Revisiting persistence of Chemical Reaction Network through Lyapunov PDE

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Abstract

This paper focuses on the chemical reaction network with a mass action kinetics. We reveal the close connection between persistence and Lyapunov function partial differential equation in [19]. Persistence is a long-term property that concerns the dynamics nearing the boundary points. Based on the form of boundary conditions of PDE, we determine the derivative of PDE’s solution of some special classes boundary points. Using this and analogizing Lyapunov Global Asymptotic Stability we derive some sufficient conditions on the non \(\omega\)-limit point for any mass action system not just weakly reversible network. And further using our conditions in a complex balanced network and a 1d \(W_I\)-endotactic network we revisit that the boundary non-equilibrium in complex balanced cannot be an \(\omega\)-limit point and obtain that 1d \(W_I\)-endotactic networks with mass action kinetics is persistent. Because the Lyapunov PDE is obtained from thermodynamics, the sufficient conditions are exactly the link between persistence and thermodynamics.

Keywords: chemical reaction network, mass-action, persistence, Lyapunov function PDE, \(\omega\)-limit point, sufficient condition, complex balanced network, 1d \(W_I\)-endotactic network.

1. Introduction

The dynamical systems arising from biology, chemistry, and engineering are often with high complexity for its nonlinear interactions. At the same time, for most common system — mass action system, the rate constant \(k\) is difficult to determine by experiments. So based on the above...
reasons, general mathematical criteria is needed. Chemical reaction network theory (CRNT) generated 40 years ago and has a wide range of applications in modeling the interaction networks. The main concern of this theory takes advantage of the algebraic property and network structure to research the dynamical property. The seminal works of CRNT are generally conducted by Fritz Horn, Roy Jackson, and Martin Feinberg \[11,13,14,15,7,8\]. They have given the essential concepts such as linkage class, weakly reversible, complex balanced network, deficiency and proved zero deficiency theorem and one deficiency theorem which about the stability and existence of equilibrium holds regardless of the choice of a rate constant \(k\). Since then this kind of chemical reaction network with its theory has interested lots of applied mathematician. There are lots of more specific directions in CRNT: the existence and stability of equilibrium, the boundedness of the trajectory, persistence and so on. We will mainly focus on the persistence property of mass action system.

Persistence is one of the most popular properties in CRNT. It originates from population dynamics: A species is called persistent if it cannot go extinct whatever the initial number of the species. Chemist and biochemist also interest in a similar question: if initial concentration of each \(S_i\) is bigger than 0, can there exist a species that will be totally used up when \(t\) trends to infinity? Persistence is a long-term behavior of the system, so it has a close connection with \(\omega\)-limit points. A bounded trajectory of a dynamical system is said to be persistence if each boundary point \(\bar{x}\) is not an \(\omega\)-limit. The representative works on persistence is mainly rewritten by Anderson, Angli, and Craciun \[2,3,4,6,9\]. They have put forward an important definition: semilocking set or siphon (they share the same meaning essentially) and give the characteristic that \(x(t_0)\) in the boundary face \(F_W\) for some \(t_0\), then this trajectory will always stay in \(F_W\) (For any point \(\bar{x}\) in \(F_W\), there exists \(\bar{x}_i = 0, i \in W\)). They also made a great contribution to persistence conjecture which is came up by Feinberg in 1987\[13\] and global attractor conjecture came from Horn and Feinberg in 1972\[7\]. After these work, there exist lots of works concerns a kind of special networks which called endotactic networks and derive some important consequences \[9,17\], such that a strong endotactic network is persistent \[17\].

The most relevant context is Lyapunov Function Partial Differential Equations for Chemical Reaction Networks \[19\]. It is activated by the context of Anderson et.al. \[5\] which construct a Lyapunov function by modeling a chemical reaction network as a Markov chain. Zhou F. researches this problem using some microscopic concepts in \[5\] and directly regarding the ap-
proximation of the scaling non-equilibrium potential as a possible Lyapunov function. Then using Kolmogorov’s forward equation, namely, Chemical Master Equation, we derive a PDE whose solution can be a Lyapunov function candidate. They also give some properties like dissipative of this solution. They further solve some special network: 1-d network, complex balanced network and some specific networks.

Our paper mainly focuses on the mass action system. And the main purpose of this context is to find the relationship between the Lyapunov PDE which is derived from thermodynamics and persistence or more exactly, \( \omega \)-limit point. Let \( \bar{x} \) be a boundary point, basing on the Lyapunov partial differential equation and the boundary conditions, we mainly do the three things:

- It is interesting that the solution of PDE \( f \) has a close connection with the semilocking set.
- Giving three sufficient conditions on non \( \omega \)-limit point and further analyzing the value of \( \lim_{x \to \bar{x}} f(x) \) we obtain another two implied sufficient conditions.
- Taking advantage of the sufficient condition and the solution of the PDE we can prove persistent properties of 1-d \( W_I \)-endotactic network and the non-equilibrium boundary points of complex balanced networks cannot be \( \omega \)-limit points.

Through our work, we have surprisingly found that the solution \( f \) of PDE and its boundary condition that we have obtained in [19] can not only judge the stability but also have a place in persistence. At least, we find it reflects the existence of boundary \( \omega \)-limit points directly. And the same time, the value of \( \lim_{x \to \bar{x}} f(x) \) is decided if \( W \) is not a semilocking set. As we all know, semilocking set and \( \omega \)-limit are the concepts which have a tight connection with persistence. And because the PDE with its boundary is established on thermodynamics. Our context contributes to finding some connection between thermodynamics and persistence.

We will organize our paper in the following form. [2] will help us know some fundamental concepts about CRNs and its dynamics. [3] tells some definitions and related results of persistence. At the same time, we also recall the modality of the Lyapunov PDE and its boundary conditions and essential property of its solution. [4] devotes to finding the value of \( f(x) \) when \( x \in (\bar{x} + \mathcal{S}) \cap \mathbb{R}_+^n \) trends to \( \bar{x} \) depending on the \( W \) and giving some sufficient conditions on the non \( \omega \)-limit. [5] contributes to applying the results in [4] to obtain some properties of 1d \( w_I \)-endotactic networks and prove that 1d \( w_I \)-endotactic network is persistent. And revisit that all the non-equilibrium boundary points in complex balanced networks can not be an \( \omega \)-limit point.
Some representative examples and conclusions are summarized in [6].

Mathematical Notation:

\( \mathbb{R}^n, \mathbb{R}_{\geq 0}^n, \mathbb{R}_>^n \): \( n \)-dimensional real space, non-negative and positive real space, respectively.

\( x^v : x^v = \prod_{j=1}^{d} x_j^{v_j} \), where \( x, v_i \in \mathbb{R}^d \) and \( 0^0 \) is defined to be 1.

\( \ln(x) : \ln(x) = (\ln x_1, \ln x_2, \cdots, \ln x_d)^T \), where \( x \in \mathbb{R}^d_{>0} \).

\( \mathcal{G}^i \): The function set whose elements are \( i \)-th continuous differentiable.

\( \text{supp} \ c : \text{supp} \ c = \{ S_j \in S | c_i \neq 0 \} \), \( \forall c \in \mathbb{R}^n_{\geq 0} \).

\( 0_n \): each element of this \( n \)-dimensional vector is zero.

2. Preliminaries on chemical reaction network

In this section, some fundamental concepts about CRN [7][15] are reviewed.

