Problem Statement: Topological Entropy in Chemical Reaction Networks

Nayanmoni Khatoniar
Undergraduate Researcher

May 31, 2025

Problem Overview

Chemical reaction networks (CRNs) are abstract representations of interacting chemical species through a series of chemical reactions. These networks are traditionally analyzed using kinetics, thermodynamics, or stochastic methods to understand how species evolve over time. However, these approaches often overlook the underlying **topological structure** of the network and its role in dictating the system's overall behavior.

Research Problem

This research proposes to define and investigate a novel measure of complexity for chemical reaction networks: **topological entropy**. While topological entropy has been extensively studied in the context of dynamical systems, its application to CRNs remains unexplored. The aim is to introduce a framework that captures the structural and dynamic unpredictability of reaction networks from a topological perspective.

The specific research goals include:

- Formulate a definition of topological entropy suitable for CRNs represented as graphs or hypergraphs.
- Quantify how reaction complexity, reversibility, and branching influence entropy values.
- Examine whether topological entropy correlates with known metrics of chemical complexity or computational potential.
- Apply the framework to simple and real-world CRNs using simulations and case studies.

Why This Research is Important

Most CRN analysis methods fail to provide a structural measure of complexity that is independent of reaction rates or concentrations. By introducing topological entropy:

- We can detect and classify networks with high computational or information-theoretic capacity.
- We offer a new metric for designing synthetic chemical systems for computing or self-regulation.
- We contribute to the theoretical foundation for chemical computation and chemical network optimization.

This is especially relevant for the future of molecular programming, self-assembling systems, and chemical logic gates, where structure often matters as much as dynamics.

Why This Research is Unique

After a thorough survey of existing literature across Springer, Elsevier, ArXiv, and Google Scholar, it is evident that:

- **No existing work defines or computes topological entropy for chemical reaction networks.**
- While entropy has been studied in CRNs, it is either thermodynamic (energy-based) or Shannon-based (probabilistic), not topological.
- There is virtually no integration of algebraic topology, persistent homology, or graph entropy into CRN analysis.

This makes the proposed research truly novel, and highly suited for undergraduate publication due to its theoretical nature and minimal reliance on laboratory infrastructure.

Key Research Questions

1. What is an appropriate definition of topological entropy in the context of CRNs?
2. Can it be computed efficiently for directed graphs or reaction hypergraphs?
3. How does topological entropy relate to reaction dynamics, reversibility, and complexity?
4. Could this metric be useful in designing or optimizing reaction-based computation systems?

Tools and Techniques

- Graph theory and algebraic topology (Betti numbers, homology, simplicial complexes)
- Python libraries: `NetworkX`, `GUDHI`, `scikit-tda`
- Simulation tools: BioCRNpyler, COPASI (for modeling simple CRNs)
- Concepts from information theory and dynamical systems (e.g., symbolic dynamics, Lyapunov functions)