Evolutional Dynamics of Interacting Autocatalytic Replicator Systems

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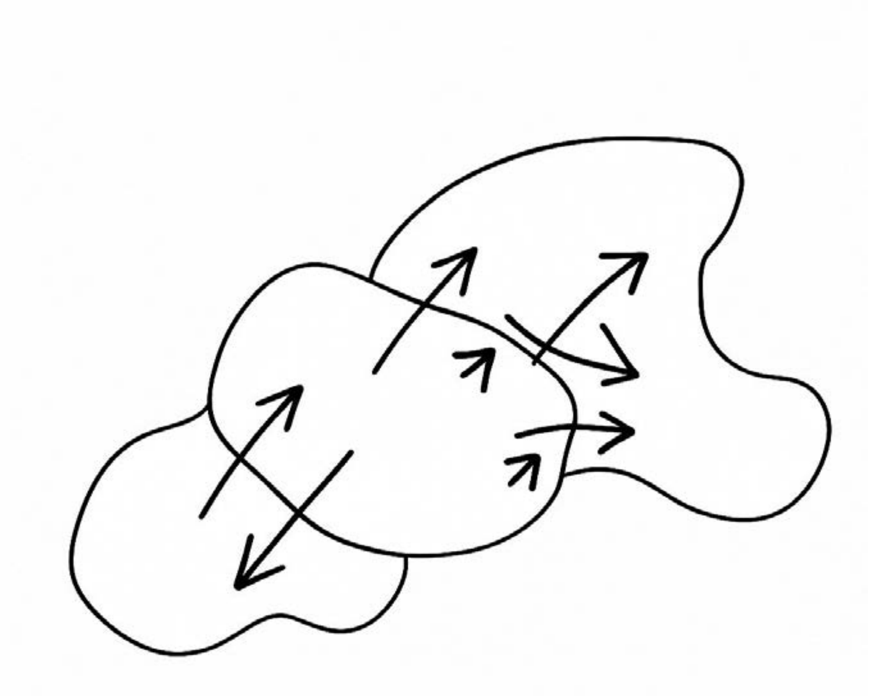
Introduction

Autocatalysis plays a pivotal role in evolutionary processes, as reactions catalyzed by their own products gain a selective advantage over those requiring external catalysts. This self-enhancing mechanism is fundamental to the emergence and sustainability of complex biochemical networks.

Building upon Turing’s seminal work on morphogenesis numerous studies have demonstrated that linear diffusion can induce significant changes in system behavior. For instance, S. Smile has been shown that two asymptotically stable four-dimensional systems, when coupled via linear diffusion, can give rise to a stable limit cycle, irrespective of initial conditions.



Paradox: If takes four asymptotically stable dynamics system connected by linear diffusion then passible obtain oscillation system in the form of limit cycle

Autocatalytic Replicator System (1/2)

Consider a system comprising n chemical or biological macromolecules M_i, $i = 1, 2, \dots, n$ with populations $N_i(t)$ as time t. The dynamics of these populations can be described by the autocatalytic equations

$$\frac{dN_i(t)}{dt} = r_i N_i^2(t), \qquad N_i(0) = N_i^0, \qquad i = 1, 2, \dots, n$$

Here r_i are quantities characterizing the rate of autocatalysis. By transitioning from absolute numbers to relative frequencies, we obtain the following equalities:

$$u_i(t) = \frac{N_i(t)}{\sum_{k=1}^{n} N_k(t)}, \qquad \sum_{i=1}^{n} u_i(t) = 1$$

Autocatalytic Replicator System (2/2)

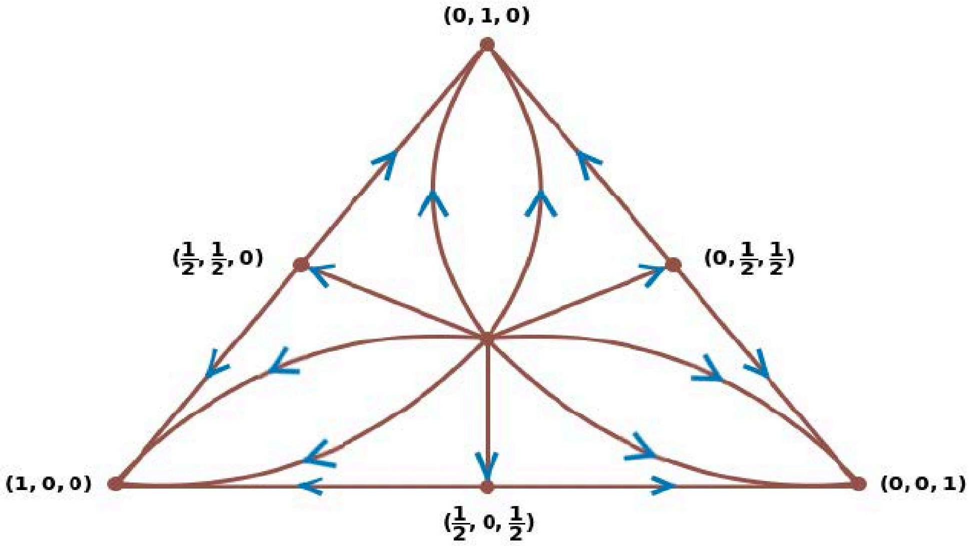
Then we obtain replicator system:

