

Changes in the Behavior of a Small Number of Molecular Systems

Yasuhiro Suzuki

Graduate School of Informatics, Nagoya University, Furocho,
Chikusa, Nagoya 464-8601, Japan

E-mail: ysuzuki@i.nagoya-u.ac.jp
<https://ysuzuki.info>

Abstract

Molecular systems in chemical reaction systems have been considered continuous systems. However, chemical reactions in living organisms involve small molecules and cannot be considered a continuous system in some cases. In this study, we examine the behaviors of the two-party Lotka-Volterra model with a small number of molecules. We then show that there are cases in which intrinsic fewness is dominant.

Keywords: systems with small number of elements, Abstract Rewriting System on Multisets

1. Introduction

Sensitivity differs from person to person. The same greeting of "Good morning" may be perceived as cheerful by some and noisy by others. There is no correct answer to sensitivity, nor can it be generalized.

We can generalize if we take the average of many people's sensitivities. Sensitivities that deviate from the average should not be ignored or directed toward sensitivities closer to the average.

A general sensitivity search system is a system in which evaluation criteria for content are modelled for each individual through instructional learning, and each user's evaluation criteria model is used for searching.

The following algorithms have been used in a sensory search; colour histogram A method to extract features of images and videos; impression analysis using the SD method A method to quantify the impression received from contents by assigning degrees to impression words, learning correspondence between impression words and contents, extracting correlation coefficients between contents, and

Extracting correlation coefficients, the distance between contents Projecting the quantified impression words and features of contents onto the feature space and measuring the distance between them.

1.1. Abstract Rewriting Systems on Multisets, ARMS

Abstract Rewriting System on Multisets, ARMS is a model of computation of chemical reactions, in which floating *molecules* can interact with each other according to given reaction rules. Technically in ARMS, a chemical solution is a finite multiset of elements denoted by symbols from a given alphabet, $A = \{a, b, \dots, j\}$; these elements correspond to *molecules*. Reaction rules that act on the molecules are specified in ARMS by reaction rules.

Let A be an *alphabet* (a finite set of abstract symbols). A *multiset* over a set of objects A is a mapping $M : A \rightarrow \mathbf{N}$, where \mathbf{N} is the set of natural numbers, $\mathbf{N}, 0, 1, 2, \dots$. The number $M(a)$, for $a \in A$, is the *multiplicity* of object a in the multiset M . We denote $A^\#$ by the set of all multisets over A , including the empty multiset, \emptyset , defined by $\emptyset(a) = 0$ for all $a \in A$.

A multiset $M : A \rightarrow N$, for $A = \{a_1, \dots, a_n\}$ is represented by the vector $w = (M(a_1) \ M(a_2) \ \dots \ M(a_n))$.

The union of two multisets $M_1, M_2 : A \rightarrow N$ is addition of vectors w_1 and w_2 that represent the each multisets respectively. If $M_1(a) \leq M_2(a)$ for all $a \in A$, then we say that multiset M_1 is included in multiset M_2 and we write $M_1 \subseteq M_2$.

A reaction rule $u \rightarrow v$, $u, v \in A^\#$ is a vector r , $r = -u + v$. Note that u and v can also be zero vector (empty). For example, the reaction $a \rightarrow b$ is the vector of $(-1 \ 1)$.

A reaction is the addition of vectors $M \in A^\#$ and $r \in R$, and it can be defined only when $r \subseteq M$. We can define a relation over $A^\#$ $a : (\rightarrow)$: for $M, M_1 \in A^\#$, $r \in R$. ARMS is a simple and conventional model of computation, but it can describe complex behaviors [3].

Because ARMS is rule based, modeling is done by creating “if-then” rules. There is no need to transform to differential equations. Less computation time. The computation in ARMS we write $M \rightarrow M_1$ if $M_1 = (M + r)$.

1.2. Lotoka-Volterra

Mathematical ecology has used the Lotka-Volterra, LV equation is the basic equation¹⁾. LV equation is a differential equations with the predator as y and the prey as x ; which is shown in the equation (1) and (2).

$$\frac{dx}{dt} = k_1x - k_2xy, \quad (1)$$

$$\frac{dy}{dt} = k_3x - k_2xy, \quad (2)$$

The equilibrium point of the LV equation can be found as the point where the derivative of x and y is zero; as shown in equation (3) and (4);

$$0 = \frac{dx}{dt} = x(k_1 - k_2y), \quad (3)$$

$$0 = \frac{dy}{dt} = y(k_3x - k_2x). \quad (4)$$

We obtain the equilibrium points,

$$(x, y) = \{(0, 0), \left(\frac{k_3}{k_2}, \frac{k_1}{k_2}\right)\}.$$

The positive and negative differential values of x or y around equilibrium points give the behavior of the LV equation.