**Definition 2.1 (Chemical Reaction Network).** A chemical reaction network is composed of three finite sets:

1. a set of species \( S = \bigcup_{j=1}^{n} \{ S_j \} \).
2. a set of complexes \( C = \bigcup_{i=1}^{c} \{ v_i, v'_i \} \) satisfying \( \text{Card}(C) = c \) and
   \[ \bigcup_{i=1,\ldots,c} \{ \text{supp} \ v_i \cup \text{supp} \ v'_i \} = S, \]
   where \( v_i, v'_i \in \mathbb{Z}_{\geq 0}^S \) with the \( j \)-th entry of \( v_i \) to express the stoichiometric coefficient of species \( S_j \) in \( v_i \).
3. a relation set \( \mathcal{R} \subset C \times C \) having the properties that (a) \( v_i \rightarrow v_i \notin \mathcal{R} \forall v_i \in C \); (b) \( \forall v_i \in C, \exists v'_i \in C \) either \( v_i \rightarrow v'_i \in \mathcal{R} \) or \( v'_i \rightarrow v_i \in \mathcal{R} \).

The triple \((S, C, \mathcal{R})\) is usually used to represent a CRN.
Each relation $v_i \rightarrow v'_i$ in the network is called a reaction with $v_i$ termed reactant complex while $v'_i$ termed resultant complex, which is equivalent to

$$\sum_{j=1}^{n} v_{ji} S_j \rightarrow \sum_{j=1}^{n} v'_{ji} S_j.$$ 

A CRN can be also viewed as a directed graph with vertices to represent complexes while directed edges to correspond to reactions. A connected component of the graph is called a linkage class.

**Definition 2.2 (Reversible and Weakly Reversible CRN).** A CRN $(S, C, R)$ is called

- **reversible** if $v_i \rightarrow v'_i \in R$ whenever $v'_i \rightarrow v_i \in R$.

- **weakly reversible** if for any reaction $v_i \rightarrow v'_i \in R$ there exists a series of reactions starting from $v'_i$ and ending with $v_i$, i.e., $v'_i \rightarrow v_{i_1} \in R, \ldots, v_{i_m} \rightarrow v_i \in R$, $m < r$.

A reversible CRN must be weakly reversible CRN, but not vice versa.

**Definition 2.3 (Dimension of Network).** For a CRN $(S, C, R)$, $v'_i - v_i$ is called the reaction vector of the $i$th ($i = 1, \cdots, r$) reaction $v_i \rightarrow v'_i$. The rank of the set of reaction vectors is the dimension of this network, denoted by $s$, i.e., $\text{rank}(v'_1 - v_1, \cdots, v'_r - v_r) = s$.

**Definition 2.4 (Stoichiometric Compatibility Class).** For a CRN $(S, C, R)$, the linear space spanned by all reaction vectors is named as the stoichiometric subspace, denoted by $\mathcal{S} = \text{span}\{v'_1 - v_1, \cdots, v'_r - v_r\}$. Let $x_0 \in \mathbb{R}^S_{\geq 0}$, the sets $\mathcal{S}(x_0) \triangleq \{x_0 + \xi \in \mathcal{S}\}$, $\mathcal{S}(x_0) \cap \mathbb{R}^S_{\geq 0}$ and $\mathcal{S}(x_0) \cap \mathbb{R}^S_{> 0}$ are called the stoichiometric compatibility class, non-negative stoichiometric compatibility class and positive stoichiometric compatibility class of $x_0$, respectively.

The reaction vectors define a stoichiometric matrix $S = (v'_1 - v_1, \cdots, v'_r - v_r) \in \mathbb{Z}^{s \times r}$. Clearly, $\dim \mathcal{S} = \dim(\text{Im } S) = s$. Geometrically, a CRN may be represented through the Cartesian coordinate system, where a complex is projected to a vector.

**Example 1.** Consider the following network with two species and four reactions

$$S_1 \rightleftharpoons S_2,$$

$$S_1 + S_2 \rightarrow 2S_2 \rightarrow 2S_1.$$
It is easy to write
\[ S = \{S_1, S_2\}, \quad C = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix}, \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix} \right\}, \]
\[ R = \left\{ \begin{bmatrix} 0 \\ 1 \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix} \rightarrow \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 2 \end{bmatrix} \rightarrow \begin{bmatrix} 2 \\ 0 \end{bmatrix} \right\}, \]
\[ \mathcal{S} = \text{span}((-1, 1)^T) \quad \text{and} \quad \dim \mathcal{S} = 1. \] Therefore, the network is a 1d (1-dimensional) CRN and contains two linkage classes. The geometric representation of this network is shown in [7]. Clearly, the stoichiometric subspace is a straight line and all reaction vectors are parallel to this line.

Utilizing the geometric property of CRNs, Craciun et al. [9] defined the concept of endotactic CRN, which serves closely for the purpose of addressing the persistence issue. They also stated that the class of endotactic networks is larger than the well-known class of weakly reversible networks. Instead, Gopalkrishnan et al. [17] redefined this concept using algebraic language and further proposed the notion of strongly endotactic CRN. Their redefinition begins with defining a partial order relation in \( \mathbb{R}^S \).

**Definition 2.5 (\( \preceq_w \)-Preorder [17]).** Let \( w \) be a vector in \( \mathbb{R}^S \). The \( \preceq_w \)-Preorder on \( \mathbb{R}^n \), denoted by \( \preceq_w \), is defined by
\[ y_1 \preceq_w y_2 \iff \langle w, y_1 \rangle \leq \langle w, y_2 \rangle, \]
where \( y_1, y_2 \in \mathbb{R}^S \), and \( \langle \cdot, \cdot \rangle \) represents standard inner product. We write \( y_1 \prec_w y_2 \) if \( \langle w, y_1 \rangle < \langle w, y_2 \rangle \).

**Definition 2.6 (\( \preceq_w \)-maximal and \( \preceq_w \)-minimal Elements [17]).** Let \( w \in \mathbb{R}^S \) and \( Y \subset \mathbb{R}^S \). The element \( y_r \in Y \) is said to be a \( \preceq_w \)-maximal element in \( Y \) if
\[ \langle w, y_r \rangle \geq \langle w, y \rangle, \quad \forall \ y \in Y. \]
The element \( y_l \in Y \) is called a \( \preceq_w \)-minimal element in \( Y \) if
\[ \langle w, y_l \rangle \leq \langle w, y \rangle, \quad \forall \ y \in Y. \]

When applying this definition to a CRN \( (S, C, \mathcal{R}) \), a complex is called leftmost relative to \( w \) if it is \( \preceq_w \)-minimal in \( C \), and rightmost relative to \( w \) if it is \( \preceq_w \)-maximal in \( C \). We then give the
Figure 1: The left graph shows the complexes, reactions and the reactant complexes polytope of the network in the phase space. The second figure is the first network in projecting into the $L$.

definition of endotactic CRN in 1D case, where 1D means that the network is a 1d CRN with single linkage class or empty set. Geometrically, all complexes in a 1D network belong to the same line [9].

**Definition 2.7 (1D Endotactic Network [9,17]).** A 1D network $(S,C,R)$ is endotactic if

1. it contains empty complex;

or

2. it contains at least two reactant complexes. Moreover, each reaction with a leftmost reactant pointing to the right while each reaction with a rightmost reactant pointing to the left. Here, the preorder $\preceq_w$ in $\mathbb{R}^S$ is defined by a basis $w \in \mathbb{R}^S_{\neq 0}$ of the stoichiometric subspace $\mathcal{S}$ of the network.

**Example 2.** The sub-network of

$$S_1 + S_2 \rightarrow 2S_2 \rightarrow 2S_1$$

is a 1D endotactic CRN since the two extreme source complexes (leftmost or rightmost reactant), $S_1 + S_2$ and $2S_2$, both react towards direction of the other source complex, as can be seen in [7]

**Definition 2.8 (Endotactic CRN [9,17]).** A CRN $(S,C,R)$ is

1. $w$-endotactic with respect to a certain $w \in \mathbb{R}^S$ if for any reactant $v_i$ that is $\preceq_w$-maximal among all reactants such that the reaction vectors are not orthogonal to $w$, we have

$$\langle w, v'_i - v_i \rangle < 0.$$
(2) an endotactic network if it is w-endotactic with respect to any \( w \in \mathbb{R}^S \).