$$\frac{du_i}{dt} = u_i(r_i u_i - f(u)), \qquad f(u) = \sum_{k=1}^{n} r_k u_k^2 ,$$
$$u_i(0) = u_i^0 \geq 0, \qquad i = 1, 2, \dots, n$$

The solution is considered on the simplex S_n:

$$S_n = \left\{ \boldsymbol{u} \in \mathbb{R}^n, \boldsymbol{u} \geq 0, \sum_{i=1}^{n} u_i = 1 \right\}$$

The dynamics of system have been extensively analyzed in previous studies. The phase portraits of this system depict trajectories originating from center of the simplex S_n. These trajectories sequentially traverse the centers of lower-dimensional simplices-specifically, from S_{n-1} to S_{n-2}, and so forth-until they converge at vertex p_k of the simplex S_n



Problem Statement

Consider an autocatalytic replicator system comprising n species, where interactions occur through the exchange of various macromolecules via linear diffusion. The dynamics of the population $v_i(t)$ of species M_i are governed by equations on the simplex S_n:

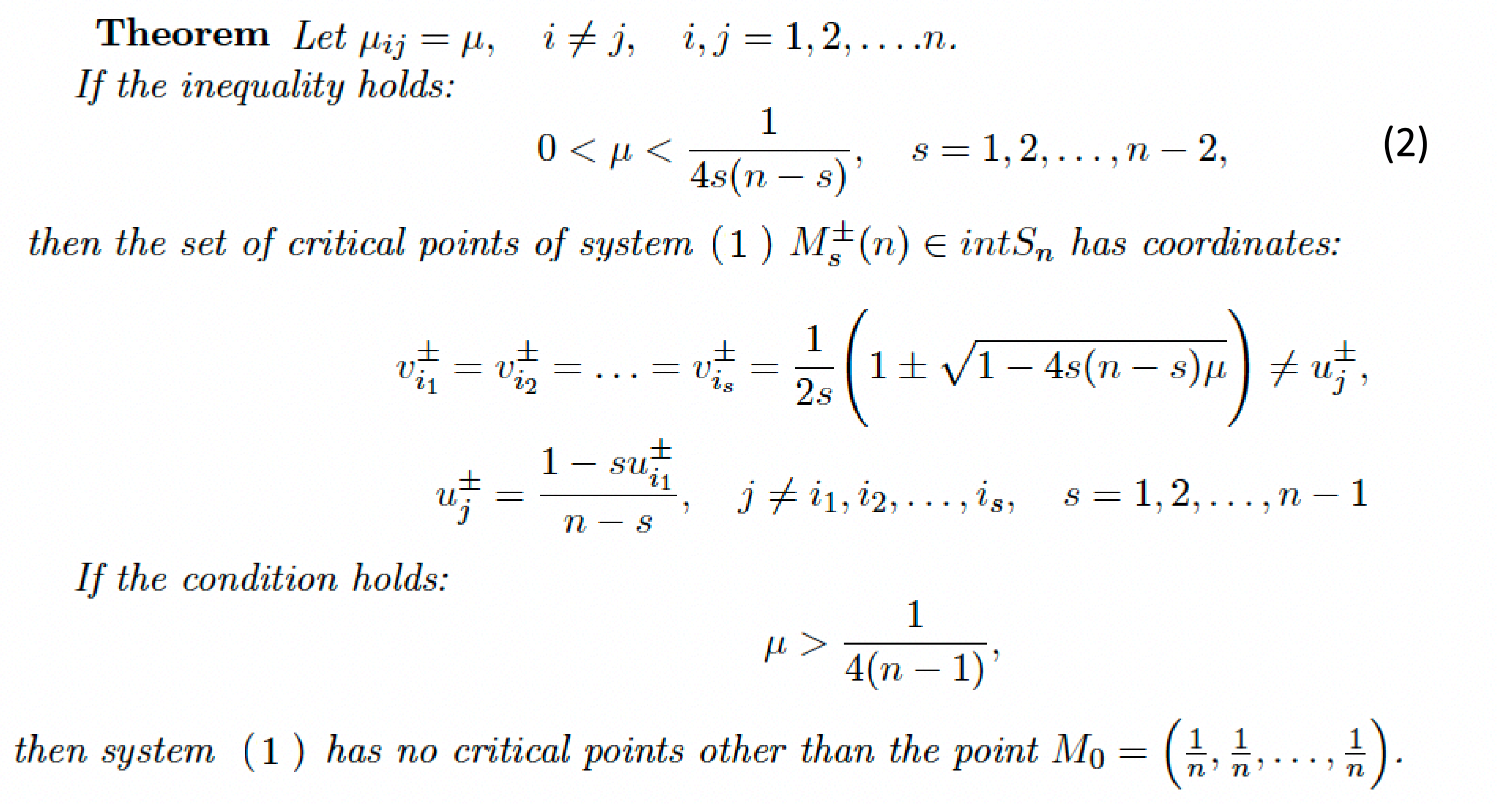
$$\frac{dv_i(t)}{dt} = v_i\left(v_i - \sum_{k=1}^{n} v_k^2\right) + \sum_{\substack{j=1,\\ j\neq i}}^{n} \mu_{ij}\left(v_j - v_i\right), \quad v_i(0) = v_i^0 \geq 0, \quad i = 1, 2, \ldots, n \tag{1}$$

