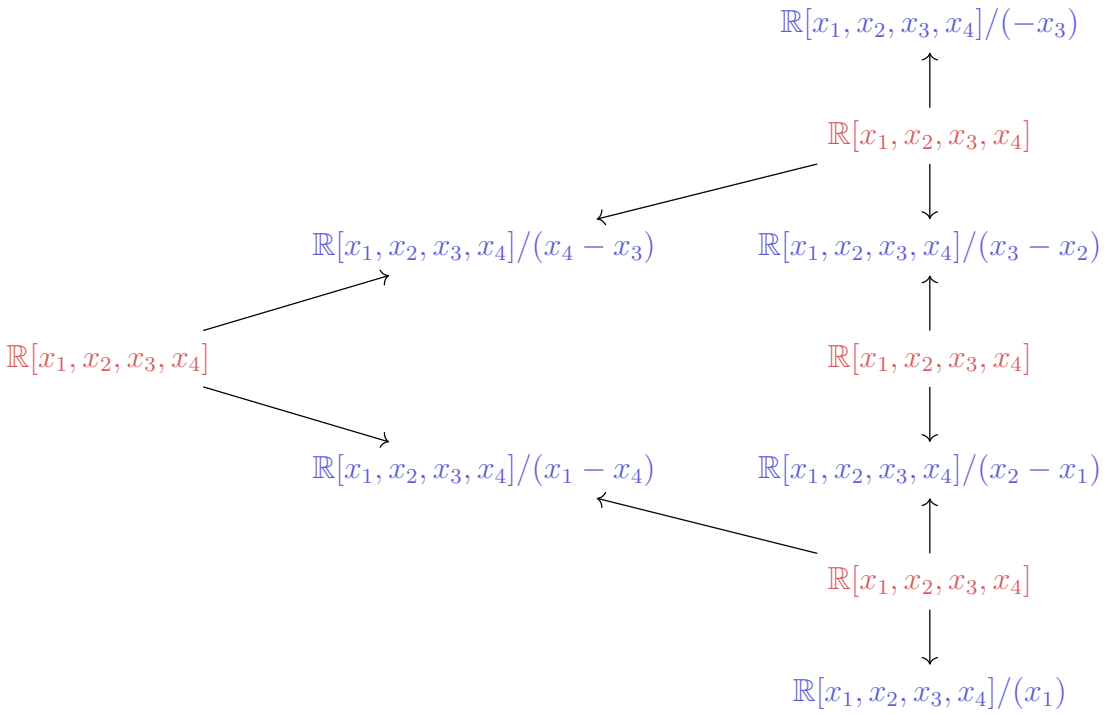
Definition 2. The *kth sheaf cochain group*, is defined to be

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

Consider the following directed graph:

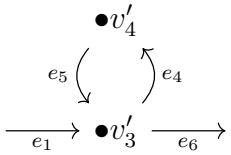


This has a corresponding sheaf:

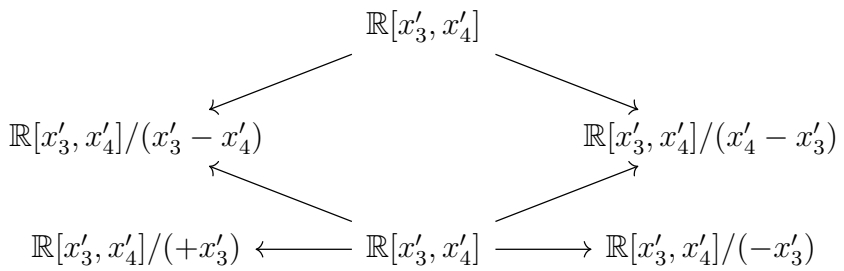


One possible reduction of this graph would be collapsing the cells on the left down to one vertex.

The corresponding reduction will have a corresponding sheaf for the new CRN. Shown below:



This will have (a priori) the corresponding CRS:



However, when we consider the direct image sheaf given by the map $\varphi : X \to X'$, $\varphi(v_1) = v'_3, \varphi(v_2) = v'_3, \varphi(v_3) = v'_3, \varphi(e_2) = e_1, \varphi(e_3) = e_1$ and the identity elsewhere. We get:

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.