Abstract

Autocatalytic sets are sets of entities that mutually catalyse each other production through chemical reactions, starting from a basic food source. Recently, the reflexively autocatalytic and food generated theory has introduced a formal definition of autocatalytic sets which has provided encouraging results in the context of the origin of life. However, the link between the structure of autocatalytic sets and the possibility of different long-term behaviours is still unclear. In this work, we study how different interactions among autocatalytic sets affect the emergent dynamics. To this aim, we develop a model in which interactions are represented by composition operations among networks, and the dynamics of the networks is performed via stochastic simulations. We find that the dynamical emergence of the autocatalytic sets depends on the adopted composition operations. In particular, operations involving entities that are sources for autocatalytic sets can promote the formation of different autocatalytic subsets, opening the door to various long-term behaviours.

The model

Reflexively Autocatalytic and Food Generated (RAF) Sets

A set R of chemical reactions is said to be a RAF set if it satisfies the following properties:
- Reflexively autocatalytic (RA): each reaction in R is catalysed by at least one molecule from R itself;
- F-generating (F): all reactants in R can be created from some food set F by using a sequence of reactions from R itself.

The union of multiple RAF sets within a chemical reaction system is still a RAF set, called the MaxRAF set.

Given a RAF set R, a subset R' of R is said to be a closed RAF set if it satisfies the additional closure property:
- R' contains each reaction r in R for which each reactant and at least one catalyst are either generated by another reaction from R' or are part of the food set F.

A MaxRAF that is the union of 3 closed RAF sets:

\[ \begin{align*}
R_1 & = \{ r_1, r_2 \} \\
R_2 & = \{ r_3, r_4, r_5, r_6 \} \\
R_3 & = \{ r_7, r_8, r_9, r_{10} \}
\end{align*} \]

Green circles represent food elements.

Stochastic Petri Nets

A stochastic Petri net consists of:
- A finite set of place P;
- A finite set of transitions R;
- Functions \[ b \in \mathbb{R}^j \times T \to \mathbb{R} \] representing edges between places and transitions;
- A marking X that assigns a number of tokens to each place;
- An array of firing rates \[ \lambda \] associated with the transitions.

In our model it is:
- \[ \lambda_r = \sum_{j \in I_r} \prod_{i \in I_r} \left( \frac{1}{\lambda_{ij}} + j \right) x_j \]

where \[ \lambda \] and \[ V \] are constants, \[ I \] are the input places of transition \[ r \] and \[ x \] is the number of tokens of place \[ j \].

Composition Operations

We introduce the following composition operations:
- CO (acts on species)
- CO_1 (acts on complexes)
- CO_2 (acts on reactions)

Main question: can composition operations prevent the dynamical emergence of the entire MaxRAF set?

We compose pairs of identical RAF sets and simulate the dynamics of the system using the standard Gillespie algorithm. Simulations start with \( \chi \neq 0 \) only if j is a food element. We assume that:

\[ M(t) = \sum_{j \notin F} \frac{1}{1 + t x_j(t)} > 1 \text{ for } t \to \infty \]

The MaxRAF does not emerge.

Otherwise, we use the time \( t \) to detect the efficiency of self-production, where \( t \) is the time necessary to perform \( i \) times all the transitions of \( R \):

\[ \tau_i = \min \{ t \mid \forall n(t) \geq i, \forall r \in R \} \]

\[ t \sim m_i + q_i \text{ for } i \to \infty \]

When a MaxRAF set emerges, different slopes of \[ t \] correspond to different efficiencies in self-reproduction. If the MaxRAF does not emerge, some transitions of the set are not performed.

Conclusions

In this work we study the impact of composition on the dynamics of simple RAF sets, in order to find some composition operations under which the dynamical emergence of the MaxRAF set is not invariant. We find that, if the composition operations do not involve the food set, the dynamics of the system always reaches the state in which all the composed MaxRAF sets appear, even if the efficiency in self-reproduction depends on the composition. On the other hand, composition operations involving food elements can prevent from the appearance of MaxRAF sets, allowing the existence of multiple long-term behaviours required for the evolvability of RAF sets.

The impact of composition on the dynamics of autocatalytic sets

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