$$\sum_{k=1}^{n} \sum_{\substack{j=1,\\ j\neq k}}^{n} \mu_{kj}\left(v_j - v_k\right) = 0, \quad \mu_{kj} = \mu_{jk}$$

Analysis of Equilibrium Points

First, we note that the existence, nature, and number of equilibrium points distinct from M_0 require separate investigation, even in the simplest case where $\mu_{ij} = \mu$ for all $i \neq j$, with $i, j = 1, 2, \dots, n$

We begin with the following result:



Theorem *Let* $\mu_{ij} = \mu, \quad i \neq j, \quad i, j = 1, 2, \dots . n.$

If the inequality holds:

$$0 < \mu < \frac{1}{4s(n-s)}, \quad s = 1, 2, \dots, n-2, \qquad (2)$$

then the set of critical points of system (1) $M_s^{\pm}(n) \in intS_n$ *has coordinates:*

$$v_{i_1}^{\pm} = v_{i_2}^{\pm} = \dots = v_{i_s}^{\pm} = \frac{1}{2s}\left(1 \pm \sqrt{1 - 4s(n-s)\mu}\right) \neq u_j^{\pm},$$

$$u_j^{\pm} = \frac{1 - s u_{i_1}^{\pm}}{n-s}, \quad j \neq i_1, i_2, \dots, i_s, \quad s = 1, 2, \dots, n-1$$

If the condition holds:

$$\mu > \frac{1}{4(n-1)},$$

then system (1) *has no critical points other than the point* $M_0 = \left(\frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n}\right)$.

General Case: $\mu_{ij} \neq \mu_0, i, j = 1, 2, \ldots, n$

The solvability of the nonlinear system:

$$F_i(v,\mu) = v_i\Big(v_i - f(v)\Big) + \sum_{\substack{j=1,\\ j\neq i}}^{n} \mu_{ij}\Big(v_j - v_i\Big) = 0, \quad i = 1, 2, \ldots, n$$

Is determined by the non-vanishing of the Jacobian determinant:

$$J = \frac{d(F_1, \ldots, F_n)}{d(v_1, \ldots, v_n)}, \quad \text{at } \bar{\mu}_0 = \Big(\mu_0, \ldots, \mu_0\Big) \text{ and } F_i(v, \bar{\mu}_0) = 0, \quad i = 1, 2, \ldots, n.$$

Further analysis confirms that these conditions are satisfied for all parameter regimes examined in this study.

