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, even before, 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. 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 and argue 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 reactions involving an element of randomness within them 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) and, in particular, Algorithmic Artificial Chemistries (Fontana & Buss, 1994a;b; Tominaga et al., 2007; Hutton, 2002; Kruszewski & Mikolov, 2022) provide a powerful framework to model these phenomena. In particular, here I focus on Combinatory Chemistry (Kruszewski & Mikolov, 2020; 2022), which is an AC where self-reproducing metabolisms emerge from the system's dynamics. The model features a mix 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. In contrast to some previous models, such as Fontana & Buss (1994a;b), the system features conservation laws and allows to represent never-ending loops as part of its dynamics[1]. 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 following auto-catalyzed reduce reactions. However, the possibility of these metabolisms undergoing variation is mostly restricted to the effect of random recombination reactions. If nothing else, 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 reduce reactions. 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). These systems are formally defined as follows. Let us consider a set of chemical species $\mathbb{S} = \{S_1, \ldots, S_i, \ldots\}$ which interact through a set of chemical reactions $\mathbb{R} = \{R_1, \ldots, R_j, \ldots\}$. While the original formulation considers *finite* sets, here I consider a generalization to countably *infinite* sets of species and corresponding reactions, which is particularly adequate for defining an *open-ended* system. Let also $x_i(t)$ denote the number of molecules of species S_i at time t and $\mathbf{x}(t) = (x_1(t), \ldots, x_i(t), \ldots)$ be the state vector of the system[2]. Each reaction R_j is characterized by *i*) a state-change vector $\boldsymbol{v}_j \equiv (v_{1j}, \ldots, v_{ij}, \ldots)$ and *ii*) a propensity function a_j such that $a_j(\boldsymbol{x})\, dt$ is the probability that one reaction R_j will occur in the next infinitesimal time interval $[t, t + dt)$ 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 $k_1, \ldots, k_n$, 1 on positions $l_1, \ldots, l_m$, and 0 everywhere else as $S_{k_1} + \cdots + S_{k_n} \rightarrow S_{l_1} + \cdots + S_{l_m}$. 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 $S_k \rightarrow \cdots$, the propensity function takes the form

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

whereas for a bimolecular reaction $S_{k_1} + S_{k_2} \rightarrow \cdots$ it takes the form[3]

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

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 $p(R_j) = a_j(\boldsymbol{x})/a_0(\boldsymbol{x})$ where $a_0 = \sum_j a_j(\boldsymbol{x})$ is the partition function, and advancing the time by an exponentially-distributed interval $\tau \sim \text{Exp}(\lambda = a_0(\boldsymbol{x}))$. Then, a new state is obtained as $\mathbf{x}(t + \tau) = \boldsymbol{x} + \boldsymbol{v}_j$.

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[1] See Kruszewski & Mikolov (2022) for a detailed discussion of how this model relates to previous proposals.

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

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

3   COMBINATORY CHEMISTRY

Combinatory Chemistry[4] (Kruszewski & Mikolov, 2020; 2022) 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 the combinators S, K, I, and, recursively, their combinations through the application operation. More formally, we define $\mathbb{S}$ be the minimal set that both satisfies $\{S, K, I\} \subset \mathbb{S}$ and $(xy) \in \mathbb{S} \; \forall x, y \in \mathbb{S}$, where (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 ($\Pi \subset \mathbb{R}$), cleavages ($X \subset \mathbb{R}$), and reductions ($A \subset \mathbb{R}$), defined as follows. On the one hand, a condensation reaction $(x + y \to (xy)) \in \Pi$ and a cleavage reaction $((xy) \to x + y) \in X$ are defined for every $x, y \in \mathbb{S}$. These reactions allow the random recombination of elements in the system. On the other hand, reduction reactions are defined in an analogous way to Combinatory Logic rewrite rules. Specifically, given $x = (\dots X \dots) \in \mathbb{S}$ with $X = (If)$ or $X = (Kfg)$ or $X = (Sfgy)$ and $f, g, y \in \mathbb{S}$, then there is a corresponding reduce reaction respectively defined as[5]

$$(\dots (If) \dots) \Rightarrow (\dots f \dots) + I, \qquad \text{(I-reduction)}$$

$$(\dots (Kfg) \dots) \Rightarrow (\dots f \dots) + g + K, \qquad \text{(K-reduction)}$$

$$\underbrace{(\dots (Sfgy) \dots)}_{\text{substrate}} \underbrace{+y}_{\text{reactant}} \Rightarrow \underbrace{(\dots (fy(gy)) \dots)}_{\text{product}} \underbrace{+S}_{\text{by-product}} . \qquad \text{(S-reduction)}$$

Furthermore, we say that x is reducible and that X is a *redex* with the additional condition that when x is the substrate of an S-reduction (see the definition above), then the corresponding reactant must be present in the state of the system at the current time t so that the reaction can take place.

