OPEN-ENDED EVOLUTION AS AN EMERGENT SELF-ORGANIZING SEARCH PROCESS

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ABSTRACT

The diversity and complexity of living systems on Earth have presumably emerged from a single common ancestor, and before that, from the inorganic components present on the surface of Earth. So far, it is unclear what are the *algorithmic* properties of a process that would display a similar trajectory in its state space. Describing such a process entails characterizing both the state space itself, the possible emergent forms, and the evolutionary process behind the diversification and complexification of forms. Because living systems are hypothesized to correspond to attractors in chemical networks, Artificial Chemistries (AC) are well suited to explore this question because they can simulate the evolution of these networks. Combinatory Chemistry is an AC in which self-reproducing metabolisms emerge from its dynamics. Here, I extend it with a set of mutation reactions, showing that said reactions coupled with the emergent structures in the system enable a more efficient search of complex structures. I conclude that the resulting dynamics constitute an emergent self-organizing search process that could capture the properties of open-ended evolutionary processes.

1 INTRODUCTION

What are the necessary conditions for the emergence of living systems? Moreover, how can a process display analogous levels of creativity and complexity as natural evolution? These are two fundamental questions that have been at the core of Artificial Life research (Varela & Maturana, 1973; Eigen & Schuster, 1978; Langton, 1989; Dyson, 1999; Pross, 2004; Banzhaf et al., 2016; Packard et al., 2019; Stanley, 2019). Both are concerned with the fundamental nature of living systems, but they are often addressed independently, with some studies focused on the emergence of evolvable units (Bagley & Farmer, 1992; Hutton, 2007; Flamm et al., 2010; Högerl, 2010; Fellermann et al., 2017; Baum, 2018; Peng et al., 2020, among others), and others starting from evolvable units to explore the space of emergent behaviours that follow (Ray, 1991; Lenski et al., 2003; Ofria & Wilke, 2004; Soros & Stanley, 2014; Williams, 2019; Taylor, 2019, among others). Even though this distinction is not completely clear-cut (e.g., Koza, 1994; Vasas et al., 2012; Young & Neshatian, 2013), there is a trend rooted in the fact that it is already hard to characterize the emergence of evolvable units, and thus it can makes sense to "shortcut" to the point where they are already part of the system (Banzhaf et al., 2016).

Here, I describe an initial attempt at producing an unifying model while focusing on the hypothesized core *algorithmic* properties of living systems. This model draws on the hypothesis that both the emergence of evolvable units and their diversification in complex forms can be construed as a the outcome of an unguided search process over a space of self-organizing chemical networks. As it has been argued before, localized self-sustaining structures (Varela & Maturana, 1973) can emerge in these networks as attractors, known as Autocatalytic Sets (Kauffman, 1993). The main observation of this paper, is that catalyzed "mutations" allow Autocatalytic Sets to explore more efficiently the space of possible organizations, thus boosting diversification and complexification of forms.

Notably, Artificial Chemistries (AC) (Dittrich et al., 2001) provide a powerful framework to model these phenomena. In particular, here I focus on Combinatory Chemistry (Kruszewski & Mikolov, 2020; 2021), which is an AC where self-reproducing metabolisms emerge from a *tabula rasa* state. The model features a combination of random recombination reactions that proceed at a slow rate and (auto-)catalyzed "reduce" reactions implementing Turing-complete rewrite rules that take place

at a much higher rate. When the system is initialized with a *tabula rasa* state featuring only atomic elements, random recombination reactions produce a wide diversity of forms, some of which then self-organize into emergent metabolisms. These take the form of recursive programs that compute themselves (think of "quines") by mean of the auto-catalyzed reactions. However, the possibility of these metabolisms undergoing variation is mostly restricted to random recombination reactions. At least, because these reactions proceed at a slow rate the evolutionary potential of such metabolisms is limited. In this paper, I introduce a new set of *mutation* reactions that simulate the *imperfect* application of some of the rewrite rules. As a result, the emergent structures can compute variants and thus, they can undergo *evolution*. I then show that even when very basic metabolisms undergo some of these mutations, they will inherit part of the structure of the originating metabolisms, and compute variants with better chances of becoming viable metabolisms. Therefore, the search process that at the base was only formed by random recombination reactions gets enriched with additional emergent search units that exploit the structure of viable metabolisms to find new ones. In other words, the system acquires a *prior* or *inductive bias* that allows it to search more efficiently for novel forms. I speculate that this process can feed into itself, continually improving its efficiency at searching for new viable forms (Pattee & Sayama, 2019). To distinguish this process from one that features random recombination on a self-organizing state space, I denote it as an *emergent self-organizing search* process, as it is the search process itself that gets updated through self-organization.