Investigation of Symmetric Equilibrium

Theorem :*Let the condition hold:*

$$\mu > \frac{1}{n^2}.$$

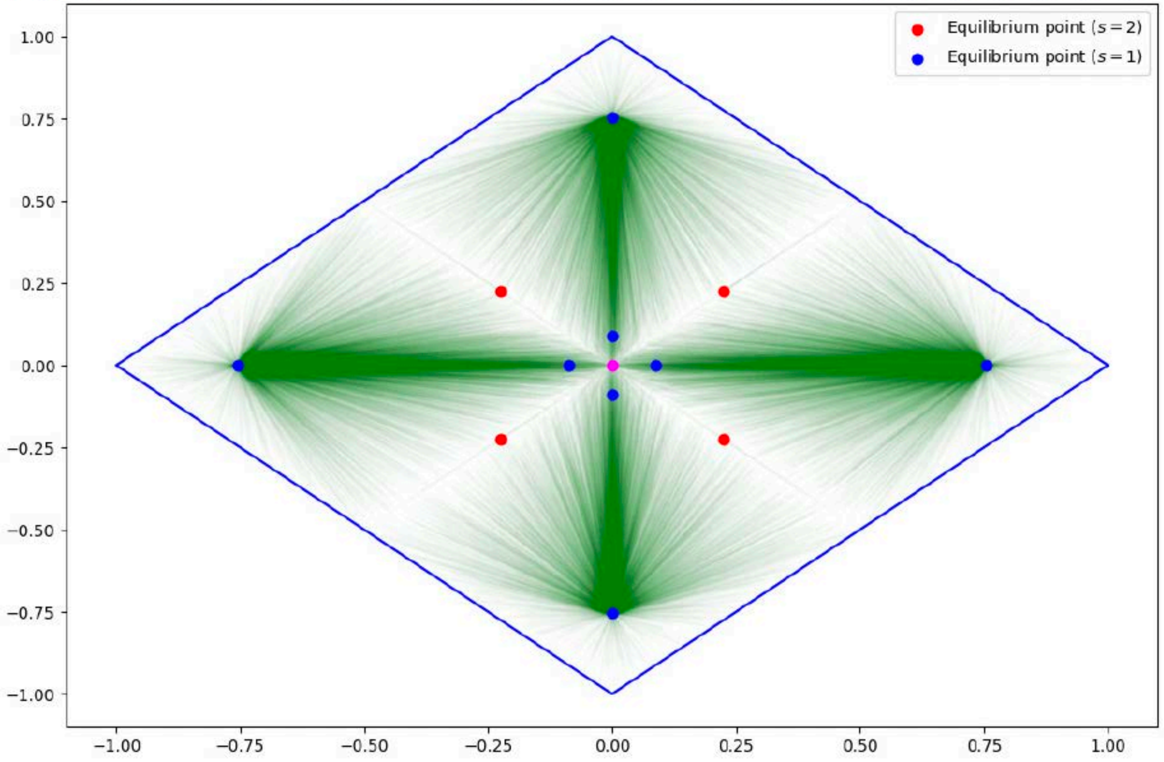
Then the equilibrium point $M_0 = \left(\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n}\right)$ *is an asymptotically stable node.*

Results of Numerical Modeling 1

Let $n = 4$, $\mu = 0.05$. In this case, inequality (2) holds for both $s = 1$ and $s = 2$.

If $s = 1$, then the four critical points of the set $M_1^+(4)$ have one coordinate equal to 0.8162, and the remaining coordinates equal to 0.0612. The four critical points of the set $M_1^-(4)$ have one coordinate equal to 0.1837, and the remaining coordinates equal to 0.2721.

If $s = 2$, then the critical points of the sets $M_2^+(4)$ and $M_2^-(4)$ coincide and have two coordinates equal to 0.3618, and the remaining coordinates equal to 0.1381.