(3) strongly endotactic if it is endotactic and for each \( w \) not orthogonal to its stoichiometric subspace \( S \), there exists a reaction \( v_i \rightarrow v_i' \) such that:

- \( \langle w, v_i' - v_i \rangle < 0 \) and
- \( v_i \) is \( \leq w \)-maximal among all reactants.

It is clear that among the above three kinds of networks, the set of \( w \)-endotactic networks is largest, and the set of strongly endotactic networks is smallest. Geometrically, a network is \( w \)-endotactic if the projection of this network to the line which \( w \) belongs to is endotactic, and a network is endotactic if its projection on any line is endotactic [9]. The strongly endotactic network means that there exists a nontrivial reaction for both leftmost and rightmost reactants in the projection of the original network to any line not orthogonal to its stoichiometric subspace [17].

**Example 3.** The following CRN

\[
S_1 \rightarrow S_2,
\]
\[
2S_2 \rightarrow 2S_1
\]

is also a 1D network with 2 linkage classes. By projecting the network to the horizontal line containing \( w = (1, 0)^\top \), as can be seen in [7], the leftmost reactant complex \( 2S_2 \) points to right and the rightmost reactant complex \( S_1 \) points to left. Hence, this network is at least a \( w \)-endotactic network. We further project it into the line \( L \) containing another \( w \), and the projection is shown not endotactic.

A look back at [7] might reveal that whatever \( w \) is, the projection of the network to the line containing \( w \) is endotactic, so the network given in [7] is endotactic. We also observe [2] again. It is obviously an endotactic network, and moreover, for any line \( L \) not orthogonal to its stoichiometric subspace, both the leftmost and the rightmost reactants of the projected 1D network on \( L \) contain nontrivial reactions. Therefore, [2] is a strongly endotactic network.

In fact, it is not easy to determine a network especially a complex network is endotactic or not for the arbitrary \( w \). The same reason for the difficulty of judging the strong endotacticity of a network. [9] gives the sufficient and necessary conditions to judge the 2-species networks.
It is not easy to testing the condition on any face of reactant ploytope. So [18] has given an algorithm to verify if a network is endotactic or not. Besides, this method can determine a network is endotactic or strong endotactic.

The endotactic structure has a close connection with persistence, a concept from population dynamics. The dynamics of a CRN system capturing the change of concentration of every species $S_j (j = 1, \cdots, n)$, identified by $x_j$, is given once the reaction rate is specified as a function $V : \mathbb{R}_{\geq 0}^n \mapsto \mathbb{R}_{\geq 0}^r$ of $x = (x_1, \cdots, x_n)^T$. The most frequently-used model to specify the reaction rate is mass action kinetics, under which the reaction rate follows power law with respect to the concentration of every species in the reactant complex. For example, for the $i$th reaction $v_i \rightarrow v'_i$, the reaction rate $V_i(x)$ is evaluated by

$$V_i(x) = k_i x^{v_i} = k_i \prod_{j=1}^n x_j^{v_{ij}}, \quad (1)$$

where $k_i \in \mathbb{R}_{> 0}$ is the reaction rate coefficient.

**Definition 2.9 (Mass Action System).** A CRN $(S, C, \mathcal{R})$ equipped with mass action kinetics is called a mass action system (MAS), which is usually represented by the quaternary $(S, C, \mathcal{R}, k)$.

The dynamical equation of a MAS $(S, C, \mathcal{R}, k)$ can be written as

$$\frac{dx}{dt} \triangleq \dot{x}(t) = \sum_{i=1}^r k_i x^{v_i}(v'_i - v_i). \quad (2)$$

**Definition 2.10 (Equilibrium).** For a MAS $(S, C, \mathcal{R}, k)$, a concentration vector $x^* \in \mathbb{R}_{> 0}^n$ is called an equilibrium if

$$\sum_{i=1}^r k_i (x^*)^{v_i}(v'_i - v_i) = 0,$$

and a complex balanced equilibrium if

$$\sum_{\{v'_j = C\}} k_j(x^*)^{v_j} = \sum_{\{v'_j = C\}} k_j(x^*)^{v_j}, \quad \forall C \in C.$$

A complex balanced equilibrium must be an equilibrium, but not vice verse. A MAS admits an (complex balanced) equilibrium is called (complex) balanced MAS. If there exists a complex balanced equilibrium in a MAS, any other equilibrium (if exists) in this MAS is also a complex balanced equilibrium [7].

9
3. Persistence

In this section, the concept of persistence and some known results to suggest persistence are introduced \([13, 6, 2, 3, 1, 9, 17]\). We also introduce the Lyapunov function PDEs \([19]\) that will be used to analyze persistence subsequently.

3.1. Definitions and Related Results

In chemical reaction network theory, persistence means that none of the concentrations of species can tend to zero if they are not zero at the beginning of reactions. Mathematically, it is defined as follows.

**Definition 3.1 (Persistence).** Consider a MAS \((S, C, R, k)\) described by 2. This MAS is called persistent if any forward trajectory \(x(t) \in \mathbb{R}_{\geq 0}^S\) with positive initial condition \(x(0) \in \mathbb{R}_{\geq 0}^S\) satisfies

\[
\liminf_{t \to \infty} x_j(t) > 0 \quad \text{for all } j \in \{1, \cdots, n\}.
\]

The above definition works for all cases, including the cases of bounded trajectory and of unbounded trajectory. In the case of bounded trajectory, the definition may be reduced to describe its \(\omega\)-limit point.

**Definition 3.2 (\(\omega\)-limit Point).** The set of \(\omega\)-limit points for the trajectory \(x(t)\) with positive initial condition \(x(0) \in \mathbb{R}_{\geq 0}^S\) is

\[
\omega(x(0)) := \{x \in \mathbb{R}_{\geq 0}^S \mid x(t_N) \to x, \text{ for some sequence } t_N \to \infty\}.
\]

**Definition 3.3 (Persistence for Bounded Trajectory).** For a MAS \((S, C, R, k)\) with bounded trajectory, it is persistent if

\[
\omega(x(0)) \cap \partial \mathbb{R}_{\geq 0}^S = \emptyset, \quad \forall x(0) \in \mathbb{R}_{\geq 0}^S.
\]

The following concepts play an important role on characterizing persistence of a MAS.

**Definition 3.4 (Semilocking set and Locking Set \([3,6]\)).** Consider a CRN \((S, C, R)\). A nonempty set \(W \subseteq S\) is said to be a semilocking set or siphon if one species of \(W\) is in a resultant complex \(v'_{i'}\), there must exist a species of \(W\) in the reactant complex \(v_i\). If for any reaction \(v_i \to v'_{i'}\) there exists a \(S_j \in W\) in reactant complex \(v_i\), then \(W \subseteq S\) is called a locking set.
Definition 3.5 (Face [3]). Consider a CRN \((S, C, R)\) and a nonempty index set \(W \subseteq S\). The set \(Z_W\), defined by
\[
Z_W = \{x \in \mathbb{R}^n_{\geq 0} | x_i = 0 \text{ for } S_i \in W\},
\]
is named the face of \(\mathbb{R}^n_{\geq 0}\). The set \(L_W\) given by
\[
L_W = \{x \in \mathbb{R}^n_{\geq 0} | x_i = 0 \text{ for } S_i \in W \text{ and } x(i) > 0 \text{ for } S_i \not\in W\}
\]
is called the relative interior of \(Z_W\).

As far as the stoichiometric compatibility class in \((S, C, R)\) is concerned, its face under a given \(W\) is \(F_W = \mathcal{S}(x) \cap Z_W\), and the relative interior of \(F_W\) is \(\mathcal{S}(x) \cap L_W\). Angeli et al. [6] also reported a necessary and sufficient condition to suggest a semilocking set. That is:

**Proposition 3.6.** A nonempty set \(W \subseteq S\) in a CRN \((S, C, R)\) is a semilocking set if and only if the face \(F_W\) is forward invariant for the dynamics [2].

