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# The Emergence of a Self-Catalysing Structure in Abstract Origin-Of-Life Models

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**Abstract**—We formalize a class of abstract and simple biochemical models that have been proposed for understanding the origin of life. We then analyse conditions under which "life-like" substructures will tend to arise in such models. 

**Keywords**—Artificial life, Autocatalysis, Random combinatorial structures.

## 1. INTRODUCTION

The emergence of properties (for example, cycles) in random combinatorial structures, such as (di)graphs has been suggested as a simple way to model and understand early biological processes, such as the origin of life (see [1,2]).

Kauffman [3,4] introduced and analysed a simple abstract origin-of-life model based on large numbers of polymers randomly catalysing the concatenation and subdivision of other polymers. He claimed that life-like subsystems ("connected, reflexively autocatalytic" sets) must spontaneously arise (with high probability) once the number of polymers becomes sufficiently large, a conclusion that was subsequently criticised by Lifson [5].

A close reading of [3,4] suggests, however, that Kauffman's original model imposes a stronger assumption, concerning the probability that a polymer calalyses any particular reaction, than the one that Lifson analyses. With that stronger assumption, Kauffman's claim holds. Nevertheless, Lifson's interpretation of what Kauffman was assuming in his model is arguably more realistic (see also [6]) and in that case, Kauffman's sufficient condition for the emergence of life-like subsystems does indeed break down. However, the question of whether this interpretation of Kauffman's model should give rise to life-like subsystems remains. In this note, we partially answer this question. First, we formalize precisely the types of model and "life" described semiformally by Kauffman. We then consider in more detail conditions for the emergence of life-like substructures in these models. In particular, we show that the degree of catalysation required for the emergence of life-like structures is less than Kauffman required, but more than some models of the type considered by Lifson.

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### 1.1. Connected, Relexively Autocatalytic (CRA) Sets

We first set up some general terminology, which allows us to consider Kauffman's model and other variations as special cases.

DEFINITIONS.

- *Let $X$ denote a set of molecules. A reaction $r$ will denote a pair $r = (\{a, b\}, c), a, b, c \in X$ which represents an allowable chemical reaction:*

$$a + b \rightleftharpoons c$$

*(both the forward and backward reactions). Note that we may allow $a = b$ in case $a + a \rightleftharpoons b$ is an allowable reaction.*
- *Let $F$ (for 'food') denote a distinguished subset of $X$.*
- *Let $\mathcal{R}$ be the set of allowable reactions. A catalysation is a pair $(x, r)$ where $x \in X$, $r \in \mathcal{R}$, denoting that molecule $x$ catalyses reaction $r$. Let $C \subseteq X \times \mathcal{R}$ be a set of catalysations.*
- *For $r = (\{a, b\}, c) \in \mathcal{R}$, let $\text{supp}(r) := \{a, b, c\}$, and for a subset $\mathcal{R}'$ of reactions define its support, written $\text{supp}(\mathcal{R}')$, by setting $\text{supp}(\mathcal{R}') = \cup_{r \in \mathcal{R}'} \text{supp}(r)$. Thus, $\text{supp}(\mathcal{R}')$ is the set of all molecules that are involved in at least one reaction from $\mathcal{R}'$.*
- *Given a subset $\mathcal{R}'$ of $\mathcal{R}$, and a subset $X'$ of $X$, define the closure of $X'$ relative to $\mathcal{R}'$, denoted $\text{cl}_{\mathcal{R}'}(X')$ to be the (unique) minimal subset $W$ of $X$ that satisfies the condition: for each reaction $a + b \rightleftharpoons c$ in $\mathcal{R}'$:*

$$a, b \in X' \cup W \Longrightarrow c \in W,$$
$$c \in W \Longrightarrow a, b \in W.$$

*Informally, $\text{cl}_{\mathcal{R}'}(X')$ is the set of all molecules that can be constructed from $X'$ by repeated application of (forward and backward) reactions in $\mathcal{R}'$. Note that $\text{cl}_{\mathcal{R}'}(X') \subseteq \text{supp}(\mathcal{R}')$, and that $\text{cl}_{\mathcal{R}'}(X)$ is well defined since the collection of subsets of $W \subseteq X$ satisfying the condition described is closed under intersection, and nonempty.*
  - *Given the quadruple $(X, F, \mathcal{R}, C)$, a subset $\mathcal{R}'$ of $\mathcal{R}$ is reflexively autocatalytic (RA), if*

$$\text{for all } r \in \mathcal{R}', \text{ there exists an } s \in \text{supp}(\mathcal{R}') : (s, r) \in C,$$

*connected to $F$ if*

$$\text{supp}(\mathcal{R}') = \text{cl}_{\mathcal{R}'}(F),$$

*connected, reflexively autocatalytic (CRA) if $\mathcal{R}'$ is both RA and connected to $F$.*

Informally, a CRA set of reactions $\mathcal{R}'$ is one in which every reaction is catalysed by an element in the support of $\mathcal{R}'$, and every element in the support can be constructed from the food set $F$ by successive applications of reactions from $\mathcal{R}'$. It thus captures the abstract idea of "life" as a self-catalysing system able to sustain itself by using a suitable food source.