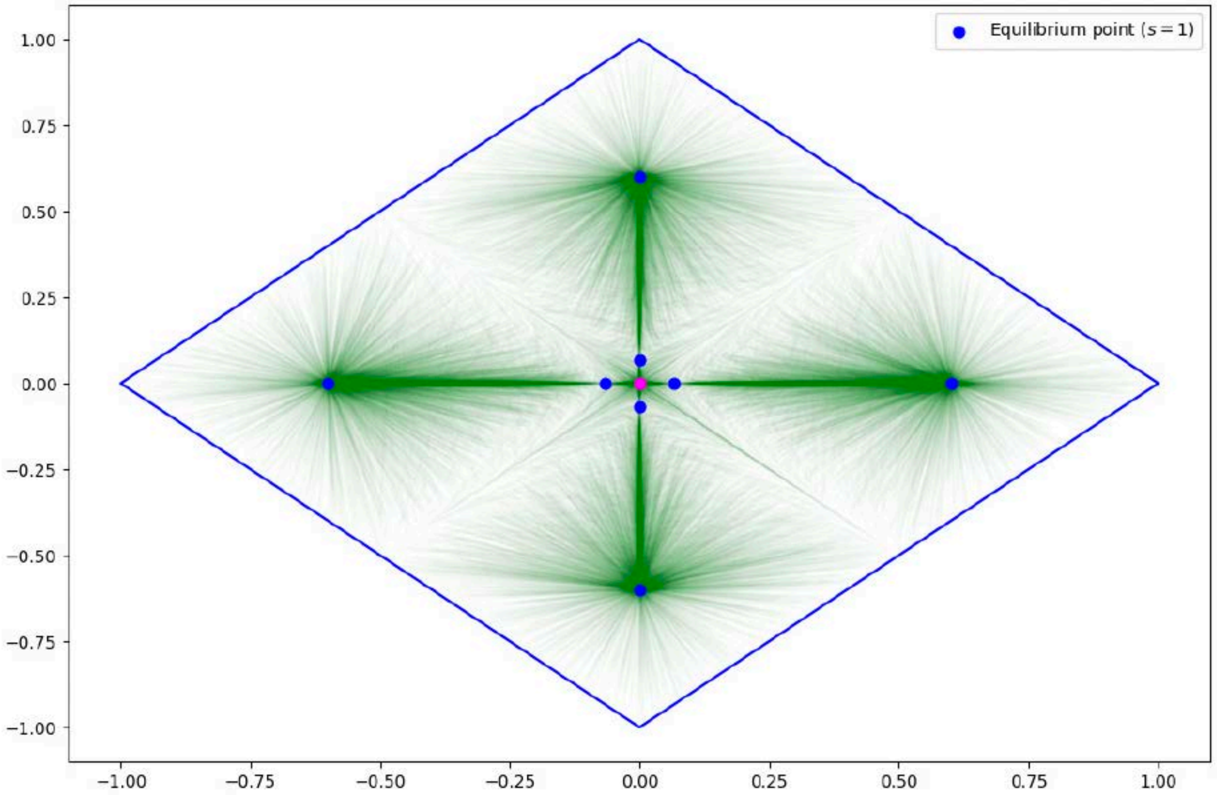


Thus, the total number of critical points (excluding the point M_0) is 12. Figure shows the phase portrait of the system. The phase trajectories from the unstable nodeat point M_0 spread over the simplex and, through a network of saddle points from the sets $M_1^-(4)$ and $M_2^\pm(4)$, concentrate depending on the initial data at the points of the set $M_1^+(4)$.

Results of Numerical Modeling 2

Let $n = 4$ with $\mu = 0.07$. In this case, the value of μ lies between $\dfrac{1}{16}$ and $\dfrac{1}{12}$. Therefore, the equilibrium point M_0 is stable. Inequality (2) holds only for $s = 1$.