2 Stochastic Chemical Reaction Systems

The name of Artificial Chemistry denotes a wide range of systems in which different elements can collide with each other to create new components (Dittrich et al., 2001). For the purposes of this article, I will restrict to Stochastic Chemical Reaction Systems of the sort introduced by Gillespie (1977; 2007). Let us consider a set of chemical species $\mathbb{S} = \{\mathrm{S}_1, \dots, \mathrm{S}_i, \dots\}$ which interact through a set of chemical reactions $\mathbb{R} = \{\mathrm{R}_1, \dots, \mathrm{R}_j, \dots\}$. While the original formulation considers *finite* sets, here I consider a generalization to countably *infinite* sets of species and corresponding reactions, which is particularly useful to define an *open-ended* system. Let also $\mathrm{x}_i(t)$ denote the number of molecules of species S_i at time t and $\mathbf{x}(t) = (\mathrm{x}_1(t), \dots, \mathrm{x}_i(t), \dots)$ be the state vector of the system[1]. Each reaction R_j is characterized by *i*) a state-change vector $\boldsymbol{v}_j \equiv (v_{1j}, \dots, v_{ij}, \dots)$ and *ii*) a propensity function a_j such that $a_j(\boldsymbol{x})\,\mathrm{d}t$ is the probability that one reaction R_j will occur in the next infinitesimal time interval $[t, t+\mathrm{d}t)$ given that $\mathbf{x}(t) = \boldsymbol{x}$. The state-change vector represents the reactants, products and by-products of the reaction. For convenience, we can write the reaction R_j with state-change vector $\boldsymbol{v}_j$ containing values -1 on positions $k_1, \dots, k_n$, 1 on positions $l_1, \dots, l_m$, and 0 everywhere else as $\mathrm{S}_{k_1} + \dots + \mathrm{S}_{k_n} \to \mathrm{S}_{l_1} + \dots + \mathrm{S}_{l_m}$. The propensity function depends on the reactants' concentration and a constant c_j that intuitively corresponds to the "speed" at which the reaction takes place. In particular, for a unimolecular reaction $\mathrm{S}_k \to \cdots$, the propensity function takes the form

$$a_j(\boldsymbol{x}) = c_j \boldsymbol{x}_k, \tag{1}$$

whereas for a bimolecular reaction $\mathrm{S}_{k_1} + \mathrm{S}_{k_2} \to \cdots$ it takes the form[2]

$$a_j(\boldsymbol{x}) = c_j \boldsymbol{x}_{k_1} \boldsymbol{x}_{k_2}. \tag{2}$$

The Gillespie algorithm (Gillespie, 1977) simulates the time evolution of a system with state $\mathbf{x}(t) = \boldsymbol{x}$ by sampling the next reaction R_j with probability $p(\mathrm{R}_j) = a_j(\boldsymbol{x})/a_0(\boldsymbol{x})$ where $a_0 = \sum_j a_j(\boldsymbol{x})$ is the partition function, and advancing the time by an exponentially-distributed interval $\tau \sim \mathrm{Exp}(\lambda = a_0(\boldsymbol{x}))$. Then, a new state is obtained as $\mathbf{x}(t+\tau) = \boldsymbol{x} + \boldsymbol{v}_j$.