If y is larger than k_1 / k_2 , x decreases, and if y is smaller, it increases. On the other hand, if x is larger than k_3 / k_2 , y increases, and if it is smaller, y decreases. Therefore, x and y oscillate around the equilibrium point; the solution to this equation is periodic [1] (Fig. 1).

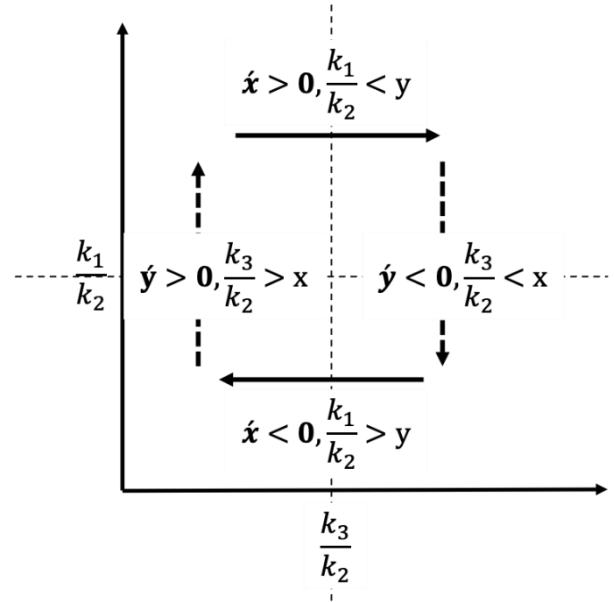


Fig.1 Behavior of LV

2. Lotoka-Volterra with small number elements

Reaction rules of Lotoka-Volterra LV is $\{x \rightarrow x, x: r_1; x, y \rightarrow y, y: r_2; y \rightarrow \text{nil}: r_3\}$, where reaction constants of each rule is k_1, k_2, k_3 and nil stands for empty set. The rules of VAS for LV are $(1, 0)$, $(-1, 1)$ and $(0, -1)$. According to chemical rate equation, probability of applying each rule is xk_1/R , k_2xy/R and yk_3/R , where $R = xk_1 + xyk_2 + yk_3$.

In case $x, y \gg$, the behaviors of LV with VAS is equal to the differential equations in the section 1.2. However, $x, y \ll$, the system shows different behaviors. For such a case, stochastic ARMS is suitable for examining.

In LV with stochastic ARMS, when the initial point (x, y) is large, the behavior is almost same as the differential equations (Fig.2 (Top)). While, initial point is small, the behavior is different (Fig.2 (Below)).

This instability caused by the initial point has pointed out by using stochastic model (Gillespie method) or Markov process. However, the mechanism of how this instability emerges have not known well.

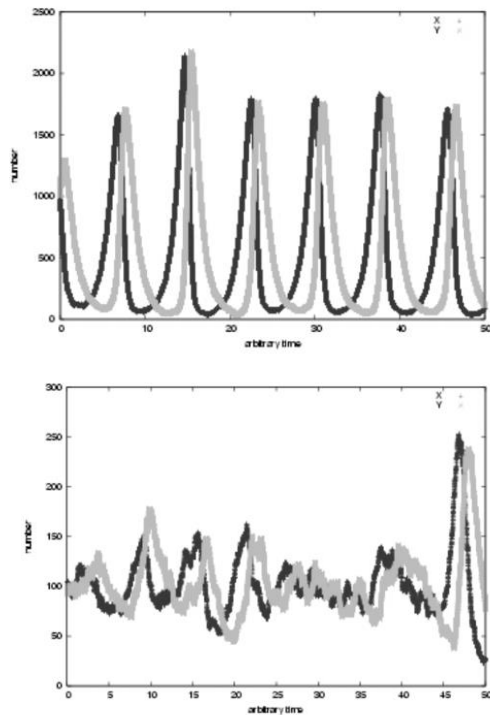


Fig. 2. Behavior of LV: (Top) x and y are large, (Below) x and y are small.

References

1. Suzuki, Y. (2010). Fluctuation Induced Structure in Chemical Reaction with Small Number of Molecules. In: Peper, F., Umeo, H., Matsui, N., Isokawa, T. (eds) Natural Computing. Proceedings in Information and Communications Technology, vol 2. Springer, Tokyo

Authors Introduction

Yasuhiro Suzuki



He is Associate professor of Graduate School of Informatics, Nagoya University