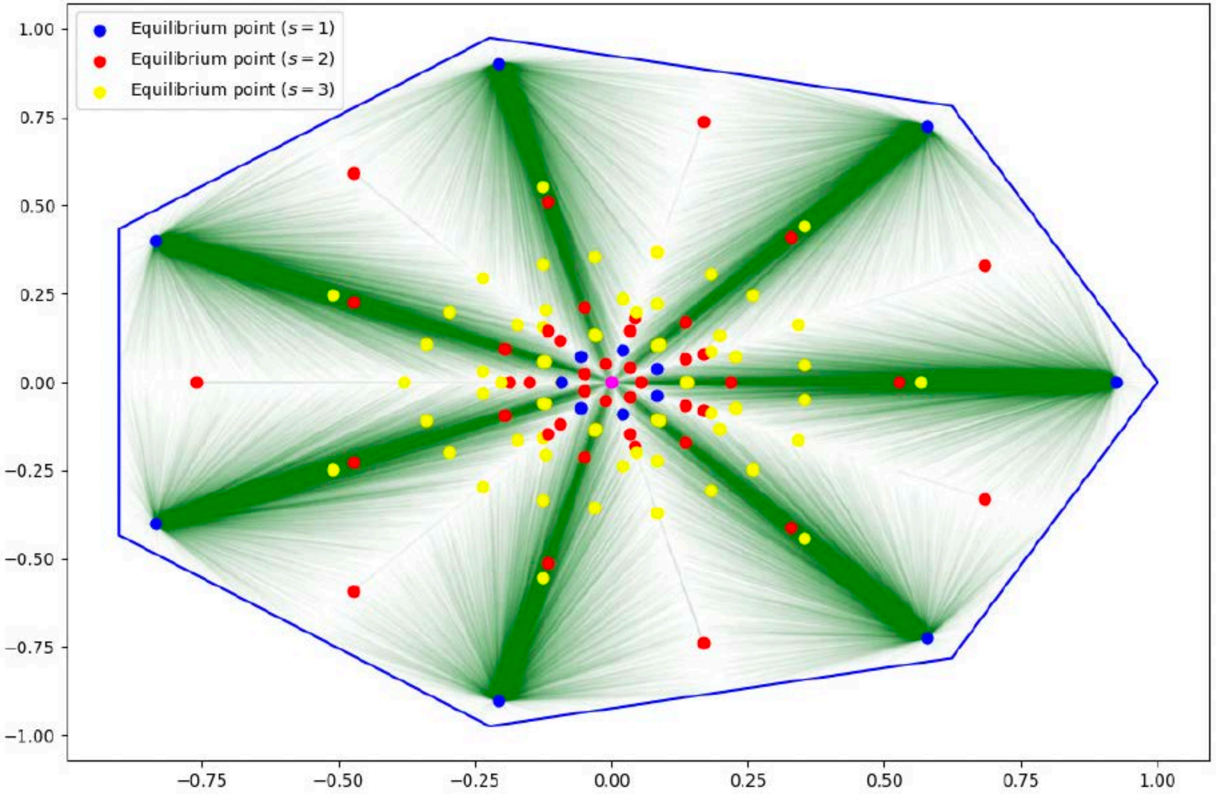
The set $M_1^+(4)$ consists of four points with one coordinate equal to 0.7, and the remaining coordinates equal to 0.1, while the set $M_1^-(4)$ consists of four points with one coordinate equal to 0.3, and the remaining coordinates equal to 0.2333. The total number of critical points in this case (excluding the point M_0) is 8.



Results of Numerical Modeling 3

Let $n = 7$ with $\mu = 0.01$. In this case, inequality (2) holds for $s = 1, 2, 3, 4$. The total number of critical points is 56 (excluding the point M_0). Of these, only the points from the set $M_1^+(7)$ are stable.

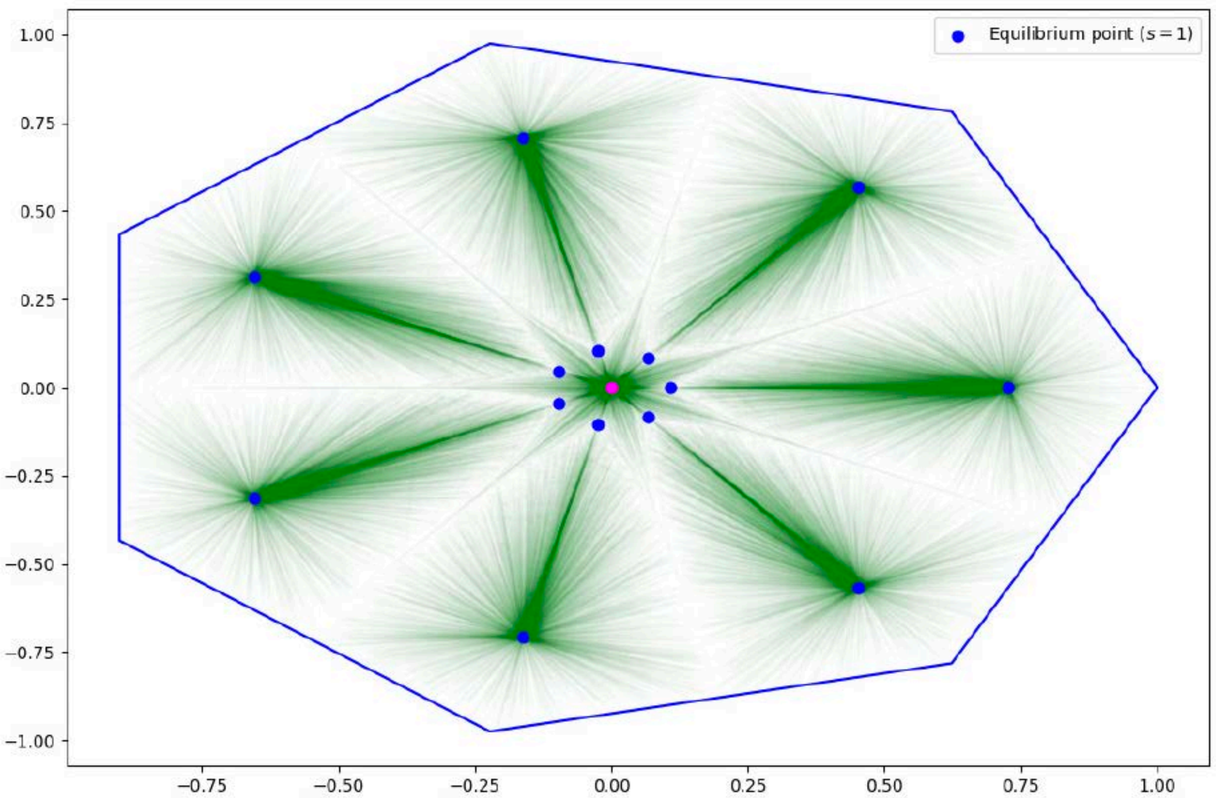
Figure shows the phase portrait of the system. As in the case of example 1 , the phase trajectories starting from the unstable node M_0, depending on the initial data, through a complex network of saddles, converge to the points from the set $M_1^+(7)$.



