An Inductive Formalization of Self Reproduction in Dynamical Hierarchies

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Abstract

Formalizing self reproduction in dynamical hierarchies is one of the important problems in Artificial Life (AL) studies. We study, in this paper, an inductively defined algebraic framework for self reproduction on macroscopic organizational levels under dynamical system setting for simulated AL models and explore some existential results. Starting with defining self reproduction for atomic entities we define self reproduction with possible mutations on higher organizational levels in terms of hierarchical sets and the corresponding inductively defined ‘meta’ - reactions. We introduce constraints to distinguish a collection of entities from genuine cases of emergent organizational structures.

1 Introduction

Self reproduction is one of ubiquitously studied phenomena in Artificial Life (ALife) studies. There are early models of self reproduction based on cellular automata and their modern simplified versions as well as other models with novel syntactical representations and corresponding semantics [Sip98]. There exist formalization aimed at various levels of abstractions and properties for self reproduction. Recent work on formalization include [BH03] where authors define a probability measure to quantify how much probable is self reproduction of a subsystem in a model under one environment with respect to some other environment.

Nonetheless we lack complete understanding of how self reproduction emerges and maintains itself across higher level organizational structures. Real life is full of examples of such higher order structures – starting with simple molecules, monomers, polymers, supra molecular structures like proteins, organelles, cells, organisms.

In [MS98] authors present a 2D lattice automaton based simulation of higher order emergent structure (upto 3rd order hyperstructure - micelle) in the spirit of actual physical dynamics. They have also presented an analysis following the formalism of hyperstructures to explain their synthesis [Baa92, RBM+01a].
working with the simulations of models (see “weak emergence” [BMP00]). Nonetheless, the hyperstructure based approach for dynamical hierarchies leave some critical aspects informally defined (e.g., emergent properties, observation process), is semi formal in nature, and thus allow trivial cases [GM01, RBM+01b]. In contrast, we adopt in this paper a more formal approach based upon the set and graph theoretic notions while precisely working with the simulations of models (see “weak emergence” [BMP+00]).

2 The Framework

The following basic definitions for multisets will be used in the paper:

A multiset $M$ on a set $E$ is a mapping associating non-negative integers with each element of $E$, that is, $M : E \rightarrow \mathbb{N}$, where $\mathbb{N} = \{0, 1, \ldots \}$. For $e \in E$, $M(e)$ is called its multiplicity in the multiset.

Set of all elements $e \in E$ with nonzero multiplicity is called the support of $M$, which is denoted as $\text{Supp}(M) = \{e \in E \mid M(e) > 0\}$.

For multisets $M$ and $M'$ on $E$, we define $M \cup M' : E \rightarrow \mathbb{N}$ such that $\forall e \in E, (M \cup M')(e) = M(e) + M'(e)$. Similarly $(M \cap M')(e) = \min(M(e), M'(e))$.

We will use the term artificial chemistry (AC) in a generic sense applicable to a wide class of ALife models with computational dynamics. ACs represent a mathematically generalized metaphors of “real chemistry” with well defined “laws of interaction or reaction semantics” between the “elements” or “molecules” of the model universe. A detailed review of ACs also appears in [DZB01].

An AC $A$ is usually started with an initial population of a multiset of molecules $P_0$. $A$ evolves over time and we have different populations consisting of different multisets of molecules during the course of evolution. We represent time progression of $A$ as an infinite sequence of multisets $P = < P_0, P_1, \ldots >$ such that $P_i$ precedes $P_j \forall j > i$. Multisets $P_0, P_1, \ldots$ are also referred to as states of $A$ and $P$ is called a run or simulation of $A$. A finite strictly consecutive subsequence of states of $A$, $< P_i, P_{i+1}, \ldots, P_{i+n} >$ is termed as a partial run of $P$. A non consecutive subsequence $< P_{i_1}, P_{i_2}, \ldots, P_{i_n} >$ with $P_{i_j}$ precedes $P_{i_k} \forall i_k > i_j$ is called subsequence of states in $P$. The set of all such different runs of $A$ is denoted by $\Gamma$. Each run of $A$ has potentially infinite states, though in case of cycles there will be repeating sub sequences of states.

