An attempt to Analyze the Dynamics of Abstract Rewriting System on Multisets

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Abstract. Under the mass action law of chemical reactions, the calculations of Abstract Rewriting System on Multisets can be regarded as linear maps. Therefore, in order to analyze the dynamical behaviors of the system, we use the method of analyzing linear dynamical systems. We consider the brusselator model and analyze its dynamical stability.

1 Introduction

Abstract Rewriting System on Multisets (ARMS) is a class of P Systems[6]. Since in ARMS we can model a system intuitively, it has been applied in various fields, such as systems biology (modeling the signaling pathway of P53 protein in a cell[4], modeling inflammation response, etc.); bio-chemistry and the science of complexity (modeling and simulation of proto-cells which is composed of membranes, modeling proto-enzyme networks and their evolution, etc.).

ARMS is not only a model of computation based on computational algebra (rewriting systems) but also a hybrid model that connects between discrete systems and continuous systems; under the mass action law of chemistry, ARMS can be regarded as a discrete expression of the master equation, which describes chemical reactions[6]. Furthermore, if we assume the system size is large enough, we have a continuous approximation of the ARMS[6].

In this paper, we consider the ARMS under the mass action law, where calculations of ARMS can be regarded as sequences of linear maps and where, in order to analyze the system, we will use methods of linear dynamical systems[3].

2 Abstract Rewriting System on Multisets, ARMS

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, $A = \{a, b, \ldots, \}$; 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 $M : A \mapsto \mathbf{N}$, where $\mathbf{N}$ is the set of natural numbers,

N, 0, 1, 2,....The number $M(a)$, for $a \in A$, is the *multiplicity* of object a in the multiset M. We denote by $A^{\#}$ the set of all multisets over A, including the empty multiset, $\emptyset$, defined by $\emptyset(a) = 0$ for all $a \in A$. A multiset $M : A \mapsto \mathbf{N}$, for $A = \{a_1, \ldots, a_n\}$ is represented by the vector $w = (M(a_1)\ M(a_2)\ \ldots\ M(a_n))$. The union of two multisets $M_1, M_2 : A \mapsto \mathbf{N}$ is addition of vectors w_1 and w_2 that represent the each multisets respectivelly. 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 $M_1 \subseteq M_2$.

Since we consider population dynamics of molecules and a reaction rule denotes the population change in this paper, we define a *reaction rule* $u \rightarrow v, u, v \in A^{\#}$ is defined as a vector $r, r = -u + v$ (it cannot express catalytic reaction such as $A + C \rightarrow B + C$). In general, a reaction rule is defined as the pair of vectors, (u, v) (in general case see [6]).

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 over $A^{\#}$ a relation: $(\rightarrow)$: for $M, M' \in A^{\#}, r \in R$ we write $M \rightarrow M'$ iff $M' = (M + r) \geq 0$.

m times of reactions from $S_0 \in A^{\#}$ corresponds to m times of vector addition, $S_m = S_0 + a_i r_i + a_j r_j + a_k r_k + \cdots, (a_i, a_j, a_k, \cdots \in \{1, 2, 3, \cdots\}, a_i + a_j + a_k + \cdots = m, r_i, r_j, r_k, \cdots \in R) = S_0 + \sum_{i=1}^{m} r_j, m = 1, 2, 3, \cdots, r_j \in R.$

Definition (cycle) The sequence of reactions such that $S_{i+m} = S_i + \sum_{i=1}^{m} r_j, m \geq 2$ is called cycle and m is the period.

Definition (Rule Matrix) The rule matrix A is composed of the transpose of all rule vectors. For example, the rule matrix of the rule vectors of {(-1 1),(1 -1)} is

$$A = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}.$$

3 Theoretical Remark on ARMS

Remark
If the rules of R of an ARMS are linearly independent, there are no cycles in any sequence of reactions.

proof: If the rules of an ARMS $r_1, r_2, \cdots, r_n$ are linearly independent, there does not exist any sequence of reactions such that $S_{i+m} = S_i + \sum_{i=1}^{m} r_j, m \geq 2$. If such a sequence existed, it would requires $a_i r_i + a_j r_j + a_k r_k + \cdots = 0$, but since we assumed that the rule vectors are linearly independent, it is satisfied only when $a_i = a_j = a_k = \cdots = 0$.

This remark also claims that if sub sets of rule vectors are not linearly independent, there can exist cycles in the sequence of reaction. [1]

It is noted that even if a set of reaction rules are linearly independent, there can exist cycles in its subspace. The rule vector

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} \equiv \begin{pmatrix} -3 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 5 \\ 1 \\ -1 \end{pmatrix}, \tag{1}$$

are linearly independent, but since the subspace of b and c is not linearly independent, there can exist cyclic reaction sequences in the $b-c$ space so that the trajectory of reaction sequences will spiral in the $a-b-c$ space.