The physical explanation of this proposition is easily caught as the concentrations of species in \(W\) are always zero and every reaction induced by the species in \(W\) will stop.

Essentially, the persistent property measures if the trajectory will tend to the face of \(\mathbb{R}^n_{\geq 0}\). Based on the notions of semilocking set, face and endotactic network, some efforts have been made to characterize persistence of CRNs. Angeli et al. [6] proved that if a boundary point (an element in \(L_W\)) is the \(\omega\)-limit point, then the set \(W\) which \(L_W\) corresponds to must be a semilocking set. They also reported that the global conservative CRNs with each semilocking set having a conservation relation between some species in it are persistent. In addition, they obtained that the global conservative CRNs with some semilocking sets without local conservation relation in it are persistent if the following two conditions are true: (a) the semilocking sets are dynamically non-emptiable; (b) there are no nested distinct locking sets without local conservation relation in the network. Johnston and Siegel [16] extended this result by putting forward that bounded networks with all weak dynamical non-emptiable semilocking sets have persistence. Anderson and his coauthors [2, 3, 4] made a systematic study on the Global Attractor Conjecture. They said that (a) deficiency zero complex balanced MASs have persistence if every equilibrium in \(\mathcal{S}(x) \cap L_W\) (\(W\) is a semilocking set in the system) is isolated for any \(x \in \mathbb{R}^S_{\geq 0}\) [2]; (b) complex balanced MASs are persistent if the equilibria are in the relative interior of \(F_W\) with \(\dim F_W = \dim \mathcal{S} - 1\) [3]; (c) all complex-balanced networks with single linkage class are persistent [4]. A recently
proposed proof of this conjecture by Craciun [10] is currently under verification. Craciun and his coauthors [1, 9, 17] also studied persistence of CRNs with endotactic structure. Pantea [1] proved any 2d endotactic MAS with bounded trajectories is persistent. Craciun et al. [9] stated that any endotactic MAS with two species is persistent, and Gopalkrishnan et al. [17] further asserted that any strongly endotactic MAS is persistent.

The above results enrich greatly the studies on persistence of CRNs. In this paper, we continue to follow this project, but use another strategy of Lyapunov function PDEs [19].

3.2. Lyapunov function PDEs

The Lyapunov function PDEs are initially proposed aiming at capturing the asymptotic stability of equilibria in MASs. By bridging between the microscopic and the macroscopic level, thermodynamics and potential theory, the Lyapunov function PDEs are yielded from Chemical Master Equation [19]. For a MAS \((S, C, R, k)\) governed by 2, they include a first-order PDE

\[
\sum_{i=1}^{n} k_i x^{v_i} - \sum_{i=1}^{n} k_i x^{v_i} \exp\{((v'_i - v_i) \cdot \nabla f(x))\} = 0, \quad x \in \mathbb{R}^S_0
\]  

(5)

and a corresponding boundary condition

\[
\lim_{x \to \bar{x}} \sum_{v \subseteq \text{supp } x} k_i x^{v_i} - \lim_{x \to \bar{x}} \sum_{v' \subseteq \text{supp } \bar{x}} k_i x^{v_i} \exp\{((v'_i - v_i) \cdot \nabla f(x))\} = 0, \quad x \in \mathbb{R}^S_0,
\]  

(6)

where \(\bar{x} \in \mathbb{R}^S_0\) represents any boundary point.

There is a good property about the solutions (if exist) of the PDEs 5,6. We exhibit it through the following proposition.

**Proposition 3.7 (Dissipation of Solutions of the PDEs [19]).** For a MAS \((S, C, R, k)\) described by 2 let \(f \in C^1\) be a solution of its Lyapunov PDEs 5,6 then

\[
\frac{df(x)}{dt} = \dot{f}(x) \leq 0, \quad x \in \mathbb{R}^S_0
\]  

(7)

with equality to hold if and only if \(\nabla f(x) \perp \mathcal{I}\). Further, assume that \(f \in C^2\) is a solution of the PDEs. If \(\exists D \subset \mathbb{R}^S_0\) such that \(\forall x \in D\) and \(\forall \mu \in \mathcal{I}\) there is

\[
\mu^T \nabla^2 f(x) \mu \geq 0 \quad \text{with equality to hold if and only if } \mu = 0_n,
\]  

(8)

then for all \(x \in D\), \(\dot{f}(x) = 0\) if and only if \(x\) is an equilibrium of the MAS.
Based on the dissipation of solutions of the PDEs, Fang and Gao [19] succeed in proving that the PDEs work well for capturing the asymptotic stability of equilibria in complex balanced MASs, all 1d MASs and some special MASs with dimension beyond 1. In this paper, we will use the PDEs to analyze the persistence of some MASs.

4. Lyapunov function PDEs for persistence

In this section, we will present some criteria for judging persistence based on different cases of solutions of the Lyapunov function PDEs, which are further applied to analyze different boundary points in MASs.

4.1. Criteria for judging persistence

The Lyapunov function PDEs might serve for analyzing the persistence of bounded MASs by judging that any boundary point is not a $\omega$-limit point according to different values-taking of solutions (if exist). To this task, we firstly reach a basic but very central theorem about the residence time of trajectories of a MAS in the positive quadrant.

**Theorem 4.1.** For a MAS $(S, C, R, k)$ given by Eq. 2, each bounded trajectory starting from a positive initial point $x(0) \in \mathbb{R}^S_{>0}$ stays in the positive stoichiometric class of $x(0)$ for infinite time, i.e.,

$$T_+ = \lim_{t \to +\infty} \int_0^t \mathbb{1}_{\{x(s) \in S(x(0)) \cap \mathbb{R}^S_{>0}\}} ds = +\infty,$$

where $\mathbb{1}_{\{\cdot\}}$ is the indicator function such that

$$\mathbb{1}_{\{A\}} = \begin{cases} 1, & A \text{ is true;} \\ 0, & A \text{ is false.} \end{cases}$$

**Proof.** For a MAS $(S, C, R, k)$ given by Eq. 2 its trajectory $x(t) \in \mathbb{R}^S_{>0}$ appears either in the interior or in the boundary of $S(x(0)) \cap \mathbb{R}^S_{>0}$. There are two kinds of possible boundary points, denoted by $\bar{x} \in \partial S(x(0)) \cap \mathbb{R}^S_{>0}$, according to $W \triangleq \text{supp}^r \bar{x}$ being a semilocking set or not. We continue the proof in two separate cases.

1. Case I: $W$ is not a semilocking set. When $x(t)$ enters into the boundary $L_W$, defined in 3.5, we have $x_j(t) = 0, \forall j \in W$. Since $W$ is not a semilocking set, $\exists p \in W$ such that $S_p \in \text{supp} v'_i$ and $\text{supp} v'_i \subseteq W^c$, i.e., for the reaction $v_i \to v'_i$ at time $t$, the inflow of species $S_p$ is larger than
zero while its outflow is zero, which means that \( \dot{x}_p(t) > 0 \) and \( x_p(t) = 0 \). This suggests that the trajectory \( x(t) \) will leave \( L_W \) once it enters into it. Therefore, the time set, given by \( \{ t | x(t) \in L_W \} \), is at most discrete. As time \( t \) goes to infinity, the trajectory \( x(t) \) will stay out of \( L_W \) for infinite time.