Of course, one may wish to restrict attention to *minimal* CRAs—that is, CRAs which have the property that no proper subset also forms a CRA. Since we are only concerned with the existence of a CRA in $\mathcal{R}$ and this is equivalent to the existence of a minimal CRA, we do not need to worry about this distinction. One may also wish to impose further restrictions on a CRA to exclude certain trivial situations—for example, one may require that not all reactions in $R$ are catalysed by elements of $F$, or, more strongly, one may require at least one element of $X - F$ to form a cycle in the digraph on $X$ defined by placing directed edges from a polymer $x$ to the elements in the support of any reaction which $x$ calalyses. However, these considerations do not affect our conclusions at all, as may be easily checked.

### 1.2. Kauffman's Abstract Model

Kauffman (see [3,4]) considered a somewhat abstract model in which the set $X$ of molecules comprises all polymers (sequences) up to a given length, $n$ over a $k$-letter alphabet—that is, $X = X_n = \{0, 1, \ldots, k-1\}^{\leq n}$, and $F$ denotes all sequences of length $\leq t$ for some small and fixed $t$ (for example, $t = 2$). Actually, Kauffman considered in detail only the case $k = 2$, but we will consider the more general case as the calculations are similar. Following [3,4], the elements of $X_n$ are regarded as oriented, and the set $\mathcal{R} = \mathcal{R}_n$ of allowable reactions (representing ligation/cleavage reactions) is the set of pairs $r = (\{a, b\}, c), a, b, c \in X_n$ for which $c = ab$ or $c = ba$ where $ab$ is the concatenation of $a$ with $b$ (in case $a = b$, $c$ is the concatenation of $a$ with itself).

$C$ is randomly generated, by assigning elements of $X_n \times \mathcal{R}_n$ as follows: each $x \in X_n$ catalyses any given reaction $r$ with probability $p_n$ (not dependent on $x$ or $r$) and these assignments are made independently over $X_n \times \mathcal{R}_n$.

In Kauffman's original model, $p_n$ is constant ("each polymer has a chance $P$ of catalysing the first reaction, the second reaction and so forth" [4, p. 307]), while in Lifson's interpretation (see [5]), $p_n$ is inversely proportional to $|\mathcal{R}_n|$ (an even more realistic extension would allow catalysation probabilities to depend on lengths of polymers, but we do not explore this here). For the general model we have described—which includes both interpretions as special cases—questions of interest include the following.

1. Let $P_n := \mathbb{P}[\exists \mathcal{R}' \subseteq \mathcal{R}_n : \mathcal{R}' \text{ is CRA}]$ and let $P_\infty = \lim_{n\to\infty} P_n$. Under what conditions on the sequence $p_n$ does $P_\infty = 1$? More generally, how does $P_\infty$ depend on $\{p_n\}$?
2. As $n$ grows, at what value will we expect to first observe a CRA, and how large (in terms of the number of reactions) will a minimal CRA be?

In this paper, we consider only the first of these two problems.

## 2. RESULTS

The number of elements of $X_n$ is clearly just the sum $\sum_{i=1}^{n} k^i$. Thus, we have

$$|X_n| = \frac{k^{n+1} - k}{k-1} \sim \frac{k^{n+1}}{k-1}, \tag{1}$$

where $\sim$ denotes asymptotic equivalence ($f(n) \sim g(n)$ precisely if $\lim_{n\to\infty} f(n)/g(n) = 1$).

Also of importance to us is the ratio of the number of reactions to polymers. Extending the argument from [3,4] from two-state to $k$-state sequences, the number of reactions $r = (\{a, b\}, c)$ can be counted by noting that, for each of the $c \in X_n$ of length $(i = 2, \ldots, n)$, there are $i - 1$ places to cut $c$ to obtain the pair $\{a, b\}$. Thus, $|\mathcal{R}_n| \sim \sum_{i=2}^{n}(i-1)k^i \sim (nk^{n+1})/(k-1)$ (where the first aymptotic equivalence fails to be an equality since we have overlooked the asymptotically negligible effect of palindromic polymers). Thus, from (1), we obtain

$$\frac{|\mathcal{R}_n|}{|X_n|} \sim n. \tag{2}$$

One of Kauffman's principal claims is that if $p_n$ is constant (as a function of $n$), then no matter how small this value is, one has

$$P_\infty = 1.$$

We generalize this result as follows, by allowing $p_n$ to tend to zero (but not too quickly).