Results of Numerical Modeling 4

Let $n = 7$ with $\mu = 0.03$. In this case, the value of μ lies between $\frac{1}{49}$ and $\frac{1}{24}$. Therefore, the equilibrium point M_0 is a stable node. Inequality (2) holds only for $s = 1$.

As in the case of example 2 , the separatrices of the saddle points from the set $M_1^-(7)$ separate the basin of attraction of the stable node M_0 and the basins of attraction of the attractors from the set $M_1^+(7)$



Main Hypothesis

Let us now consider the obtained results in the context of the system's potential for further evolution after reaching a limiting state. When condition (3) holds, the system's trajectories converge asymptotically to the symmetric equilibrium point $M_0 = (\frac{1}{n}, \frac{1}{n}, \ldots, \frac{1}{n})$, independent if initial conditions. This scenario, characterized by uniformity, is not interest from an evolutionary perspective, as it implies a lack of diversification.

In contrast, under multistable (adaptive) dynamics, the long-term behavior of the system depends on the initial data. In this case, the limiting state comprises a set of non-degenerate, stable equilibria $M_1^+(n)$. Due to symmetry, when initial conditions are uniformly distributed over the simplex, the probability of converging to any particular point in $M_1^+(n)$ is $\frac{1}{n}$.

Assuming a sufficiently large number of independent realizations with varied initial conditions, each of the macromolecules corresponding to points in $M_1^+(n)$ can appear in the limiting states. Since these equilibria have distinct frequency distributions, the set $M_1^+(n)$ can be interpreted as a pool of potential macromolecular types capable of engaging in new interactions in subsequent replicator systems. Hence, multistability provides a foundation for the evolutionary expansion of macromolecular systems.

Testing of Main Hypothesis (1/2)

To illustrate this, let us revisit Example 4 ($n = 7, \mu = 0.03$). In this case, the seven stable nodes from the set $M_1^+(7)$ each have one coordinate equal to 0.7645 and six coordinates equal to 0.0392.