(2) Case II: \( W \) is a semilocking set. In this case, assume that at time \( T (T < +\infty) \) the trajectory \( x(t) \) enters into \( L_W \), i.e., \( x(T) = \bar{x} \in L_W \). For simplicity of symbols, denote \( \dot{x}(t) = g(x) \) for the dynamics. \(^2\) This ODE together with the initial condition \( x(t) = x(0) \) at \( t = 0 \) has the same solution with the following initial value problem

\[
\begin{align*}
\frac{dx(t-t)}{dt} &= -g(x(T-t)), \quad t \in [0, T]; \\
x(T) &= \bar{x}, g(x(t)) = g(\bar{x}), \quad t = 0.
\end{align*}
\]

Since \( g(x(T-t)) \) is a polynomial function and \( x(T-t) \) is bounded, which support the conditions for existence and uniqueness of solution of the above ODE, the solution written by \( x(t) = (x_1(T-t), \cdots, x_n(T-t))^T \) is unique. Further, let \( X_1 \in \mathbb{R}_{\geq 0}^W \) and \( X_2 \in \mathbb{R}_{\geq 0}^W \), then each \( g_j(x(T-t)) = g_j(X_1(T-t), X_2(T-t)), \ j = 1, \cdots, n, \) is a linear combination of \( k_1X_1^{|v_1|w}X_2^{|v_2|w}, \cdots, k_rX_1^{|v_r|w}X_2^{|v_r|w} \), where \( v_i|w \) represents a sub-vector of \( v_i \) with every entry orientated by \( W \). By denoting \( k_iX_2^{|v_i|w} \) as \( k_i(t), \ i = 1, \cdots, r, \) we rewrite \( g_j(X_1(T-t), X_2(T-t)) = g_j(X_1(T-t), t) \). The initial value problem \(^1\) with respect to \( X_1 \) can be rewritten as

\[
\begin{align*}
\frac{dX_1(T-t)}{dt} &= -g_j(X_1(T-t), t)|_W, \quad t \in [0, T]; \\
X_1(T) &= 0, g_j(0, 0) = 0, \forall j \in W, \quad t = 0.
\end{align*}
\]

Note that this ODE is sole since the uniqueness of \( x(T-t) \) implies \( X_1(T-t) \) and \( k_i(t) \) to be unique, so is \( g(X_1(T-t), t)|_W \). It is not difficult to verify \( g_j(0, t) = 0 \) for all \( j \in W \) from the fact that every \( g_j(X_1(T-t), t) \) is a linear combination of \( k_1(t)X_1^{|v_1|w}, \cdots, k_r(t)X_1^{|v_r|w} \). Whatever the species in a semilocking set \( W \) acts as a reactant or a resultant, the term \( X_1^{|v_i|w} = 0 \) \( (i = 1, \cdots, r) \).

We thus have that \( X_1(T-t) \equiv 0 \) is the unique solution of the above equation. Naturally, at \( t = T \) one should get \( X_1(0) = 0 \). This is contradicted against \( x(0) \in \mathbb{R}_{\geq 0}^W \). Therefore, the assumption that the trajectory \( x(t) \) enters into \( L_W \) in a finite amount of time is not true.

By combining (1) and (2), we conclude that each bounded trajectory in a MAS with a positive initial point will stay in the positive stoichiometric compatibility class for infinity time when time trends to infinity.

The proof process also indicates the time that a bounded trajectory of a MAS stays in the...
boundary.

**Corollary 4.2.** Given a MAS \((S, C, R, k)\) with the dynamics of 2, the time set for any bounded trajectory starting from a positive initial point to stay in the boundary \(L_W\), given in 3.5, is at most discrete if \(W\) is not a semilocking set. Also, it is impossible for the mentioned trajectory to enter into a semilocking boundary in a finite amount of time.

4.1 and 4.2 report definitely the time allocation for a bounded trajectory of a MAS to stay in the positive quadrant and the non-semilocking boundary, respectively. The infinite time for the former implies great possibility for a MAS to be persistent while the discrete time set for the latter might suggest a non-semilocking boundary to be not a convergence region. The difficulty in proving persistence may lie in analyzing semilocking boundary, which has been confirmed in Anderson’s work [2]. The results of 4.1 and 4.2 keep it unknown whether a bounded trajectory can enter into a semilocking boundary in infinite time. Despite these facts, it is still possible to infer persistence of a MAS through different values-taking of solution of its Lyapunov function PDEs.

**Lemma 4.3.** Consider a MAS \((S, C, R, k)\) described by 2. Assume that \(f \in \mathcal{C}^{1}\) is a nonnegative solution of its Lyapunov PDEs 5 and \(\bar{x} \in \mathbb{R}^{S} \geq 0\) represents any boundary point. \(\bar{x}\) is not a \(\omega\)-limit point if the solution \(f(x)\) satisfies

\[
\lim_{x \to \bar{x}} \dot{f}(x) = -\infty \text{ or } \lim_{x \to \bar{x}} \dot{f}(x) \leq -M,
\]

where \(x \in \mathbb{R}^{S}_{\geq 0} \cap \mathcal{A}(\bar{x})\) and \(M\) is a positive constant.

**Proof.** For any initial point \(x(0) \in \mathbb{R}^{S}_{\geq 0} \cap \mathcal{A}(\bar{x})\), we have \(f(x(0)) \geq 0\) and

\[
f(x(t)) = f(x(0)) + \int_{0}^{t} \dot{f}(x(s))ds.
\]

Since \(f \in \mathcal{C}^{1}\) and \(\lim_{x \to \bar{x}} \dot{f}(x) = -\infty\) (or \(-M\)), there exists a \(\epsilon\)-neighbourhood of \(\bar{x}\), denoted by \(N_{\epsilon}(\bar{x})\), such that \(\dot{f}(x) < -M_1, \forall x \in N_{\epsilon}(\bar{x})\), where \(\epsilon, M_1 > 0\). In the following, we use rebuttals of evidence to continue the proof.

Assume that \(\bar{x}\) is a \(\omega\)-limit point under the given initial conditions. By defining

\[
W \triangleq \text{supp}^c \bar{x},
\]

15
Now we note that we can find a \( \epsilon \)-neighbourhood of \( \bar{x} \), denoted by \( N_{\epsilon}(\bar{x}) \), such that \( \bar{f}(x) \prec -M_1, \forall x \in N_{\epsilon}(\bar{x}) \) and the total time \( t(x) \) stays in it:

\[
T_\epsilon = \lim_{t \to \infty} \int_0^t \mathbb{1}_{[\bar{f}(x) \in N_{\epsilon}(\bar{x})]} ds = +\infty.
\]

(13)

If we can not find, from the continuous of \( \bar{f}(x) \), we can find \( \epsilon_1 \) and \( \epsilon_2 \) with \( \epsilon_2 - \epsilon_1 > 0 \) such that \( \bar{f}(x) \) is less than \( -M_2 \) and \( -M_3 \) when \( x \in N_{\epsilon_1}(\bar{x}) \) and \( x \in N_{\epsilon_2}(\bar{x}) \) respectively. Besides, \( x(t) \) spends finite time in \( N_{\epsilon_2}(\bar{x}) \) when \( t \to \infty \). And the time of trajectory staying out of \( N_{\epsilon_1} \) is infinite as the time \( t(x) \) in positive stoichiometric compatibility class is infinity from [4.1]. Otherwise we can choose \( \epsilon = \epsilon_2 \) and \([13]\) holds. Next we define \( \Omega \) as:

\[
\Omega \triangleq \{ x \in \mathbb{R}^{\omega_0}, \epsilon_1 \leq |x - \bar{x}| \leq \epsilon_2 \}
\]

is obvious a bounded region. \( \bar{x} \) is the \( \omega \)-limit point of trajectory \( x(t) \), so for any \( t_1 > 0 \), we can find \( t_2 > t_1 \), such that \( x(t_2) \in N_{\epsilon_1} \). Combining this with the infinity time out of \( N_{\epsilon_2} \), we can obtain that the trajectory will pass through the region \( \Omega \) infinity times.