THEOREM 1. *If $p_n \geq cn^2/|\mathcal{R}_n|$, where $c > \log_e(k)$, then $\lim_{n\to\infty} \mathbb{P}[\mathcal{R}_n$ is a CRA$] = 1$ and in particular, $P_\infty = 1$.*

PROOF. First, since $\text{supp}(\mathcal{R}_n) = X_n = \text{cl}_{\mathcal{R}_n}(F)$, $\mathcal{R}_n$ is connected to $F$. Thus, it suffices to show the probability of $\mathcal{R}_n$ being reflexively autocatalytic converges to 1, as $n \to \infty$. We have

$$\mathbb{P}[\mathcal{R}_n \text{ is RA}] = 1 - \mathbb{P}[\exists r \in \mathcal{R}_n : \forall x \in X_n, (x, r) \notin C] \geq 1 - \sum_{r\in\mathcal{R}_n} \mathbb{P}[\forall x \in X_n, (x, r) \notin C],$$

by the Bonferroni inequality. Now, for any $r \in \mathcal{R}_n$, we have

$$\mathbb{P}[\forall x \in X_n, (x,r) \notin C] = (1-p_n)^{|X_n|},$$

by the assumptions of the model. Thus,

$$\mathbb{P}[\mathcal{R}_n \text{ is RA}] \geq 1 - |\mathcal{R}_n|(1-p_n)^{|X_n|}.$$

Thus, if $p_n \geq cn^2/|\mathcal{R}_n|$, then, letting $g(n) = (n|X_n|)/(|\mathcal{R}_n|)$,

$$|\mathcal{R}_n|(1-p_n)^{|X_n|} \leq ng(n)^{-1}k^{n+1}e^{-cng(n)} = kng(n)^{-1}e^{(\log_e(k)-cg(n))n},$$

by virtue of (1) and the inequality, $(1-a)^b \leq e^{-ab}, a, b > 0$. Now, from (2), $\lim_{n\to\infty} g(n) = 1$ and so if $\log_e(k) - c < -\delta < 0$, then, there exists some $n_0$, such that for all $n \geq n_0$, $\log_e(k) - cg(n) < -\delta/2$. Consequently, for all $n \geq n_0$, $|\mathcal{R}_n|(1-p_n)^{|X_n|} \leq kng(n)^{-1}e^{-n\delta/2}$ and so $\lim_{n\to\infty} |\mathcal{R}_n|(1-p_n)^{|X_n|} = 0$, as required. ∎

Thus, if each polymer catalyses on average $n^2$ reactions in total, then it becomes increasingly certain that the entire system of reactions is a CRA (under Kauffman's original model, the average number of reactions catalysed by a given polymer grows even faster than $n^2$—it is proportionally to $|\mathcal{R}_n|$ and thus grows exponentially with $n$). However, this assumption that the average number of reactions catalysed by a given polymer grows quickly (or at all) with $n$ has been questioned by Lifson, so it is useful to explore slower rates of growth, and see under what conditions a CRA (not necessarily all of $\mathcal{R}_n$) will arise.

### 2.1. Lifson's Interpretation

A major criticism of Kauffman's model (see [5,6]) is the assumption that $p_n$ should be constant with $n$. Lifson analyses a more modest scenario whereby each element $x \in X_n$ has a fixed probability $p$ of catalysing some reaction, but in that case, only one (uniformly selected) reaction is catalysed by $x$. We may model this by taking $p_n = p/|\mathcal{R}_n|$. In [5], Lifson showed that Kauffman's proof (which shows that $\mathcal{R}_n$ is a increasingly certain to be CRA) is no longer valid, but this leaves open the question of what value $P_\infty$ might take, since it could conceivably be the case that $\mathcal{R}_n$ could contain a CRA, $\mathcal{R}'$. The next theorem partially answers this question—in particular, it shows that the analogue of Theorem 1 no longer holds (for the existence of CRAs), at least if $p$ is small.

THEOREM 2. *Suppose $p_n = p/|\mathcal{R}_n|$. Then, we have the following.*

1. *For all $\epsilon > 0$, there exists $\delta > 0$ such that if $p < \delta$, then*

$$\lim_{n\to\infty} \mathbb{P}[\exists \mathcal{R}' \subseteq \mathcal{R}_n : \mathcal{R}' \text{is RA}] < \epsilon.$$

2. *If $p < 1/3e^{-1}$, then $P_\infty = 0$.*

PROOF.