We assume in this paper that reaction semantics defined in the ALife model is deterministic. More general case of probabilistic or stochastic reactions will be dealt in future. For a reaction $r$ defined in terms of the inputs and the corresponding outputs (ignoring other conditions), we define $input_r$ as a multiset of input molecules and $output_r$ as the multiset of the outputs of $r$. For a sequence of reactions $r = < r_1, r_2, \ldots, r_n >$, we define $\text{Input}(r) = \bigcup_{r_j \in r} input_{r_j}$ as the multiset of all participating input molecules in the reaction sequence. Similarly $\text{Output}(r) = \bigcup_{r_j \in r} output_{r_j}$ is the multiset of all output molecules in $r$.

**Definition 1 (Feasible Reaction).** A reaction $r$ is said to be feasible in a state $P_i$ iff $\forall g \in \text{Supp}(input_r), P_i(g) > input_r(g)$.
Informally this means reaction \( r \) may execute if all required input molecules are available in the state \( P_i \) of \( A \). If state \( P_i \) is in run \( P = < P_0, P_1, \ldots > \) of \( A \), \( r \) is also said to be a feasible reaction in run \( P \). In actual ALife models there can be many other global conditions or environmental constraints associated with the feasibility of reactions defined by the designer. We have though ignored, these can be added without much difficulty when applying the framework on these models. Note that feasibility of a reaction does not imply automatically that it will be executed as well since that depends on the scheduling algorithm defined by the designer of the chemistry which selects the reactions to execute at any state of the chemistry.

We can extend above definition to a sequence of reactions as follows: define \( r = < r_1, r_2, \ldots, r_n > \) as a feasible reaction sequence in a state subsequence \( < P_i, P_{i+1}, \ldots, P_n > \) of run \( P \) iff \( r_j \) is a feasible reaction in state \( P_j \) \( \forall j = 1, 2, \ldots, n \). \( r \) is also called a feasible reaction sequence in the run \( P \).

**Definition 2** (Potential Causality). Let \( \Omega_0 \) be the set of molecules for a run \( P \in \Gamma \) of \( A \). We define potential causal relation \( \Rightarrow \) between two molecules as follows: \( \Rightarrow \subseteq \Omega_0 \times \Omega_0 \) such that for molecules \( g_1, g_2 \in \Omega_0 \), \( (g_1, g_2) \in \Rightarrow \) if and only if there exists a feasible reaction \( r \) in the state \( P \) such that \( g_1 \in \text{input}_r \) and \( g_2 \in \text{output}_r \). \( r \) is termed as potential causal link between \( g_1 \) and \( g_2 \) and we represent this using \( g_1 \Rightarrow_r g_2 \).

There can be multiple causal links between two molecules and each molecule can be causally linked to multiple other molecules. We can also define a multi-graph using all the potential causal reactions at any state of the chemistry.

**Definition 3** (Potential Reaction Graph). Define a multi-graph \( G_i = (V_i, E_i) \) for the state \( P_i \) such that for each molecule \( g \in \text{Supp}(P_i) \) there is a node \( e_g \) in \( E_i \) and if \( g \Rightarrow_r g' \) then we have a directed edge from \( e_g \) to \( e_{g'} \) in \( E_i \) with label \( r \), where \( r \) is feasible in \( P_i \).

Next consider a feasible reaction sequence \( r = < r_1, r_2, \ldots, r_n > \) and define for \( g, g' \in \Omega_0 \), \( g \Rightarrow_{r} g' \) when \( \exists g_0, g_1, \ldots, g_n \) such that \( g_0 = g \), \( g_n = g' \) and \( g_i \Rightarrow_{r} g_{i+1} \forall 0 \leq i < n \). Such a feasible reaction sequence \( r \) will be termed as a potential causal path between \( g, g' \). There can be multiple such potential causal paths present between \( (g, g') \). Note that potential causal path is not a path in potential reaction graph but is constructed when chemistry evolves over time.

Now we can define potential self replication using the principle of preservation of overall resources (dilution flux) along with the concept of potential causality.

