DYNAMICS OF TWO-GENE ANDRECUT-KAUFFMAN SYSTEM: CHAOS AND COMPLEXITY

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Abstract. Evolutionary dynamics of a two-gene model for chemical reactions, corresponding to gene expression and regulation, has been studied in detail. Bifurcation analysis has been carried out to understand behavior of steady state solutions leading to chaotic evolution for different cases. Numerical simulations have been performed and measurable quantities like Lyapunov exponents, topological entropies and correlation dimensions have been calculated for certain sets of parameter values. These measures explain complexity and chaotic nature of evolution.
Keywords: chaos, Lyapunov exponents, bifurcation, topological entropy.

1. Introduction

Mathematical equations dealing with natural and biological systems are nonlinear in nature and are mostly in complicated form. Nonlinearity can be defined by parameters involved in these systems. Behavior of such systems can be understood during evolution by varying parameters under different initial conditions. Computers have added much to the numerical study of this subject by producing many exciting and interesting results. A simple system evolves in simple ways but a complex or complicated system evolves in complicated ways and between simplicity and complexity there cannot be a common ground [1]. Complex systems have features like cascading failures, far from energetic equilibrium, often exhibit hysteresis, bistability, may be nested, network of multiplicity, emergent phenomena and some more properties. All these are related to the nonlinearity. A systematic evolutionary description and emergence of chaos can be obtained in the beginning chapters of the book edited by Hao-Bin-Lin [2]. Chaos and

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irregular phenomena may not require very complicated equations. During evolution, biological systems may display the properties like complexity and chaos. Complexity can be viewed via its systematic nonlinear properties and it is due to the interaction among multiple agents within the system [3, 4]. Chaotic systems display varied forms of attractors, depending on different sets of parameter values. Complexity and chaos observed in a system can be well understood by measuring elements like Lyapunov exponents (LCEs), topological entropies, correlation dimension etc. Topological entropy, a non-negative number, provides a perfect way to measure complexity of a dynamical system. For a system, more topological entropy signifies more complexity. Actually, it measures the exponential growth rate of the number of distinguishable orbits as time advances [5, 6, 7]. Since complexity and chaos appear mostly in nonlinear systems, it is necessary to find certain measure of the quantities causing these. Positive measure of LCEs signifies presence of chaos [8, 9, 10, 11]. Measure of topological entropy signifies the complexity [5, 11, 12, 13], and the correlation dimension provides the dimensionality of the attractor of the system [14, 16].

While dealing with natural systems, principles of nonlinear dynamics have been extensively used in diverse areas of sciences. In biochemical context nonlinear equations are obtained from chemical reactions appearing in a two-gene model [6, 15]. Here, chemical reactions are assumed to correspond to gene expression and regulation.

The studies performed in the present article deal with a two-gene Andrecut-Kauffman model [6]. In this two-dimensional discrete system, dynamical variables describe the evolution of the concentration levels of transcription factor proteins. To study the characteristics of complex nature of evolutionary phenomena, bifurcation diagrams have been drawn by varying a certain parameter. Then, some numerical investigations are carried forward to obtain LCEs, topological entropies and correlation dimensions for different sets of parameters of the system. Results obtained are shown through graphics. Finally, the complex nature of evolutions has been discussed on the basis of results obtained through this study.

2. Two-gene Andrecut-Kauffman system

In the present study, we consider a two-dimensional map proposed by Andrecut and Kauffmann [6, 7]. The map was used to investigate the dynamics of two-gene models for chemical reactions corresponding to gene expression and regulation. The discrete dynamical variables, denoted by x_n and y_n, describe the evolutions of the concentration levels of transcription factor proteins. The map is given by the following pair of difference equations:

$$\begin{aligned} x_{n+1} &= \frac{a}{1+(1-b)x_n^t+by_n^t}+cx_n, \\ y_{n+1} &= \frac{a}{1+(1-b)y_n^t+bx_n^t}+dy_n, \end{aligned} \tag{1}$$

with parameters $a = 25$, $b = 0.1$, $c = d = 0.18$, and $t = 3$, one obtains four different fixed points with coordinates $(2.30409, 2.30409)$, $(-2.52688, 2.44162)$, $(2.44162, -2.52866)$, $(-2.39464, -2.39464)$, and all are unstable.