Because \( g(x) \) is continue, there exists \( \|g(x)\|_\infty < M_4, \forall x \in \Omega \) where \( M_4 \) is bounded. If the trajectory enters into \( \Omega \) at any time \( a \) and leaves at time \( b \), we have:

\[
e_2 - e_1 \leq |x(b) - x(a)| = \int_a^b g(x(s)) ds \leq (b - a) M_4 \Rightarrow b = a \geq \frac{e_2 - e_1}{M_4}.
\]

From above equation, we know at least take \( t = (e_2 - e_1)/M_4 \) to go across \( \Omega \). And we know that the total time that \( x(t) \) spends in \( \Omega \) is infinity. It conflicts with limited of the time in \( N_{\epsilon_2}(\bar{x}) \).

So from above, we conclude that we can find \( N_{\epsilon} \) such that \( \bar{f}(x) \leq -M_1 \) and \([13]\) holds, then:

\[
\lim_{t \to \infty} f(x(t)) = f(x_0) + \lim_{t \to \infty} \int_0^t \bar{f}(x(s)) ds \\
\leq f(x_0) - M_1 \int_{t \to \infty} \mathbb{1}_{[\bar{f}(x) \in N_{\epsilon}]} ds = -\infty.
\]

This will violate \( f(x) \geq 0 \). Thus \( \bar{x} \) is not an \( \omega \)-limit point. \( \square \)

**Lemma 4.4.** For a MAS \((S, C, R, k)\) given by \([2]\) let \( f \in \mathcal{G}^1 \) be a nonnegative solution of its Lyapunov PDEs \([S, R] \) and \( \bar{x} \in \mathbb{R}^{\omega_0} \) be any boundary point. If \( \bar{x} \) is the local maximal point for the solution \( f(x) \) or \( \lim_{t \to \infty} f(x) \), then \( \bar{x} \) is not a \( \omega \)-limit point.

**Proof.** We also use rebuttals of evidence to conduct proof. Assume that \( \bar{x} \) is a \( \omega \)-limit point. Namely, for any initial point \( x(0) \in \mathbb{R}^{\omega_0} \cap \mathcal{S}(\bar{x}) \), there exists a time series \( \{t_k\} \) such that \( \bar{x} \in \mathcal{S}(\bar{x}) \)
\( \omega(x(0)) \). Also, for all \( \epsilon > 0 \), there exists a moment \( t_\epsilon < t_N \to +\infty \) such that \( x(t_\epsilon) \in N_\epsilon(\bar{x}) \), where \( N_\epsilon(\bar{x}) \) is a \( \epsilon \)-neighborhood of \( \bar{x} \). Note that \( \dot{f}(x) \leq 0 \), so it is impossible that \( f(\bar{x}) \) (\( f(x) \) can be defined at \( x = \bar{x} \)) or \( \lim_{x \to \bar{x}} f(x) \) (\( f(x) \) cannot be defined at \( x = \bar{x} \)) is local maximal. Therefore, \( \bar{x} \) is not a \( \omega \)-limit point.

The above results suggest that we can judge a boundary point in a MAS not a \( \omega \)-limit point utilizing the solutions of its Lyapunov function PDEs. We thus can further deduce persistence of MASs from these results for the bounded trajectories.

**Theorem 4.5.** For a MAS \((S, C, R, k)\) governed by \([2]\) let its Lyapunov function PDEs \([5,6]\) contain a nonnegative solution \( f \in \mathcal{A}^1 \), and its trajectories be bounded. Then the MAS is persistent if one of the following conditions holds for any boundary point \( \bar{x} \in \mathbb{R}^n_{>0} \):

1. \( \lim_{x \to \bar{x}} \dot{f}(x) = -\infty \);
2. \( \lim_{x \to \bar{x}} \dot{f}(x) = -M \) with \( M \) a positive constant;
3. \( \bar{x} \) is the local maximal value point for \( f(x) \) or \( \lim_{x \to \bar{x}} f(x) \).

**Proof.** Combining 4.3, 4.4, we have that if one the above three conditions holds, then \( \bar{x} \) is not a \( \omega \)-limit point. Since \( \bar{x} \) is any boundary point, the result means that \( \omega(x(0)) \cap \partial \mathbb{R}^n_{>0} = \emptyset \) for any initial point \( x(0) \in \mathcal{A}(\bar{x}) \cap \mathbb{R}^n_{>0} \). This together with the known condition of bounded trajectories proves the MAS persistent. \( \square \)

When addressing the issue of persistence, a key point is to identify whether the set related to boundary points \( \bar{x} \), defined through \( W \triangleq \text{supp}^c \bar{x} \), is a semilocking set or not. The result is quite clear in the case of \( W \) being not a semilocking set. Anderson \([2]\) has proved that a MAS is persistent if \( W \) is not a semilocking set for any boundary point. In the following, we will revisit this result through the Lyapunov function PDEs method, and discuss some possibilities to reach persistence in the case of \( W \) being a semilocking set.

**4.2.** \( W \triangleq \text{supp}^c \bar{x} \) is not a semilocking set

**Lemma 4.6.** Consider chemical reaction system \((S, C, R, k)\). Let \( f(x) \in C^1 \) is a solution of Lyapunov function \([5]\) and its boundary condition \([6]\). If \( W \) is not the semilocking set, \( \lim_{x \to \bar{x}} \dot{f}(x(t)) = -\infty \) where \( x \in \mathbb{R}^n_{>0} \).
Proof. W is not a semilocking set. \( \dot{f}(x(t)) \) is the derivative of \( f \) respect to time \( t \). From the form of boundary conditions of Lyapunov PDE, it also can be written as:

\[
\dot{f}(x(t)) = \nabla f(x) \cdot \dot{x} = \sum_{i=1}^{n} k_i x^i (v'_i - v_i)^T \cdot \nabla f(x)
\]

\[
= \sum_{\text{supp } v_i \subseteq \text{supp } \bar{x}} k_i x^i (v'_i - v_i)^T \nabla f(x) + \sum_{\text{supp } v_i \nsubseteq \text{supp } \bar{x}} k_i x^i (v'_i - v_i)^T \nabla f(x)
\]

\( W \triangleq \text{supp } \bar{x} \) is not a semi-locking set, then there at least exist a reaction \( v_i \rightarrow v'_i \) which satisfies \( \text{supp } v_i \subseteq \text{supp } \bar{x}, \text{supp } v'_i \nsubseteq \text{supp } \bar{x} \). Note that

\[
\sum_{i=1}^{n} k_i x^i (v'_i - v_i)^T \nabla f(x) = -\infty
\]

In fact, \( f \) as a solution of the PDE satisfies its boundary condition (a) [6] For \( \forall x \in (\bar{x} + S) \cap \mathbb{R}^n \) and \( x \rightarrow \bar{x} \):

\[
\lim_{x \rightarrow \bar{x}} \sum_{\text{supp } v_i \subseteq \text{supp } \bar{x}} k_i x^i \geq \lim_{x \rightarrow \bar{x}} \sum_{\text{supp } v'_i \subseteq \text{supp } \bar{x}} k_i x^i \exp((v'_i - v_i)^T \nabla f(x))
\]

Let \( a = (v'_i - v_i)^T \nabla f(x) \), from \( e^a \geq a - 1 \), then we can get

\[
\lim_{x \rightarrow \bar{x}} (\sum_{\text{supp } v_i \subseteq \text{supp } \bar{x}} k_i x^i - \sum_{\text{supp } v'_i \subseteq \text{supp } \bar{x}} k_i x^i \exp((v'_i - v_i)^T \nabla f(x))) \geq \lim_{x \rightarrow \bar{x}} \sum_{\text{supp } v'_i \subseteq \text{supp } \bar{x}} k_i x^i (v'_i - v_i)^T \nabla f(x)
\]

(14)

Because \( \text{supp } v_i \subseteq \text{supp } \bar{x} \), \( \lim_{x \rightarrow \bar{x}} x^i > 0 \). Thus, there must exist a constant \( C \) that

\[
\lim_{x \rightarrow \bar{x}} \sum_{\text{supp } v_i \subseteq \text{supp } \bar{x}} k_i x^i = C
\]

Then [14] can be written as:

\[
\lim_{x \rightarrow \bar{x}} \sum_{\text{supp } v_i \subseteq \text{supp } \bar{x}} k_i x^i (v'_i - v_i)^T \nabla f(x) \leq C - 0 = C
\]

(15)

The solution PDE \( f(x) \) also satisfies boundary condition (b) [18] When \( x \rightarrow \bar{x} \), it can be written as:

\[
0 = \lim_{x \rightarrow \bar{x}} \sum_{\text{supp } v_i \subseteq \text{supp } \bar{x}} k_i x^i = \lim_{x \rightarrow \bar{x}} \sum_{\text{supp } v'_i \subseteq \text{supp } \bar{x}} k_i x^i \exp((v'_i - v_i)^T \nabla f(x)).
\]

18
Theorem 4.7. Considering a MAS any \( \bar{\omega} \) constant. For arbitrary boundary point \( \bar{x} \) from above condition, we know the solution of the PDE \( f \) from 4.4. We can easily prove that any \( \bar{x} \) is not a semi-locking set. So there exists a trajectory \( v \) such that \( \lim_{x \to \bar{x}} v(x) = 0 \).