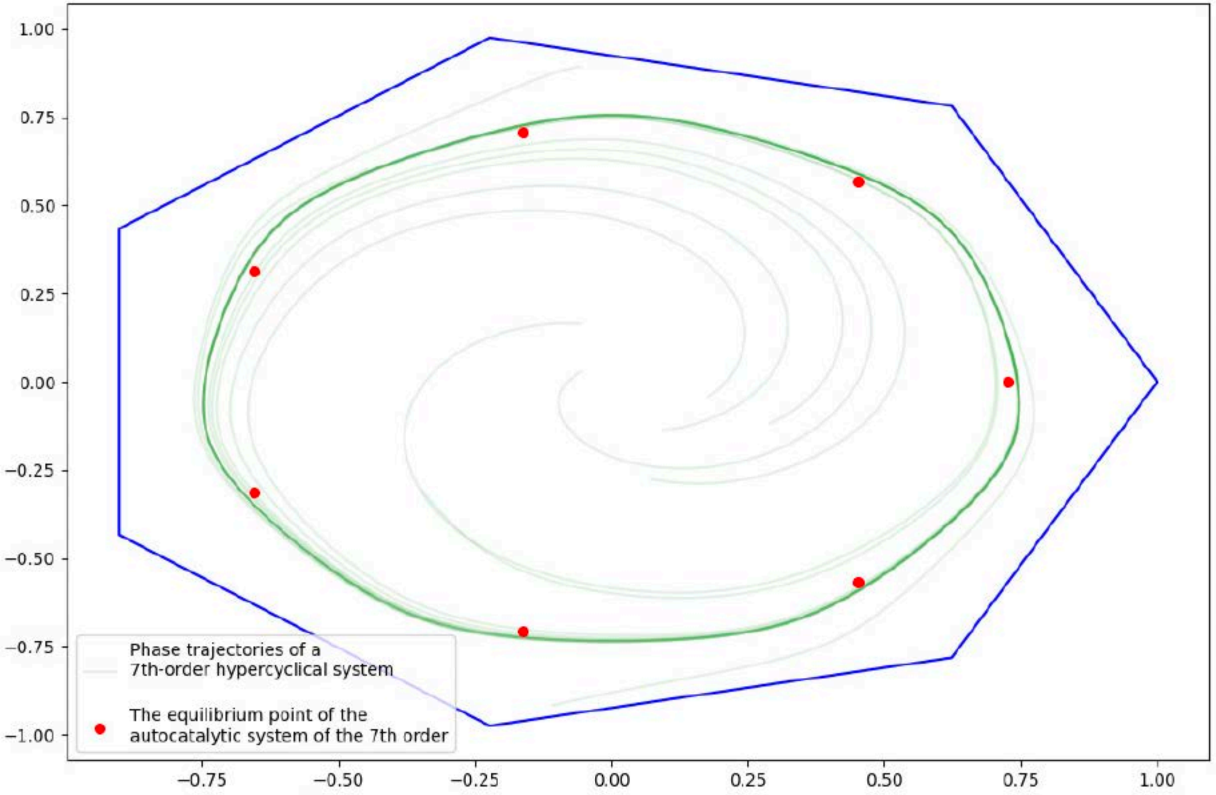
Now consider a hypercyclic replicator system of the same dimensionality, described by the following system of equations:

$$\frac{dw_i(t)}{dt} = w_i\Big(w_{i-1} - f(w)\Big) + \nu \sum_{\substack{j=1,\\ j\neq i}}^{n} \Big(w_j - w_i\Big), \quad i = 1, 2, \ldots, 7,$$

$$f(w) = \sum_{i=1}^{7} w_{i-1} w_i, \quad w_0(t) = w_7(t) \tag{4}$$

Testing of Main Hypothesis (2/2)

In contrast to the frozen limiting dynamics of autocatalysis, this hypercyclic system has a much more complex behavior, characterized by the formation of a stable limit cycle. Moreover, the hypercycle satisfies the requirements of Darwin's triad: variability, heritability, and differential fitness. Numerical implementation of the dynamics of system with $\nu = 0.0025$ shows that the points of the set $M_1^+(7)$ belong to the limit cycle of system (4).



This finding supports the hypothesis that macromolecules produced through multistable dynamics in interacting autocatalytic systems can engage in interactions within more complex replicator systems. In summary, the adaptive behavior observed in interacting autocatalytic systems can be viewed as an initial evolutionary step towards the development of more sophisticated replicator systems, such as the hypercycle.

References

- Turing A. M. “The Chemical Basis of Morphogenesis”. Phil. Trans. of the Royal Society of London Phys. 1952. Vol. 237: P., 37 - 42.
- Smale S. “A Mathematical Model of Two Cells Via Turing’s Equation”. J. Oiff. Geom. 1972. № 7: P., 193 - 210.
- Eigen M., Shuster P. “The Hypercycle. A Principle of Natural Self-Organization”. Springer, 1979.
- Arnold V. “Mathematical Methods of Classical Mechanics”. Springer-Verlag, 1989.
- Hofbauer J., Sigmund K. “Evolutionary Games and Population Dynamics”. Cambridge University Press. 2003.
- Bratus A. S., Novozhilov A. S., Platonov A. P. “Dynamical Systems and Models in Biology”. Fizmatlit, Moscow. 2010.
- Hofbauer J., Sigmund K. “The Theory of Evolution and Dynamical Systems”. Cambridge University Press. 1978.
- Bellman R. “Introduction to Matrix Analysis”. New York, McGraw-Hill. 1960.

Thank you for Attention