4 Analysis of the dynamics of Brusselator

The brusselator model is a mathematical model of an autocatalytic, oscillating chemical reaction, known as the Belousov Zhabotinsky reaction (BZ reaction)[2]. The brusselator model is given by:

$$\begin{aligned} A &\xrightarrow{k_1} X && r_1 \\ B + X &\xrightarrow{k_2} Y + D && r_2 \\ 2X + Y &\xrightarrow{k_3} 3X && r_3 \\ X &\xrightarrow{k_4} E && r_4 \end{aligned}$$

Fig. 1. Brusselator

where A and B are input and are continuously supplied to or richly exist in the system. Since we are interested in the behavior of the number of X and Y, we will use the two-dimensional rule vector $\mathbf{x}=(x\ y)$ where:

$$\boldsymbol{r}_1 = (1,0),\ \boldsymbol{r}_2 = (-1,1),\ \boldsymbol{r}_3 = (1,-1),\ \boldsymbol{r}_4 = (-1,0), \tag{2}$$

respectively. Although there are some of simulation based works on this model by using various models, basically they follow:

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{ax_n^2 y_n}{C} \begin{pmatrix} 1 \\ -1 \end{pmatrix} + \frac{bx_n}{C} \begin{pmatrix} -1 \\ 1 \end{pmatrix} + \frac{x_n}{C} \begin{pmatrix} -1 \\ 0 \end{pmatrix}.$$

where C is a constant for normalization and defined by $ax^x y_n + bx_n + x_n = C$. For simplicity, we assume that k_1 and k_4 are equal to 1, $k_2 = b$ and $k_3 = b$. The moleculaes A and B are assumed to be in large excess so that their concentrations do not change with time. Furthermore, in analyzing dynamics we ignore the constant C (we can ignore it without loss of generality).

[1] $rank(R)$ illustrates the ARMS may have cycles or not in its sequences of reactions

Equilibria

Since (1 0) + (1 1) + (-1 1) + (-1 0) = (0 0) when $ax^2y = bx = x = 1$, obviously these rule vectors are not linearly independent and there can exist cyclic reaction sequences. It is apparent that $ax^2y = bx = x = 1$ is satisfied only when $(x, y) = (1, \frac{b}{a})$, so this is the only equilibrium of the system.

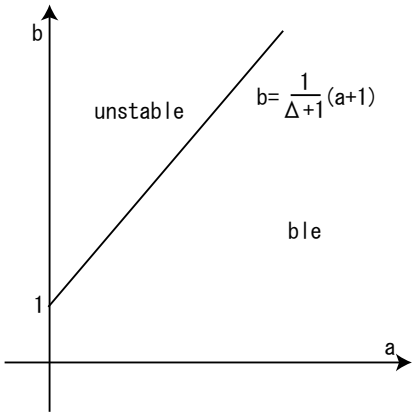

Fig. 2. When the system on macroscopic $\epsilon <<$

Stability

Since $X, Y \in A^{\#}$, by calculating partial difference we obtain the Jacobian of the system:

$$Jf(x, y) = \begin{pmatrix} -b\epsilon - \epsilon + 2axy\epsilon + ay\epsilon^2 & ax^2y \\ b\epsilon - 2ax\epsilon - ay\epsilon^2 & -ax^2\epsilon \end{pmatrix}, \tag{3}$$

where ϵ is given as;

$$\epsilon = \frac{([X] + [Y]) + \delta}{[X] + [Y]}, (0 < \delta < [X] + [Y]) \tag{4}$$

where δ denotes the change of concentration of $x \in X$ or $y \in Y$. While δ is fixed, if $[X] + [Y]$ (system size) is getting larger (macroscopic), δ is getting smaller in relation to the system size, on the other hand, if $[X] + [Y]$ is getting smaller (mesoscopic), the δ is relatively getting larger ($\epsilon > 1$). It is noted that $\epsilon \in$ the set of quotient, $\mathbf{Q}$.

Evaluated at $(x, y) = (1, \frac{b}{a})$,

$$Jf(1, \frac{b}{a}) = \begin{pmatrix} -b\epsilon + b\epsilon^2 & a\epsilon \\ -b\epsilon - b\epsilon^2 & -a\epsilon \end{pmatrix}. \tag{5}$$

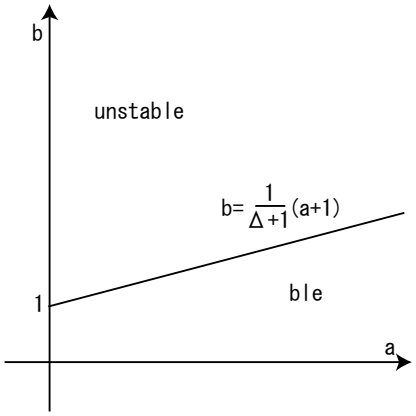

Fig. 3. When the system on mesoscopic $\epsilon >>$

Thus the trace, τ and determinant, det are

$$\tau = Trace\Big(Jf(1, \frac{b}{a})\Big) = (b - a - 1 + b\epsilon)\epsilon, \tag{6}$$

$$\det = Det\Big(Df(a, \frac{b}{a})\Big) = a\epsilon^2, \tag{7}$$

Since $a > 0, \epsilon > 0$, this implies that $(1, \frac{b}{a})$ is not a saddle point. If $b < \frac{1}{\epsilon+1}(a+1)$, then $\tau < 0$ and the equilibrium is an attractor, while if $b > \frac{1}{\epsilon+1}(a+1)$, it is a repellor. This shows that when a system is macroscopic, its stability is close to the model of differentional equations, while when the system is mesoscopic, $\frac{1}{\epsilon+1}(a+1), \epsilon >>$ is getting smaller and the unstable region is expanding. Thus, the behavior of a system on a mesoscopic scale is likely to be destabilized by fluctuations.

5 Conclusion

On the simulation of the brusselator model, especially, on a mesoscopic scale, Vladimir[7], using the Monte-Carlo simulation on two-dimensional lattice, reported that decreasing the system size down to mesoscopic may result in the periodic kinetic oscillations becoming aperiodic and disappearing. We have also found this behavior throughout simulations by using ARMS [5]. We believe that it is the descritization that makes the system unstable. However, its physical significance is still open to discussion.

Since under the mass action law ARMS can be regarded as a linear map, we attempted to use methods of analyzing linear dynamical systems in our investigation of the stability of the system. It is a challenge to apply this method to P Systems or the reaction map systems[1] will be the subject of our future study.

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