If we also let \( a = (v' - v) \) \( \bar{\omega} \) and \( \bar{x} \) from 4.4, then we have:

\[
\lim_{x \to \bar{x}} \sum_{\supp v' \subset \supp \bar{x}} k_i x^{i'} \exp((v' - v_i) \bar{\omega} \supp f(x)) = 0.
\]

If we also let \( a = (v' - v) \supp f(x) \), from e\( \geq 1 \)In this case,

\[
\lim_{x \to \bar{x}} \sum_{\supp v' \subset \supp \bar{x}} k_i x^{i'} (v' - v_i) \bar{\omega} \supp f(x) = \lim_{x \to \bar{x}} \sum_{\supp v' \subset \supp \bar{x}} k_i x^{i'} \leq 0.
\]

So

\[
\lim_{x \to \bar{x}} \sum_{\supp v' \subset \supp \bar{x}} k_i x^{i'} (v' - v_i) \bar{\omega} \supp f(x) \leq 0.
\]  \hspace{1cm} (16)

For all reactions: \( \supp v_i \) which satisfy \( \supp v_i \supset \supp \bar{x} \) and \( \supp v_i \subset \supp \bar{x} \), we have:

\[
k_i x^{i'} \exp((v' - v_i) \bar{\omega} \supp f(x)) \leq \sum_{\supp v' \subset \supp \bar{x}} k_i x^{i'} \supp F(x)
\]

and \( \lim_{x \to \bar{x}} F(x) = 0 \). So:

\[
\lim_{x \to \bar{x}} k_i x^{i'} (v' - v_i) \bar{\omega} \supp f(x) \leq \lim_{x \to \bar{x}} (\ln F(t) - \ln k_i - \ln x^{i'}) \supp F(x)
\]

Because \( W \) is not semi-locking set, there exist reaction \( R \) satisfies \( \supp v_i \supset \supp \bar{x} \) and \( \supp v_i \subset \supp \bar{x} \). Thus \( \ln F(x) \) tends to infinity and \( \ln k_i x^{i'} \) trends to a constant \( C \). So:

\[
\lim_{x \to \bar{x}} \sum_{\supp v' \subset \supp \bar{x}} k_i x^{i'} (v' - v_i) \bar{\omega} \supp f(x) = -\infty.
\]  \hspace{1cm} (17)

From equation[15][16][17] we can easily prove

\[
\lim_{x \to \bar{x}} f(x) = \lim_{x \to \bar{x}} \sum_{i=1}^{r} k_i x^{i'} (v' - v_i) \bar{\omega} \supp f(x) = -\infty.
\]

\( \square \)

**Theorem 4.7.** Considering a MAS \((S, C, R, k)\), where \( k \in \mathbb{R}_{\geq 0} \) is the vector of reaction rate constant. For arbitrary boundary point \( \bar{x} \), if \( W \supseteq \supp \bar{x} \) is not a semilocking set and the solution of the PDE \( f \geq 0 \), then all the bounded trajectories in \((S, C, R)\) are persistent.

**Proof.** From above condition, we know \( f(x) \geq 0 \) and \( W \) is not a semilocking set. Thus from 4.6, any \( \bar{x} \) is not an \( \omega \)-limit point. So each bounded trajectory is persistent. \( \square \)
4.3. \( W \triangleq \text{supp}' \bar{x} \) is semilocking set

**Remark 4.8.** If we use 5 minus 6 then we can obtain another boundary condition:

\[
\lim_{x \to \bar{x}} \sum_{\text{supp } v_i \not\subseteq \text{supp } \bar{x}} k_i x^{v_i} \exp(\langle v'_i - v_i \rangle^\top \nabla f(x)) = 0, \quad x \in \mathbb{R}_{>0}^n. \tag{18}
\]

where \( x \in (\bar{x} + \mathcal{F}) \cup \mathcal{R}_{>0}^n \). Then we call 6 and 18 as boundary (a) boundary (b) respectively.

In order to make the writing more convenient, we give the following stipulation.

**Remark 4.9.** The value of \( \lim_{x \to \bar{x}} \hat{f}(x) \) can be written as:

\[
\lim_{x \to \bar{x}} \hat{f}(x) = \lim_{x \to \bar{x}} \sum_{i=1}^r k_i x^{v_i} (v'_i - v_i)^\top \nabla f(x)
\]

\[
\begin{align*}
&= \lim_{x \to \bar{x}} \sum_{\text{supp } v_i \not\subseteq \text{supp } \bar{x}} k_i x^{v_i} (v'_i - v_i)^\top \nabla f(x) + \lim_{x \to \bar{x}} \sum_{\text{supp } v'_i \subseteq \text{supp } \bar{x}} k_i x^{v_i} (v'_i - v_i)^\top \nabla f(x) \\
&\quad + \lim_{x \to \bar{x}} \sum_{\text{supp } v'_i \not\subseteq \text{supp } \bar{x}} k_i x^{v_i} (v'_i - v_i)^\top \nabla f(x) + \lim_{x \to \bar{x}} \sum_{\text{supp } v_i \not\subseteq \text{supp } \bar{x}} k_i x^{v_i} (v'_i - v_i)^\top \nabla f(x)
\end{align*}
\]

We denote the parts of right side of above equation as \( *1, *2, *3, *4 \). Then when considering the boundary point \( \bar{x} \) whose corresponding \( W \triangleq \text{supp}' \bar{x} \) is a semi-locking set we can not find reaction \( R_i \) which satisfy \( \text{supp } v_i \subset \text{supp } \bar{x} \) and \( \text{supp } v'_i \subset \text{supp } \bar{x} \), so the value of \( *2 \) is zero. Hence \( f = *1 + *3 + *4 \) when \( W \) is a semi-locking set. So we only need to analyse the \( *1, *3 \) and \( *4 \) by using the boundary conditions of Lyapunov PDE when \( W \) is a semi-locking set.