PART 1. Consider the pair $(\mathcal{R}', S')$, where $S' := \text{supp}(\mathcal{R}')$. Let $r := |\mathcal{R}'|$; $s := |S'|$. Under the assumptions of the model, the probability that each element of $\mathcal{R}'$ is catalysed by (at least) one element of $S'$ is $(1-(1-p/|\mathcal{R}_n|)^s)^r \leq (ps/|\mathcal{R}_n|)^r \leq (3rp/|\mathcal{R}_n|)^r$, where the last inequality follows from the observation that, for any reaction $r$, $|\text{supp}(r)| \leq 3$ and so, $s \leq 3r$. Thus, by the Bonferroni inequality,

$$\mathbb{P}[\exists \mathcal{R}' \subseteq \mathcal{R}_n : \mathcal{R}' \text{ is RA}] \leq \sum_{r\geq 1} \sum_{\mathcal{R}':|\mathcal{R}'|=r} \mathbb{P}[\mathcal{R}' \text{ is RA}] \leq \sum_{r\geq 1} \binom{|\mathcal{R}_n|}{r} \left(\frac{3rp}{|\mathcal{R}_n|}\right)^r \leq \sum_{r\geq 1} \frac{(3rp)^r}{r!}.$$

By Stirling's formula, $(r^r/r!) \leq (e^r/\sqrt{2r\pi})$. Thus, if we write $p = (1/3)e^{-1}\alpha$, where $\alpha < 1$, we have $\sum_{r\geq 1}((3rp)^r/r!) \leq \sum_{r\geq 1} r^{-0.5}\alpha^r \leq \alpha/(1-\alpha)$, which establishes Part 1 of the theorem.

PART 2. Note that if a subset $\mathcal{R}'$ of $\mathcal{R}_n$ is connected to $F$, then $\text{supp}(\mathcal{R}') \cap F \neq \emptyset$. Let $f := |F|$. The number of $r \in \mathcal{R}_n$ such that $\text{supp}(r) \cap F \neq \emptyset$ is at most $2|X_n|f$, since for each $x \in X, f \in F$ there exists at most two elements $g \in X$ such that $f + g \rightleftharpoons x$ is a reaction (and in case $x \in F$, $f' + g' \rightleftharpoons x$ implies $f', g' \in F$). Thus,

$$|\{\mathcal{R}' \subseteq \mathcal{R}_n : |\mathcal{R}'| = r, \text{supp}(\mathcal{R}') \cap F \neq \emptyset\}| \leq \binom{|\mathcal{R}_n|}{r} - \binom{|\mathcal{R}_n| - 2|X_n|f}{r}.$$

Consequently, if we let $P_n^{(r)} := \mathbb{P}[\exists \mathcal{R}' \subseteq \mathcal{R}_n : |\mathcal{R}'| = r, \mathcal{R}' \text{ is CRA}]$ and once again apply the Bonferroni inequality, we have

$$P_n^{(r)} \leq \left(\binom{|\mathcal{R}_n|}{r} - \binom{|\mathcal{R}_n| - 2|X_n|f}{r}\right)\left(\frac{3rp}{|\mathcal{R}_n|}\right)^r \leq \left(\frac{|\mathcal{R}_n|^r - (|\mathcal{R}_n| - 2|X_n|f - r)^r}{|\mathcal{R}_n|^r}\right)\frac{(3rp)^r}{r!}.$$

Thus,

$$P^{(r)} \leq \left(1 - \left(1 - \frac{2|X_n|f}{|\mathcal{R}_n|} - \frac{r}{|\mathcal{R}_n|}\right)^r\right)\frac{(3rp)^r}{r!} \leq \left(\frac{2|X_n|fr}{|\mathcal{R}_n|} + \frac{r^2}{|\mathcal{R}_n|}\right)\frac{(3rp)^r}{r!}. \tag{3}$$

Now, if $p < (1/3)e^{-1}$, the series $\sum_{r\geq 1}(r^t(3rp)^r/r!)$ converges (for $t = 1, 2$) and the result now follows from (1)–(3) and the bound $P_\infty \leq \lim_{n\to\infty}\sum_{r\geq 1} P_n^r$ from the Bonferroni inequality. ∎

The question of determining $P_\infty$ under Lifson's interpretation for $p$ in the range $(1/3)e^{-1} \leq p \leq 1$ appears more difficult, however, I conjecture that $P_\infty = 0$ in this case also, and make a further conjecture (whose truth would improve Theorem 1): for some *sub*-quadratic function $f$, the model in which each polymer catalyses on average $f(n)$ reactions in total, satisfies $P_\infty = 1$.

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