**Definition 4** (Potentially Self Reproducing Entities). A molecule/entity \( g \) is defined as potentially self reproducing in a chemistry \( A \), if \( \exists \) a run \( P \) of \( A \) for which the following holds:

\( \exists g' \in \Omega_0 \) such that the following conditions are satisfied:

**Observational Equivalence** \( g' \sim g \), where exact definition of \( \sim \subseteq \Omega_0 \times \Omega_0 \) is dependent on the underlying chemistry and its designer or the observer.
For example if molecules are represented as graphs then $\sim$ can be defined as graph isomorphism, or if molecules are strings then it will be character by character string equivalence. $\sim$ can even be defined by the designer as functional equivalence.

**Reflexive Autocatalysis** $\exists$ feasible sequence of reactions $C_p$ so that $g \Rightarrow_{C_p} g'$, that is, $C_p$ is a potential causal path between $g$ and $g'$.

**Material Basis** For every such potential causal path $C_p$ between $(g, g')$, which is a feasible reaction sequence in a partial run $< P_{i_1}, P_{i_2}, \ldots, P_{i_n} >$ of $\mathcal{P}$, we have $P_{i_n}(g) > P_{i_1}(g)$ and $\exists X \subseteq \text{Input}(C_p) - \{ g \}$ (where $X \neq \emptyset$) such that $\forall g_x \in X : P_{i_n}(g_x) < P_{i_1}(g_x)$.

Informally, this states that there should be an increase in the size of population of $g$ and corresponding decrease in some other populations of participating entities ($X$) in the state $P_{i_n}$ as compared to the sizes of these populations in initial state $P_{i_1}$.

Let me now discuss the above conditions in the context of ALife studies: the first requirement of observational equivalence is fundamental to any ALife study because otherwise in the model universe itself there cannot have some fundamental embodied equivalence between two entities and therefore always some external observer is needed who imposes the equivalence ($\sim$) between the molecule $g$ and the product $g'$ to define self reproduction. The apparently objective alternatives to this view where one might consider structural or functional equivalences can themselves be considered as externally imposed criterion not inherent in the model universe unless the underlying chemistry evolves or possesses some kind of structural or functional recognition capability. For most of the ALife studies, it is upon the observer or the designer to define the recognition process which can be used to determine the equivalence between molecules $g$ and $g'$. This can also be seen in light of the Valera’s theory of autopoisis which emphasizes upon the “emergence” of autonomy in life forms [Zel81]. Also note that by equivalence we may not require that $g$ and $g'$ are identical and thus $g$ can reproduce with mutations under some observable limit.

The second requirement of reflexive autocatalysis should be obvious since all molecules not present in the chemistry at the beginning should be the result of some reactions. Reflexive autocatalysis denotes one or more reaction steps in the reaction sequence starting from $g$ and yielding another molecule $g'$ finally, which should be observationally equivalent to $g$.

The last requirement of material basis is to capture the essence of entity - environment interaction quantitatively along the lines of real chemistry. This condition dictates that new molecule appearing in the chemistry must not be the result of some sort of magical appearance out of nothing. This requirement is most often ignored in ALife studies and alternately weakly captured by imposing dilution flux which keeps the volume of the chemistry constant. Our formulation makes clear connection between the transformation of reacting molecules as per the reactions in $C_p$. 


Each potential causal path $C_p$ leading to potential self replication for $g$ is also called potential self reproducing path of $g$. Note that potential self replication does not necessarily guarantee that self replication of $g$ will occur in every run in which $C_p$ is potentially feasible. The only thing which is guaranteed is that there exists at least one run of $A$, where $C_p$ will actually execute and thus lead to self replication of $g$. This further highlights the importance of emergence of membrane structures in real life which had very profound role in making potential self reproducing paths actual execution paths since due to the presence of membrane boundaries these potential self reproducing reactions could actually execute with high probability.

Furthermore it is not again guaranteed that in all those runs where $C_p$ executes, there is no spontaneous emergence of same entity $g$ in some other way not involving $g$ in the reactions. Indeed this is bit unfortunate because then in that case it will not be possible for any outside observer to establish reflexive autocatalysis just by looking at entities at different states of the chemistry.