3 Combinatory Chemistry

Combinatory Chemistry (Kruszewski & Mikolov, 2020; 2021) is an Artificial Chemistry endowed with Turing-complete reactions, derived from Combinatory Logic (Schönfinkel, 1924; Curry et al., 1958) rewriting rules. In particular, chemical species are defined to be as the individual combinators S, K, I, which can be recusively combined through the application operation. More formally, let $\mathbb{S}$ be the minimal set such that $\{\mathrm{S}, \mathrm{K}, \mathrm{I}\} \subset \mathbb{S}$ and if $x, y \in \mathbb{S}$, then it is also true that $(xy) \in \mathbb{S}$, where

[1] Even if the vector is infinite, it is possible to tractably operate on it if all but a finite set of elements are 0.

[2] See (Gillespie, 2007) for a more precise formulation

(xy) denotes the application of x onto y. By convention, application is left-associative, and thus $((xy)z)$ is equivalent to (xyz). There are three kinds of reactions: condensations (Π), cleavages (X), and reductions (A). Each of these possible kinds of reactions $\mathbb{R} = \Pi \cup X \cup A$ are defined, as follows. Given $x, y \in \mathbb{S}$, both a condensation reaction $(x + y \rightarrow (xy)) \in \Pi$ and a cleavage reaction $((xy) \rightarrow x + y) \in X$ are defined. On the other hand, reduction reactions are analogous to Combinatory Logic rewrite rules. Given $x = (\cdots X \cdots) \in \mathbb{S}$ where $X = (\mathrm{I}f)$ or $X = (\mathrm{K}fg)$ or $X = (\mathrm{S}fgz)$ with $f, g, z \in \mathbb{S}$, then we say that x is reducible, that X is a *redex*, and there is a corresponding reduce reaction defined as follows[3]:

$$(\cdots(\mathrm{I}f)\cdots) \Rightarrow (\cdots f \cdots) + \mathrm{I} \tag{I-reduction}$$

$$(\cdots(\mathrm{K}fg)\cdots) \Rightarrow (\cdots f \cdots) + g + \mathrm{K} \tag{K-reduction}$$

$$\underbrace{(\cdots(\mathrm{S}fgy)\cdots)}_{\text{substrate}} \underbrace{+y}_{\text{reactant}} \Rightarrow \underbrace{(\cdots(fy(gy))\cdots)}_{\text{product}} \underbrace{+\mathrm{S}}_{\text{by-product}} \tag{S-reduction}$$

In contrast to combinatory logic's rewrite rules, these reductions ensure "conservation of mass", namely, the total number of combinators in the system does not change over time. Reaction propensities for reduce reactions are chosen to be much larger than for cleavages and condensations (in other words, reduce reactions are auto-catalyzed): $a_j(\boldsymbol{x}) \gg a_{j'}(\boldsymbol{x})$ for $j \in A$ and $j' \in X \cup \Pi$. In this way, *computation takes precedence* over random recombination, allowing for the emergence of self-organizing structures (see next section). For further details on the system's definition, see Kruszewski & Mikolov (2021).

4 Emergent Self-Organizing Structures

As shown by Kruszewski & Mikolov (2021), if initialized with only atomic S, K and I uniformly distributed combinators, the above-mentioned dynamics give rise, first, driven by random condensation and cleavages, to a diversity explosion of combinatory logic expressions, which then gives way to emergent self-organizing structures. More in detail, because many of the new-found expressions by random recombination admit reduce reactions, they will often undergo these reactions before additional condensations or cleavages. Notably, some expressions can follow a chain of such reduce reactions that leads back to the original expression (or an expression which contains the original one), thus perpetuating their organization in time. In other words, these expressions will tend to *recursively compute* themselves via reduce reactions, forming a *limit cycle* under these dynamics. As shown by Kruszewski & Mikolov (2021), these limit cycles constitute Autocatalytic Sets. For example, one such structure can be identified with the expression $\Omega = (\mathrm{SII}(\mathrm{SII}))$, which undergoes the following cycle or a small variation around it:

$$\begin{aligned}
(\underline{\mathrm{SII}(\mathrm{SII})}) + (\mathrm{SII}) &\Rightarrow \quad (\mathrm{I}(\mathrm{SII})(\mathrm{I}(\mathrm{SII}))) + \mathrm{S} \\
(\underline{\mathrm{I}(\mathrm{SII})}(\mathrm{I}(\mathrm{SII})) &\Rightarrow \quad (\mathrm{SII}(\mathrm{I}(\mathrm{SII}))) + \mathrm{I} \\
(\mathrm{SII}(\underline{\mathrm{I}(\mathrm{SII})})) &\Rightarrow \quad (\mathrm{SII}(\mathrm{SII})) + \mathrm{I}
\end{aligned}$$

where the corresponding redex at each step is underlined. Note that on each cycle, this structure will "consume" one copy of (SII), and release back the individual combinators into the environment as by-products of each reduction, in close analogy to real-world metabolisms. Furthermore, this structure is composed of two juxtaposed copies of the same expression $A = (\mathrm{SII})$. This pattern of an expression applied one or more times to itself is a common factor in the emergent structures of this system. Another interesting pattern is displayed in Figure 1, also with the form (AA), but with $A = (\mathrm{SI}(\mathrm{S}(\mathrm{SK})\mathrm{I}))$. Over a full cycle, it "absorbs" three copies of the expression A: one is decomposed into the elementary combinators, while the other two are released as (AA) at the same time as the expression returns to its original (AA) form. In other words, this structure self-reproduces. Importantly, however, if there are no other copies of A in the environment, the reduction of the S combinator cannot take place, and the expression could be cleaved or condensed with another one, probably provoking it to lose its function.

[3]The notation using the $\Rightarrow$ symbol is meant to distinguish reduce reactions from random condensation and cleavage ones.

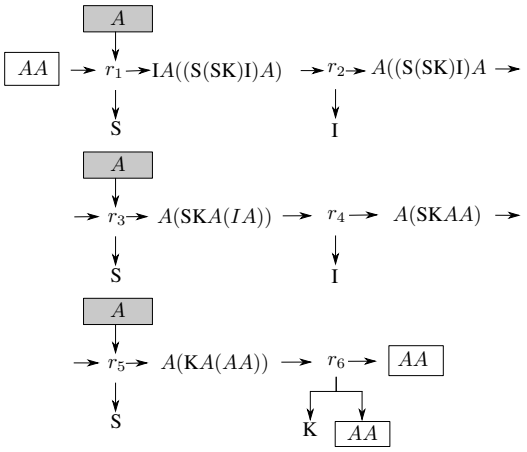

Figure 1: Cycle of a self-reproducing structure that emerges from the dynamics of Combinatory Chemistry. Starting from (AA), where $A = (\text{SI}(\text{S}(\text{SK})\text{I}))$, it acquires three copies of A from its environment and uses two to create a copy of itself, metabolising the third one to carry out the process. (Reproduced from Kruszewski & Mikolov (2021).)

5 Emergent Search Process

Combinatory Chemistry defines a walk over multi-sets of combinatory logic expressions, some of them acting as (attracting) fixed-points or limit cycles. While random condensation and cleavages allow it to explore the space of possible expressions, reduce reactions define the underlying search landscape, including the fixed points, limit cycles and their basins of attraction. Thus, even though there are no explicit goals or objectives in this system, *we* can construe it to be *searching* for these fixed points and limit cycles. This search is made more efficient thanks to the basins of attraction that effective prune the search space. Consider for instance, that a condensation reaction is produced between the two irreducible expressions $(\text{S}(\text{SI}(\text{SI})(\text{SI}))$ and $(\text{S}(\text{SK})\text{I})$, to obtain $(\text{S}(\text{SI}(\text{SI})(\text{SI}))(\text{S}(\text{SK})\text{I}))$. This new expression does not constitute *per se* an emergent structure. Yet, following the chain of reduction reactions that it admits, we see that it leads to the emergence of the self-reproducing expression (AA) with $A = (\text{SI}(\text{S}(\text{SK})\text{I}))$. To see this, let's denote $B = (\text{S}(\text{SK})\text{I})$, and note that $A = (\text{SI}B)$, then the following set of reduce expressions are very likely to follow:

$$
\begin{aligned}
(\underline{\text{S}(\text{SI}(\text{SI}))(\text{SI})B}) + B \Rightarrow &\quad (\text{SI}(\text{SI})BA) + \text{S} \\
(\underline{\text{SI}(\text{SI})B}A) + B \Rightarrow &\quad (\text{I}BAA) + \text{S} \\
(\underline{\text{I}B}AA) + B \Rightarrow &\quad (BAA) + \text{I} \\
(\underline{BA}A) + A \Rightarrow &\quad (\text{SK}A(\text{I}A)A) + \text{S} \\
(\text{SK}A(\underline{\text{I}A})A) \Rightarrow &\quad (\text{SK}AAA) + \text{I} \\
(\underline{\text{SK}AA}A) + A \Rightarrow &\quad (\text{K}A(AA)A) + \text{S} \\
(\underline{\text{K}A(AA)A}) \Rightarrow &\quad 2(AA) + \text{K}
\end{aligned}
$$

Therefore, we can see that the system found a limit cycle by first forming a new expression through random condensation of the available material, and then, because the resulting expression was in the basin of attraction of a limit cycle point, it arrived to it by following a chain of reduce reactions. Nonetheless, the search for novel expressions is still exclusively done though random recombination of existing components.

6 Mutation Reactions

Thanks to the self-organizing properties discussed in the previous section, the random recombination process in Combinatory Chemistry is not entirely random. For instance, it will be very unlikely for some of the reducible expressions to be selected in a condensation or cleavage reaction because

reducible expressions are very unstable and short-lived. Consider (IKK). This expression is expected to undergo the reduce reaction $(\mathrm{IKK}) \Rightarrow (\mathrm{KK}) + \mathrm{I}$ with much higher probability than any other kind of reaction.

Hence, because self-organization prunes the space, the exploration process defined by random recombination reactions is more efficient than purely random search, as it has been previously argued (Kauffman, 1993). Nonetheless, random recombination as discussed so far has its limits. Discovering larger and more complex structures can quickly become hard as the search space grows exponentially large. Meanwhile random recombination reactions exploring this exponentially large space occur at a relatively low rate. Yet, we know that nature has found a way to explore this space, given the evidence of the living systems we see today on Earth (including ourselves).

I hypothesize that in contrast to the model described thus far, the open-ended evolutionary process in earth relies on *imperfect* computation, which allows it to search this space more efficiently. To this end, I introduce a new set of mutation reactions (μ), defined as follows:

$$(\cdots(\mathrm{S}fgy)\cdots) + z \overset{!}{\Rightarrow} (\cdots(fy(gz))\cdots) + \mathrm{S} \qquad \text{(inner-mutation)}$$

$$(\cdots(\mathrm{S}fgy)\cdots) + z \overset{!}{\Rightarrow} (\cdots(fz(gy))\cdots) + \mathrm{S} \qquad \text{(outer-mutation)}$$

Both of these reductions take the shape of S-reductions, but instead of being only defined for a reactant equal to the third argument y, they are defined for any reactant present in the system. Note that this reactant is placed in either of the two locations where y is usually located in the product. An intuitive argument for why such reactions could be a natural choice is that catalyzing a reaction that requires an exact copy of a sub-expression is an error-prone process, and other reactants can sneak in instead.

These reactions are also catalyzed, even though with lower propensity than regular S-reductions: $a(j_{X\cup\Pi}) < a(j_\mu) \ll a(j_A)$ with $j_\mu \in \mu$, $j_{X\cup\Pi} \in X \cup \Pi$, and $j_A \in A$. In this way, imperfect non-deterministic computation can take place at a faster rhythm than chance reactions, but not so fast as to interfere with the regular course of deterministic computation.