For $c \neq d$, and when $a = 25$, $b = 0.1$, $c = 0.18$, $d = 0.42$, and $t = 3$, again, four unstable fixed points exist as $(2.2832, 2.5413)$, $(-2.5458, 2.6566)$, $(2.4613, -2.7288)$, and $(-2.3744, -2.61705)$. Threrefore, for all of these cases, orbit with initial point taken nearby any of the fixed points may be unstable and may be chaotic as well.

We intend to investigate certain dynamic behavior of system (1) for cases when $c = d$ and when $c \neq d$ for evolutions showing irregularities due to presence of chaos and complexity.

3. Numerical simulations

Performing various numerical simulations, the dynamics of evolution have been investigated by obtaining bifurcation diagrams, calculating LCEs, topological entropy and correlation dimensions of the system for different cases. For the values of control parameters within the system the following ranges have been proposed: $a \in [0, 50]$, $c \in [-0.4, 0.4]$, $b = 0.1$, $d = 0.5$, $t = 3, 4, 5$.

Taking $c = d$, bifurcation diagrams are drawn along the directions x and y, by varying c for cases $t = 3, 4, 5$ and certain fixed values of other parameters as show in Fig. 1. Then, plots of attractors have been obtained for parameters $a = 25$, $b = 0.1$, $t = 3$ and (i) for regular case $c = d = 0.32$ and (ii) for chaotic case $c = d = 0.18$ and shown in Fig. 2. In each case when $t = 3, 4, 5$, bifurcations show period doubling leading to chaos and then to regularity. Also, bistability and folding nature of phenomena are appearing here.

3.1 Lyapunov Exponents and Topological Entropies

For chaotic evolution, when $a = 25$, $b = 0.1$, $t = 3$, $c = d = 0.18$, LCEs are obtained and their plots are shown in Fig. 3. Numerical investigations further proceeded for calculation of topological entropies. In Fig. 4, plots of topological entropies are presented for $t = 3, 4, 5$ and for different ranges of parameter c. Analysis of these plots, gives an impression that for the case $t = 3$, system shows enough complexity in the range $0.05 \leq c \leq 0.23$. For the case $t = 4$, the system shows high complexity in the range $0 \leq c \leq 0.22$ and in the case $t = 5$, high complexity appears in $0 \leq c \leq 0.44$.

In Fig. 6, plots of LCEs for chaotic evolution for different cases discussed above are shown in the upper row and plots of topological entropies are shown in the lower row for these cases. For all the plots, parameters $a = 25$ and $b = 0.1$ are common. Here, topological entropy plots are drawn for different ranges of parameter c.

3.2 Correlation Dimensions

Correlation dimension gives its measure of dimensionality. Chaotic evolutions in dynamical systems are characterized by a chaotic set, "strange attractor", which has fractal structure. Being one of the characteristic invariants of non-linear system dynamics, the correlation dimension actually gives a measure of complexity for the underlying attractor of the system. A statistical method can be used to determine correlation dimension. It is an efficient and practical method in comparison to other methods, like box counting etc. The procedure to obtain correlation dimension follows from some steps calculation [14, 17, 16].

Extending further the numerical study, the correlation dimensions of system (1) have been calculated for various chaotic cases discussed above. For this the method used is that of Martelli with Mathematica codes [16]. In briefly, the method can be described as follows:

Consider an orbit $O(\mathbf{x}_i) = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \ldots\}$ of a map $f : U \to U$, where U is an open bounded set in $\mathbb{R}^n$. To compute correlation dimension of $O(\mathbf{x}_i)$, for a given positive real number r, we form the correlation integral,

$$C(r) = \lim_{n\to\infty} \frac{1}{n(n-1)} \sum_{i\neq j}^{n} H(r - \|\mathbf{x}_i - \mathbf{x}_j\|) \tag{2}$$

where

$$H(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0 \end{cases}$$

is the unit-step function. The summation indicates the number of pairs of vectors closer to r when $1 \leq i, j \leq n$ and $i \neq j$. $C(r)$ measures the density of pair of distinct vectors $\mathbf{x}_i$ and $\mathbf{x}_j$ that are close to r. The correlation dimension D_c of $O(\mathbf{x}_1)$ is then defined as

$$D_c = \lim_{r\to 0} \frac{\log C(r)}{\log(r)} \tag{3}$$

To obtain D_c, $\log C(r)$ is plotted against $\log(r)$, Fig. 8, and then we find a straight line fitted to this curve. The intercept of this straight line on y-axis provides the value of the correlation dimension D_c.