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 (2022).

4   EMERGENT SELF-ORGANIZING STRUCTURES

As shown by Kruszewski & Mikolov (2022), the above-described system initialized with only atomic S, K and I combinators gives rise, first, to a diversity explosion of Combinatory Logic expressions driven by random condensation and cleavages and then, gives way to emergent self-organizing structures. These structures emerge because many of the new-found expressions by random recombination admit reduce reactions and so, they will often undergo these reactions before additional condensations or cleavages. In particular, some expressions can follow a chain of 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 argued by Kruszewski & Mikolov (2022), these limit cycles constitute Autocatalytic Sets (Kauffman, 1993). For example, one such structure can be identified with the expression $\Omega = (SII(SII))$, which undergoes the following cycle (or a variation within its basin of attraction):

$$(\underline{SII(SII)}) + (SII) \Rightarrow (I(SII)(I(SII))) + S,$$

$$(\underline{I(SII)}(I(SII))) \Rightarrow (SII(I(SII))) + I,$$

$$(SII(\underline{I(SII)})) \Rightarrow (SII(SII)) + I.$$

Underlined expressions correspond to the reaction's redex. Note that on each cycle, this structure will "consume" one copy of (SII), and release back the individual combinators into the environment

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[4]Code and materials can be found in `https://germank.github.io/combinatory-chemistry/`.

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

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 $A = (\text{SII})$. 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 $A = (\text{SI}(\text{S}(\text{SK})\text{I}))$. 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, if there are no other copies of A in the environment for any the above mentioned metabolisms, 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.
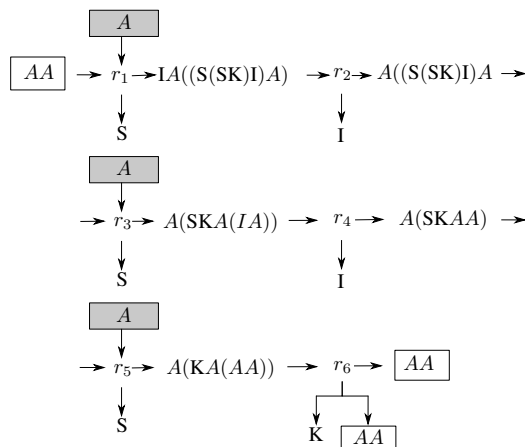

Figure 1: Cycle of a self-reproducing structure that emerges from the dynamics of Combinatory Chemistry. Starting from (AA), where $A = (\text{SI}(\text{S}(\text{SK})\text{I}))$, it acquires three copies of A from its environment and uses two to create a copy of itself, metabolising the third one to carry out the process. (Reproduced from Kruszewski & Mikolov (2022).)

5 EMERGENT SEARCH PROCESS

Combinatory Chemistry defines a walk over multisets of Combinatory Logic expressions, some of them acting as (attracting) fixed-points or limit cycles. While random condensation and cleavages allow to explore the space of possible expressions, reduce reactions shape the underlying search landscape, including the fixed points, limit cycles and their basins of attraction. Even though there are no explicit goals or objectives in this system, *we* can construe it to be *searching* for limit cycles, which constitute the emergent structures of the system.

As it has been previously noted by Kauffman (1993), the search for new structures is made more efficient by self-organization. In Combinatory Chemistry, this happens in at least two ways. One the on hand, 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, for instance, the expression (IKK). This expression is expected to undergo the reduce reaction $(\text{IKK}) \Rightarrow (\text{KK}) + \text{I}$ with much higher probability than any other kind of reaction, and therefore there will be almost no $z + (\text{IKK}) \rightarrow (z(\text{IKK}))$ or $(\text{IKK}) \rightarrow (\text{IK}) + \text{K}$ reactions, corresponding to a condensation and a cleavage, respectively. In this way, the system prunes the space of possible reactions that it explores.