Next we will consider more strict characterization self reproduction for special class of chemistries which employ sequential scheduling where at any state of the chemistry during simulation only one reaction is selected for the execution. For these chemistries we consider cyclic runs and prove that every potentially self reproducing entity indeed self reproduces.

**Definition 5** (Cyclic Run). A run $\mathcal{P} = < P_0, P_1, \ldots >$ of $A$ is cyclic iff $\exists n \geq 0, l > 0$ such that $\forall k \geq 1, 0 < r \leq l, P_{n+kl+r} = P_{n+r}$. Subsequence $< P_{n+1}, \ldots P_{n+l} >$ is the cycle in $\mathcal{P}$ and a cyclic run is therefore represented as $\mathcal{P} = < P_0, P_1, \ldots P_n, [P_{n+1}, \ldots P_{n+l}]^\infty >$.

**Theorem 1.** For a cyclic run $\mathcal{P} = < P_0, P_1, \ldots P_n, [P_{n+1}, \ldots P_{n+l}]^\infty >$ of $A$, a potentially self reproducing entity $g \in \Omega_0$ actually self reproduces if $\exists$ potential self reproducing path $C_p$ for $g$ which is feasible in the cycle $\mathcal{P} = [P_{n+1}, \ldots P_{n+l}]$.

**Proof.** This is because the feasible reaction sequence $C_p$ indeed executes in the cycle $\mathcal{P}$, otherwise there will be different states of the chemistry not present in $\mathcal{P}$ because of the execution of some other reactions not in $C_p$, contradicting the very structure of the cycle. Furthermore due to sequential scheduling of the reactions during simulations there is always only one potential reaction which is executed in every state of the cycle.

Though above characterizations only specify self replication of a single molecule, it can be seamlessly extended to the case of simultaneous self replication of multiple molecules. In such cases either scheduling algorithm will have to execute several reactions in parallel or the potential self reproducing paths for several molecules might be intermixed with each other.

Next we will discuss an important extension to above definitions to handle more realistic scenarios whereby sets of molecules forming higher level organizational structures reproduce collectively.
3 Self Reproduction on Higher Organizational Levels

3.1 Entities on Higher Organizational Levels

To achieve this aim, we will inductively define the hierarchical sets as entities at different levels. Consider the level 0 entities as all “syntactically valid” molecules appearing at any state of the chemistry during its dynamical progression through time. \( \Omega_0 \) used above denotes the set of all such level 0 entities.

Then level 1 entities are any finite subsets of \( \Omega_0 \) of size > 1. Let \( \Omega_1 \) be the set of all such level 1 entities. Thus

\[
\Omega_1 = \{ x | x \subseteq \Omega_0 \} \land [x \cap \Omega_0 \neq \emptyset] \land [|x| > 1] \}
\]

Note that we do not consider a singleton set consisting of only one level 0 entity as an level 1 entity. Similarly Level 2 entities consist of finite number of level 0 and level 1 entities. That is, each level 2 entity is finite subset of \( \Omega_0 \cup \Omega_1 \) of size > 1. Let \( \Omega_2 \) be set of all such level 2 entities. This way we can inductively define the set of level \( n \) entities as

\[
\Omega_n = \{ x | x \subseteq \bigcup_{0 \leq i < n} \Omega_i \} \land [x \cap \Omega_{n-1} \neq \emptyset] \land [|x| > 1] \}
\]

The above classification of higher level entities in the chemistry, though captures syntactical essence of hierarchical structures, does not specify their dynamical structure, which is one of the important problems to be addressed in ALife theories. In this paper we will focus our attention to only the characterization of self replication for such higher level structures and will not provide analysis on how these structures emerge per se in the chemistry and maintain themselves.

3.2 Defining Meta Reactions

I will proceed by defining higher level “meta” reactions which form the counter part of higher level entities defined above.

Let us consider a level 1 entity \( \zeta_1 = \{ e_1, e_2, \ldots, e_r \} \in \Omega_1 \), where \( e_i \in \Omega_0 \) and a feasible reaction sequence \( R = < r_1, r_2, \ldots, r_k > \), satisfying the following:

\[
\forall 1 \leq i \leq k. input_i \cap \zeta_1 \neq \emptyset
\]

Then in that case we say that (level 1 entity) \( \zeta_1 \) takes part in level 1 (meta) reaction \( R \).