Computation of correlation dimension has been carried out for all the cases described in this article for different set of values of parameters as shown in Table 1.

4. Discussion

Two-gene Andrecut-Kauffmann system represented by map (1) has been studied carefully to understand chaotic phenomena during its evolution together with complexities present in the system. Investigation is made for cases $t = 3, 4, 5$ only but one can extend it for cases $t > 6$ also. Bifurcation plots in Fig. 1 and

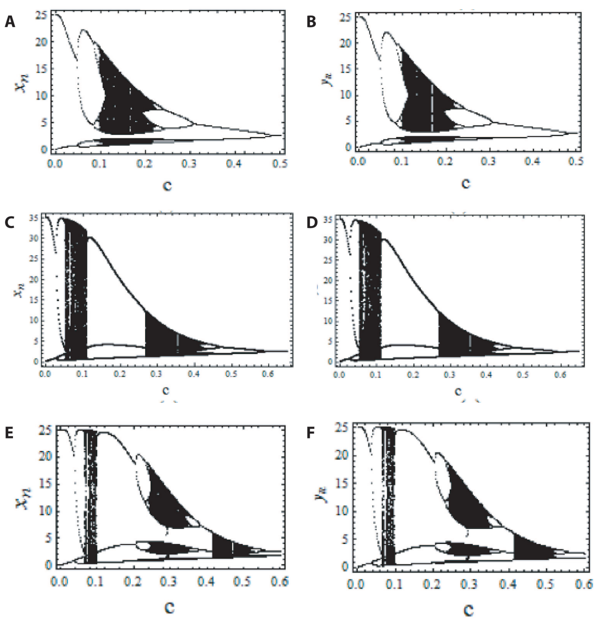
t	a	b	c	d	dimension
3	25	0.1	0.18	0.18	3.81869
4	25	0.1	0.18	0.18	3.05258
5	25	0.1	0.18	0.18	3.11754
3	25	0.1	0.28	0.12	3.16201
4	25	0.1	0.28	0.12	3.96724
5	25	0.1	0.28	0.12	4.05859
3	35	0.1	0.20	0.20	3.80410
4	35	0.1	0.20	0.20	3.41640
5	35	0.1	0.20	0.20	4.73368

Table 1: Table showing correlation dimension for different set of parameter values.

in Fig. 5, show the phenomena of period doubling and bistability in all these cases. Chaotic evolutions with periodic windows are clearly visible. Presence of complexity in the system can be observed by plots of topological entropies in Fig. 3, Fig. 4 and Fig. 6. Variations of topological entropies can be observed in 3D plots shown in Fig. 7. Numerical values of correlation dimensions, shown in Table 1, provide approximate dimensionality of chaotic attractors.

List of Figures

Figure 1: Three cases of bifurcations along x-axis (A, C, E) and y-axis (B, D, F) for map (1)



when $c = d$ are shown: (A) $t = 3, a = 25, b = 0.1$ and $0 \leq c \leq 0.5$; (B) $t = 3, a = 25, b = 0.1$ and $0 \leq c \leq 0.5$; (C) $t = 4, a = 35, b = 0.1$ and $0 \leq c \leq 0.65$; (D) $t = 4, a = 35, b = 0.1$ and $0 \leq c \leq 0.65$; (E) $t = 5, a = 25, b = 0.1$ and $0 \leq c \leq 0.5$; (F) $t = 5, a = 25, b = 0.1$ and $0 \leq c \leq 0.5$.