7 Emergent Self-Organizing Search

Let's now examine the result of adding these reactions in the simplest limit cycle, namely, the $\Omega = (\mathrm{SII}(\mathrm{SII}))$ combinator introduced in Section 4 . Normally, this structure would react with (SII) using an S-reduction. However, let's suppose that it reacts with an expression z from the environment following an inner-mutation. Then, the ensuing chain of reductions would be as follows.

$$\begin{aligned}
(\underline{\mathrm{SII}(\mathrm{SII})}) + z &\overset{!}{\Rightarrow} (\mathrm{I}(\mathrm{SII})(\mathrm{I}z)) + \mathrm{S} \\
(\underline{\mathrm{I}(\mathrm{SII})}(\mathrm{I}z) &\Rightarrow (\mathrm{SII}(\mathrm{I}z)) + \mathrm{I} \\
(\mathrm{SII}(\underline{\mathrm{I}z})) &\Rightarrow (\mathrm{SII}z) + \mathrm{I} \\
(\mathrm{I}z(\underline{\mathrm{I}z})) &\Rightarrow (\mathrm{I}zz) \\
(\underline{\mathrm{I}z}z) &\Rightarrow (zz)
\end{aligned}$$

Therefore, if an inner-mutation occurred on Ω with reactant z, then the system will very likely produce the expression (zz). This is interesting because of our observation above: limit cycles tend to have the form of an expression applied to itself. Therefore, the system is *searching* for new expressions with a given structure, which is expected to be favourable in contrast to other random combinations. Therefore, by introducing inner-mutations with sufficiently high reaction rate constant c_μ, the collision of two arbitrary expressions z will be catalyzed at least by the following

factor:[4]

$$\frac{a(\Omega + z \overset{!}{\Rightarrow} \cdots)}{a(z + z \rightarrow \cdots)} = \frac{c_\mu \boldsymbol{x}_\Omega \boldsymbol{x}_z}{c_\Pi \boldsymbol{x}_z^2} = \frac{c_\mu \boldsymbol{x}_\Omega}{c_\Pi \boldsymbol{x}_z} \tag{3}$$

The outer-mutation has a different effect, constructing an expression in which a randomly acquired reactant from the environment is applied to the $A = (\text{SII})$ expression:

$$\begin{aligned}
(\underline{\text{SII}(\text{SII})}) + z \overset{!}{\Rightarrow} &\quad (\text{I}z(\text{I}(\text{SII}))) + \text{S} \\
(\underline{\text{I}z}(\text{I}(\text{SII})) \Rightarrow &\quad (z(\text{I}(\text{SII}))) + \text{I} \\
(z(\underline{\text{I}(\text{SII})})) \Rightarrow &\quad (z(\text{SII})) + \text{I}
\end{aligned}$$

Here, it is interesting to note that here we are sending the defining function of the Ω combinator as an argument to an arbitrary function z, which is in line with the algorithmic mutations explored by Chaitin (2011).

8 Discussion and Conclusions

In summary, Combinatory Chemistry displays emergent structures, which take the form of (attracting) limit cycles. The system discovers these structures both thanks to the random recombination of expressions and to the self-organization of the space. When mutation reactions are introduced, the emergent structures can expand the search process capabilities by catalyzing the formation of new structures which are unlikely to be formed through random condensation alone.

This study still requires empirical confirmation, but some limitations are foreseeable. Particularly, the mutation reactions as they are currently defined will react from a randomly sampled expression from the full population. However, the distribution of expressions is heavily skewed towards simpler forms, such as atomic combinators. For this reason, the application of such reactions will often result in very simple forms such as (SS), (KK) or (II). Therefore, if simulations are not performed at a very large scale, then at least it might be worth exploring ways in which the space of random reactants can be restricted (for instance, limiting their minimum length) to reduce the amount of time that the system spends in computing these elementary forms (which are already well covered by random mixing).

To conclude, this paper introduces mutation reactions for Combinatory Chemistry. Furthermore, I have argued that through them, the system acquires new strategies to explore the space of possible chemical organizations in what constitutes a self-organizing search process. Speculatively, as new structures are discovered, they can expand the repertoire of exploration strategies. As the system becomes more efficient at discovering new complex forms, it is possible that it can display open-ended evolutionary properties, rather than just stalling on the set of forms that it could have reached when only using random recombination to search the space.

[4] Ignoring the chain of reduce reactions following the mutation which we can assume almost instantaneous for they will have very high propensity. On the other hand, Ω is not the only expression that would catalyze this reaction and thus, the factor should probably be considerably larger.

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