Also consider some other level 1 entity \( \zeta_2 \) such that

\[
\zeta_2 \subseteq (Output(R) - Input(R))
\]

Then in that case we say that \( \zeta_2 \) is potentially causally related to \( \zeta_1 \) and write it as \( \zeta_1 \Rightarrow_R \zeta_2 \).
For example, consider a sequence of reactions feasible in three consecutive states of a chemistry as

\[ R = \langle r_1 : a + a_1 \rightarrow 2c, r_2 : a + c \rightarrow d, r_3 : e + e_1 \rightarrow d + f \rangle \]

Now we can define \( \zeta_1 = \{a, c, e_1\} \) which takes part in \( R \) because \( \text{input}_{r_1} = \{a, a_1\} \) and \( \{a, a_1\} \cap \zeta_1 = \{a\} \neq \emptyset \). Similarly \( \text{input}_{r_2} \cap \zeta_1 \neq \emptyset \) and \( \text{input}_{r_3} \cap \zeta_1 \neq \emptyset \). If we consider \( \zeta_2 = \{c, d, f\} \) then \( \zeta_2 \subseteq (\text{Output}(R) - \text{Input}(R)) \) Therefore we can also infer that \( \zeta_2 \) is potentially causally related to \( \zeta_1 \) through \( R \), i.e., \( \{a, b, c\} \Rightarrow_r^1 \{c, d, f\} \). Note that the given formulation also allows trivial cases where certain collections of entities are inferred as causally connected while in reality only the individual elements appearing in those collections are independently causally connected. For illustration let me consider another feasible sequence

\[ R' = \langle r_1 : a + a_1 \rightarrow 2d', r_2 : b + b_1 \rightarrow b', r_3 : e + e_1 \rightarrow e' + f \rangle \]

Also define \( \zeta' = \{a, b, e_1\} \) which takes part in \( R' \). Next let us select \( \zeta'' = \{d', b', f\} \) then \( \zeta'' \subseteq (\text{Output}(R') - \text{Input}(R')) \). Therefore we can infer that \( \zeta' \Rightarrow_r^1 \zeta'' \) even though this is merely because of the fact that component elements in \( \zeta' \) and \( \zeta'' \) are independently causally connected, i.e., \( a \Rightarrow_e a' \) through \( r_1 \), \( b \Rightarrow_e b' \) through \( r_2 \), and \( e \Rightarrow_e f \) through \( r_3 \). It is clear that, to be meaningful, we need to exclude such trivial cases while defining potential self replication for emerging higher level entities.

**Constraint of non-triviality:** This is done by enforcing another constraint to ensure that total number of potential causal paths between \( \zeta' \) and \( \zeta'' \) are strictly more than \( |\zeta''| - |\zeta'| \) - this is because - then in that case there will be at least one component in \( \zeta'' \) which must be causally connected to more than one element in \( \zeta' \). An even more strict constraint using the concept of reaction graphs can be formulated where we can demand absence of cliques in the reaction graph consisting of potential causal paths between elements of \( \zeta' \) and \( \zeta'' \) to ensure non triviality of causality but we will not pursue it here.

Also it should be pointed out that level 1 reactions have to have time progression built into them, that is, should be feasible reaction sequences. Thus not every subset of level 0 reactions can be considered as a level 1 reaction.

Now we are in a position to define a potential causal path which will be then used to define self replication of level 1 entities in terms of level 1 reactions.

Consider two such level 1 reactions \( R = \langle r_1, r_2, \ldots, r_n \rangle \) and \( S = \langle s_1, s_2, \ldots, s_m \rangle \). We say \( R \) temporally precedes \( S \) if and only if \( r_1 \) precedes \( s_1 \) and \( r_n \) also precedes \( s_m \) over some sequence of states \( < P_1, P_2, \ldots, P_k > \) in the run \( P \), where \( \max(m, n) \leq k \leq m + n \). Then \( < R, S > \) can be considered as a level 1 feasible reaction sequence.