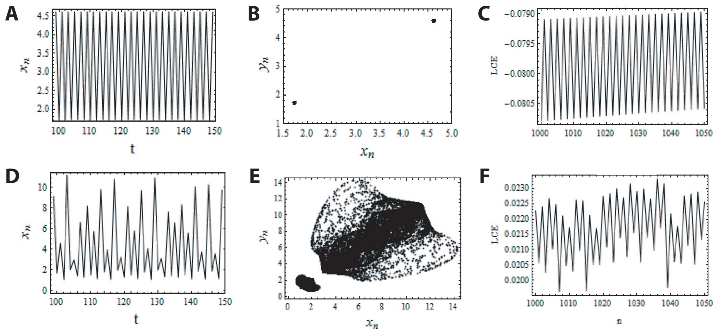


Figure 2: Time series, phase plane attractors and LCEs for regular (A, B, C) and chaotic (D, E, F) case of map (1). Parameter values are taken as: (A) time series for $a = 25, b = 0.1, t = 3, c = d = 0.32$; (B) phase plane attractors for $a = 25, b = 0.1, t = 3, c = d = 0.32$; (C) LCEs for $a = 25, b = 0.1, t = 3, c = d = 0.32$; (D) time series for $a = 25, b = 0.1, t = 3, c = d = 0.18$; (E) phase plane attractors for $a = 25, b = 0.1, t = 3, c = d = 0.18$; (F) LCEs for $a = 25, b = 0.1, t = 3, c = d = 0.18$.

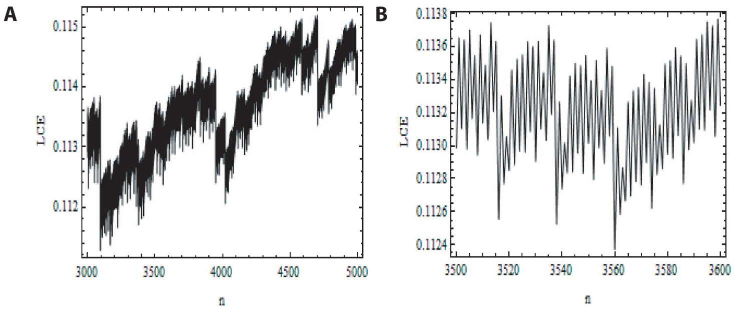


Figure 3: Plots of LCEs for chaotic evolution of map (1). Parameter values are $a = 25, b = 0.1, t = 3, c = d = 0.18$ while evolving from initial point $(2.1, 2.1)$.

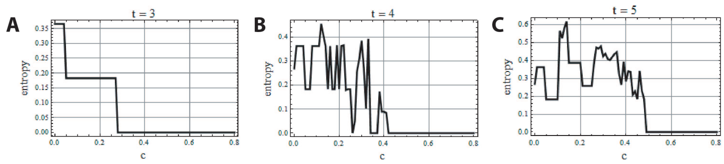


Figure 4: Plots of topological entropy for map (1) when $c = d$. The three different cases arise for the following values: (A) $t = 3, a = 25, b = 0.1$ and $0 \leq c \leq 0.5$; (B) $t = 4, a = 35, b = 0.1$ and $0 \leq c \leq 0.65$; (C) $t = 5, a = 25, b = 0.1$ and $0 \leq c \leq 0.8$.