On the other hand, basins of attraction allow some structures to be more easily discovered. 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 $B = (S(SK)I)$, and note that $A = (SIB)$, then the following set of reduce expressions are very likely to follow:

$$
\begin{aligned}
(\underline{S(SI(SI))(SI)B}) + B &\Rightarrow & (SI(SI)BA) + S \\
(\underline{SI(SI)BA}) + B &\Rightarrow & (IBAA) + S \\
(\underline{IB}AA) + B &\Rightarrow & (BAA) + I \\
(\underline{BA}A) + A &\Rightarrow & (SKA(IA)A) + S \\
(SKA(\underline{IA})A) &\Rightarrow & (SKAAA) + I \\
(\underline{SKAAA}) + A &\Rightarrow & (KA(AA)A) + S \\
(\underline{KA(AA)A}) &\Rightarrow & 2(AA) + K
\end{aligned}
$$

Therefore, we can see that the system found the self-reproducing structure by first forming a new expression through random condensation of some of the existing expressions, 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, it is worth noting that the search for novel expressions is exclusively done though random recombination of existing components.

6 MUTATION REACTIONS

Thanks to the self-organizing properties discussed in the previous section, the exploration process defined by random recombination reactions is more efficient than purely random search, an aspect that has been hypothesized to be behind the emergence of living systems on Earth (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:
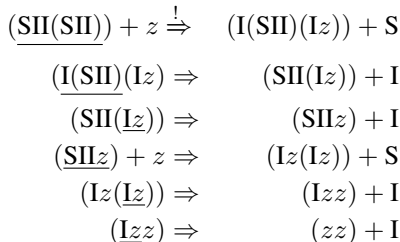
$$
(\cdots (Sfgy) \cdots) + z \overset{!}{\Rightarrow} (\cdots (fy(gz)) \cdots) + S \qquad \text{(inner-mutation)}
$$

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

Both of these reduce-like reactions 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 possible reactant. This "wrong" reactant is placed in either of the two locations where y is usually located within 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 therefore, other reactants in the system can take its place 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 happen at a faster rhythm than chance reactions, but not so fast as to interfere with the regular course of the deterministic computation over which emergent structures are defined.

7 EMERGENT SELF-ORGANIZING SEARCH

Let's now examine the result of adding these reactions in the simplest limit cycle, namely, the $\Omega = (SII(SII))$ 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.
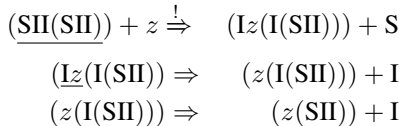
$$(\underline{\text{SII}(\text{SII})}) + z \overset{!}{\Rightarrow} \quad (\text{I}(\text{SII})(\text{I}z)) + \text{S}$$
$$(\underline{\text{I}(\text{SII})}(\text{I}z) \Rightarrow \quad (\text{SII}(\text{I}z)) + \text{I}$$
$$(\text{SII}(\underline{\text{I}z})) \Rightarrow \quad (\text{SII}z) + \text{I}$$
$$(\underline{\text{SII}z}) + z \Rightarrow \quad (\text{I}z(\text{I}z)) + \text{S}$$
$$(\text{I}z(\underline{\text{I}z})) \Rightarrow \quad (\text{I}zz) + \text{I}$$
$$(\underline{\text{I}z}z) \Rightarrow \quad (zz) + \text{I}$$

Therefore, if an inner-mutation occurred on Ω with reactant z, then the system will very likely produce the expression (zz)[6]. This is interesting because of our earlier observation that emergent structures tend to have the form of an expression applied to itself. Therefore, the system is *searching* for new expressions with a given structure, and this structure is expected to be favourable with respect 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:[7]

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

This means that if z is a rare expression ($\boldsymbol{x}_z$ is small), then these reactions could improve the probability of exploring (zz).

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

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

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 notion of algorithmic mutations explored by Chaitin (2011).

Yet, some limitations are foreseeable. Particularly, because the empirical distribution of expressions is heavily skewed towards simpler forms, then, for instance, the application of an inner-mutation, will often result in very simple forms such as (SS), (KK) or (II). Therefore, 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). Otherwise, it might be important to simulate systems of suficiently large scale for the predicted effects to appear.

8 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 that were unlikely to be found through random condensation alone. The emergence of new strategies to explore the space of possible chemical organizations defines a self-organizing search process. Whereas exploration through random recombination alone is expected to stall at

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[6]A similar analysis for the self-reproducing expression (AA) where $A = (\text{SI}(\text{S}(\text{SK})\text{I}))$ yields a similar result, but where *two* copies of (zz) are produced at the end.

[7]Ignoring the factors corresponding to 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.

some point, I speculate that as new structures are discovered they will continue to expand the repertoire of exploration strategies, which in turn will lead to other new structures to be found. In other words, the above described system can potentially display an open-ended evolutionary process over the space of Combinatory Chemistry organizations. Future work will focus in validating or rebutting these predictions through empirical explorations.

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