Let \( R = \langle R_1, R_2, \ldots, R_n \rangle \) and define for \( \zeta, \zeta' \in \Omega_1 \), \( \zeta \Rightarrow_{R}^1 \zeta' \) when \( \exists \zeta_0, \zeta_1, \ldots, \zeta_n \in \Omega_1 \) such that \( \zeta_0 = \zeta, \zeta_n = \zeta' \) and \( \zeta_i \Rightarrow_{R_i}^1 \zeta_{i+1} \forall 0 \leq i < n \). Such feasible reaction sequence \( R \) will be termed as the level 1 potential causal path between \( \zeta \) and \( \zeta' \). There can be multiple such potential causal paths present between \( (\zeta, \zeta') \).
As discussed before, this definition permits trivial scenario of level 1 potential causal paths which are the result of the presence of independent level 0 potential causal paths between the elements of $\zeta = \{e_1, e_2, \ldots, e_l\}$ and $\zeta' = \{e'_1, e'_2, \ldots, e'_m\}$. In order to eliminate this situation we need to enforce the constraint of non-triviality: we say $R$ is a non-trivial potential causal path between $\zeta$ and $\zeta'$ if and only if number of potential causal paths between pairs of elements from $\zeta$ and $\zeta'$ are more than $m$ indicating network dependence. This is because in case of trivial potential causal path between $\zeta$ and $\zeta'$ there will in turn be exactly $m$ level 0 independent potential causal paths producing each of $e'_i$, $1 \leq i \leq m$.

**Definition 6 (Potentially Self Reproducing Sets of Entities).** A level 1 entity $\zeta$ is defined as potentially self reproducing in chemistry $A$, if $\exists$ a run $P$ of $A$ for which the following holds:

$\exists \zeta' \in \Omega_1$ such that the following conditions are satisfied:

**Observational Equivalence** $\zeta' \sim^1 \zeta$, where exact definition of $\sim^1 \subseteq \Omega_1 \times \Omega_1$ is again dependent on the underlying chemistry structure and its designer or the observer. An observer might, for example, define $\zeta' \sim^1 \zeta$ if both sets are equivalent under $\sim$, that is, there exists an one to one equivalence between the elements of $\zeta$ and $\zeta'$.

**Reflexive Autocatalysis** $\exists$ non trivial causal path $C_p$ consisting of level 1 reactions so that $\zeta \Rightarrow^1_{C_p} \zeta'$.

**Material Basis** For every such non-trivial potential causal path $C_p$ between $(\zeta, \zeta')$, which is a feasible reaction sequence in a subsequence of states $< P_{i_1}, P_{i_2}, \ldots, P_{i_n} >$ of $P$, there should be a resultant increase in the size of population of $\zeta$ and corresponding decrease in some other entity populations participating the the reaction sequence ($C_p$) in state $P_{i_n}$ as compared to the sizes of these populations in initial state $P_{i_1}$.

The above approach can be extended without much difficulty to inductively define meta reactions on even higher levels in the chemistry.

Due to space limitations detailed case study illustrating the formalism would be presented a forthcoming paper [Mis].

4 Conclusion

In this paper we presented a rigorous formalism to define higher level organizational structures in terms of hierarchal sets and corresponding non trivial meta
reactions. The formalism can adequately capture syntactical representations of important higher order structures and meta reaction sequences these structures can take part in. The constraint of non triviality allows us to distinguish the genuine case of higher level organization with a collection of reacting entities. The formalism allowed us to define concretely the case of self reproduction even when we allow mutations under observable limitations. The definition of self reproduction is quite generic and captures the essence of self in terms of observed equivalence.

5 Further Work

This is an ongoing work with the aim to capture the necessary and sufficient conditions for evolution to occur in important ALife studies. We need to introduce explicitly a notion of mutations, heredity and most importantly selection by considering a population of reproducing entities. We need to define certain closure properties for such higher level entities which will ensure that even under mutations which change the syntactical structure of entities they can nonetheless semantically retain their properties e.g. self reproduction. Detailed case studies will be used to further refine the formalism. We also need to extend the current formalism by considering the more generic scenario involving probabilistic reactions or stochastic dynamics, whereby we can address the questions involving how do developmental pathways get selected and fixed over the course of evolution.

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