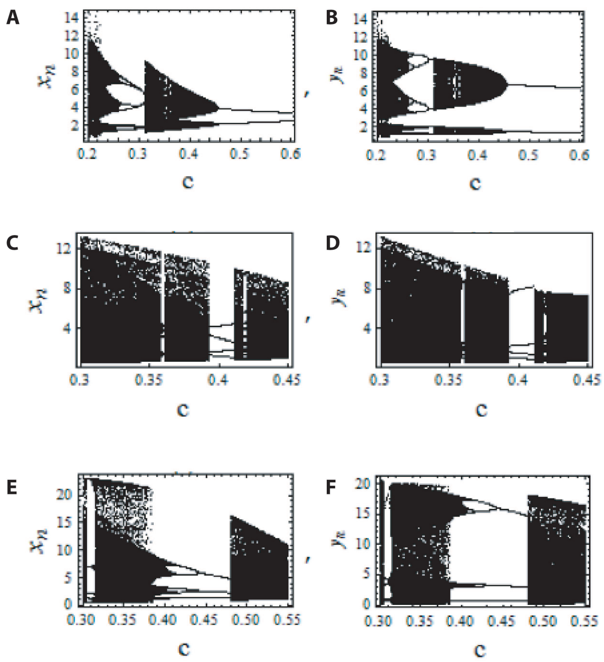


Figure 5: Bifurcation plots along x-axis (A, C, E) and y-axis (B, D, F) when $c \neq d$ for different ranges of parameter c: (A) $t = 3, a = 25, b = 0.1$ and $d = 0.2$; (B) $t = 3, a = 25, b = 0.1$ and $d = 0.2$; (C) $t = 4, a = 25, b = 0.1$ and $d = 0.3$; (D) $t = 4, a = 25, b = 0.1$ and $d = 0.3$; (E) $t = 5, a = 25, b = 0.1$ and $d = 0.2$; (F) $t = 5, a = 25, b = 0.1$ and $d = 0.2$.

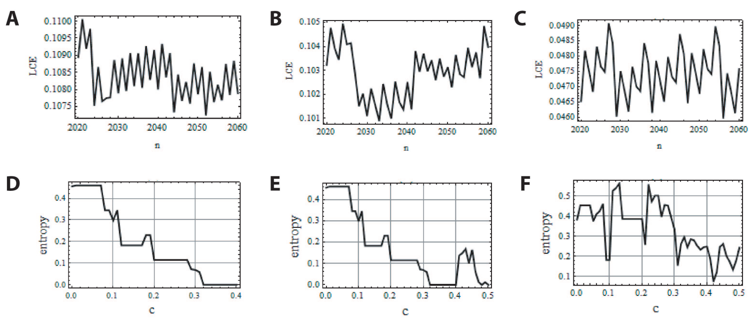


Figure 6: The plots for LCEs (A, B, C) and topological entropies (D, E, F) are shown here. Parameter values are taken as: (A) $t = 3, a = 25, b = 0.1, c = 0.2$ and $d = 0.15$; (B) $t = 4, a = 25, b = 0.1, c = 0.2$ and $d = 0.15$; (C) $t = 5, a = 25, b = 0.1, c = 0.28$ and $d = 0.12$; (D) $t = 3, a = 25, b = 0.1$ and $d = 0.15$; (E) $t = 4, a = 25, b = 0.1$ and $d = 0.15$; (F) $t = 5, a = 25, b = 0.1$ and $d = 0.15$.

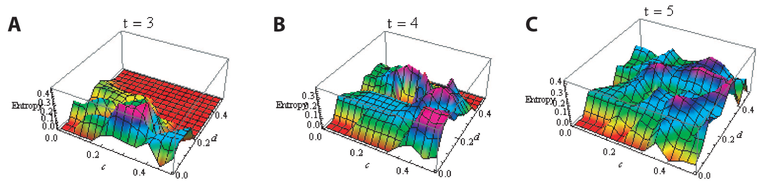
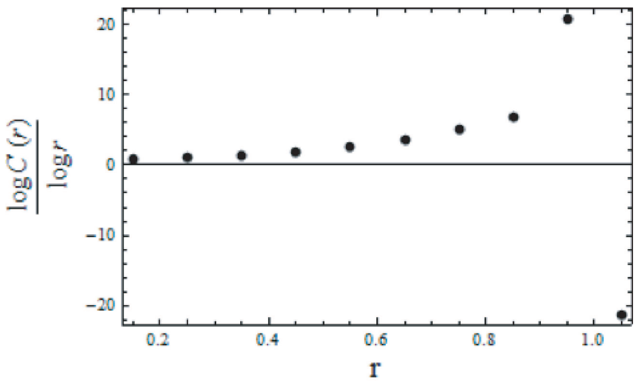


Figure 7: Three-dimensional plots for topological entropy variations. Parameter values are taken as: (A) $t = 3, a = 25, b = 0.1, 0 \leq c \leq 0.5$ and $0 \leq d \leq 0.5$; (B) $t = 4, a = 25, b = 0.1, 0 \leq c \leq 0.5$ and $0 \leq d \leq 0.5$; (C) $t = 5, a = 25, b = 0.1, 0 \leq c \leq 0.5$ and $0 \leq d \leq 0.5$. Figure 8: Plot of correlation integral curve for



the case $t = 3$. Parameter values are $a = 25, b = 0.1, c = 0.28, d = 0.12$.

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