Above theorem tells us that boundary \( \omega\text{-limit} \) points must be the points whose corresponding \( W \) is a semilocking set. In other words, if \( W \) is not semilocking set, boundary point \( \bar{x} \) cannot be an \( \omega\text{-limit} \) point. Namely, we just need to consider \( \bar{x} \) whose underlying \( W \) is a semilocking set in order to make sure which conditions \( \bar{x} \) should have to not to be an \( \omega\text{-limit} \) point.

\[
\lim_{x \to \bar{x}} \hat{f}(x) = -\infty \text{ if the corresponding } W \text{ of } \bar{x} \text{ is not a semi-locking set. So if } W \text{ is a semi-locking set, when does the } \lim_{x \to \bar{x}} \hat{f}(x) = -M? \text{ Next we use } 4.3 \text{ to derive the following two lemmas.}
\]
Lemma 4.10. \((S, C, R, k)\) is a chemical reaction system. \(f \in \mathbb{C}^2\) is the solution of Lyapunov PDE for this system. \(\dot{x}\) is a boundary non-equilibrium point of this network. \(\dot{x}\) is not an \(\omega\)-limit point if Lyapunov PDE of this network has the solution which satisfies the following conditions:

- \(f \geq 0\)
- \(f\) is convex function
- \(\Delta f(x)\) is a diagonal matrix

Proof. Let \(W \triangleq \text{supp} \dot{x}\). If \(W\) is not a semilocking set, from \(4.7\) \(\dot{x}\) is not an \(\omega\)-limit point. Considering \(W\) as a semilocking set, when \(\dot{x}\) is not an equilibrium, then \(W\) is not a locking set and \(\dot{f}\) is strictly negative. As a result, when \(W\) is a semilocking set, we’ll have:

\[
\lim_{x \to \bar{x}} \dot{f}(x) = *1 + *3 + *4
\]

\(W\) is a semilocking set, thus:

\[
\lim_{x \to \bar{x}} \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i} = \lim_{x \to \bar{x}} \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i}
\]

\[
= \lim_{x \to \bar{x}} \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i} + \lim_{x \to \bar{x}} \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i}
\]

From above equation and boundary condition (a), we can obtain the following equation:

\[
\lim_{x \to \bar{x}} \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i} = \lim_{x \to \bar{x}} \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i} \exp((v'_i - v_i) \cdot f(x))
\]

What’s more, we perform the Taylor expansion of \(\exp((v'_i - v_i) \cdot f(x))\) with respect to zero, then have:

\[
\lim_{x \to \bar{x}} \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i}(v'_i - v_i) \cdot f(x) + \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i} e^{\alpha_i} \frac{1}{2}[(v'_i - v_i) \cdot f(x)]^2 = 0
\]

where \(\alpha_i \in \mathbb{R}\) lies between 0 and \((v'_i - v_i) \cdot f(x)\). So further we have:

\[
\lim_{x \to \bar{x}} \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i}(v'_i - v_i) \cdot f(x) = -\lim_{x \to \bar{x}} \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i} e^{\alpha_i} \frac{1}{2}[(v'_i - v_i) \cdot f(x)]^2
\]

\[
-\lim_{x \to \bar{x}} \sum_{\text{supp } v \subseteq \text{supp } \dot{x}} k_i x^{v_i} e^{\alpha_i} \frac{1}{2}[(v'_i - v_i) \cdot f(x)]^2
\]
It is obvious that (b) is no bigger than zero. Now we consider (a). Without loss of generality, we assume \( W = \{ m + 1, \cdots, n \} \) with \( m < n \). Because \( \text{supp} \, \nu' \subseteq \text{supp} \, \bar{x} \) and \( \text{supp} \, \nu \subseteq \text{supp} \, \bar{x} \), the \( k \)-th component of \( \nu'_i - \nu_i \) is zero for all \( k \in W \). In that case, we can get:

\[
(\nu'_i - \nu_i)\nabla f(x) = \sum_{i=1}^{m} (\nu_i)\nabla f(x)
\]

where \( (\nu_i) \) denotes the \( l \)-th component of \( \nu'_i - \nu_i \).

\( \Delta f(x) \) is a diagonal matrix, namely:

\[
\frac{\partial^2 f}{\partial x_k \partial x_k} = 0 = \frac{\partial \nabla_k f}{\partial x_k},
\]

therefore, \( \nabla_k f(x) \) doesn’t contain \( x_k \), where \( k_1 \notin W \) and \( k_2 \in W \). Consequently, if we project this network \( (\mathcal{S}, C, \mathcal{R}, k) \) into \( (\mathcal{S}', C', \mathcal{R}', k') \) where \( \mathcal{S}' = \{ S_1, \cdots, S_m \} \), \( \mathcal{R}' \) is composed of reactions \( \mathcal{R} \), such that \( \text{supp} \, \nu \subseteq \text{supp} \, \bar{x} \) and \( \text{supp} \, \nu' \subseteq \text{supp} \, \bar{x} \). \( C' \) is the set of complexes which appear in \( \mathcal{R}' \) and \( k' \) is the rate constant of \( \mathcal{R}' \). And we use \( x' \) and \( \bar{x}' \) to denote the projection of \( x \) and \( \bar{x} \), then we can see that \( \bar{x}' \) is an interior point of \( (\mathcal{S}', C', \mathcal{R}', k') \). Thus \( \lim_{x \to \bar{x}'} \nabla f(x') = \nabla f(\bar{x}') \) for any \( l \notin W \). At this consequence, there exists:

\[
\lim_{x \to \bar{x}'} \sum_{\nu \subseteq \text{supp} \, \bar{x}} \sum_{\nu' \subseteq \text{supp} \, \bar{x}} k_i \nu'^i e^{\nu_i} \frac{1}{2} [(\nu'_i - \nu_i)\nabla f(x)]^2 = \lim_{x \to \bar{x}'} \sum_{\nu \subseteq \mathcal{R}} k_i (x'^i e^{\nu_i}) \frac{1}{2} \left( \sum_{i=1}^{m} (\nu_i)\nabla f(x') \right)^2
\]

where \( x' \) denotes the vector which is composed of the first \( m \) components of \( \bar{x} \).

Because the convexity of \( f(x) \), the value of above equation is zero if and only if \( x' \) is an equilibrium of \( (\mathcal{S}, C, \mathcal{R}, k) \). But if \( x' \) is an equilibrium, \( \bar{x} \) is also an equilibrium. This is obvious contradict to our assumption. In this case, above equation can not be zero, further with its non-negativity, we obtain:

\[
\lim_{x \to \bar{x}'} \sum_{\nu \subseteq \text{supp} \, \bar{x}} \sum_{\nu' \subseteq \text{supp} \, \bar{x}} k_i \nu'^i e^{\nu_i} \frac{1}{2} [(\nu'_i - \nu_i)\nabla f(x)]^2 = M
\]

is strictly positive where \( M \) is a constant. Thus \( (a) = -M \) and \( (b) \leq 0 \), we can obtain:

\[
\lim_{x \to \bar{x}'} \sum_{\nu \subseteq \text{supp} \, \bar{x}} k_i \nu'^i (\nu'_i - \nu_i)\nabla f(x) < -M.
\]

Next we consider the value of \( \ast 4 \). From \([16] \) of \([4.6] \) we have \( \ast 4 \leq 0 \). So we obatin that \( \lim_{x \to \bar{x}'} f(x) \leq -M \). Thus \( \bar{x} \) is not an \( \omega \)-limit point from \([4.3] \). \( \square \)
Lemma 4.11. Let chemical reaction network denoted by \((S, C, R, k)\). The solution of Lyapunov PDE for this system is denoted by \(f(x) \in \mathbb{R}^2\). \(\bar{x}\) is a boundary non-equilibrium point of this network. \(\bar{x}\) is not an \(\omega\)-limit point, if Lyapunov PDE of this network has the solution which satisfies the following condition:

- \(f \geq 0\)
- \(f\) is convex function
- there exist at least one reaction satisfies \(\text{supp } v \ni \text{ supp } \bar{x}\) and \(\text{supp } v' \subseteq \text{ supp } \bar{x}\) that makes \(x^{v_i}\) and \(\exp\left[-(v'_j - v_j)^T \nabla f(x)\right]\) the same order infinitesimal.

Proof. Let \(W \triangleq \text{supp } c_{\bar{x}}\). If \(W\) is not a semilocking set, from 4.7, \(\bar{x}\) is not an \(\omega\)-limit point. Considering \(W\) as a semilocking set, when \(\bar{x}\) is not an equilibrium, then \(W\) is not a locking set. At the same time, from 4.9, we know \(\lim_{x \to \bar{x}} \dot{f}(x) = \ast 1 + \ast 3 + \ast 4\).

Consider boundary condition (a):

\[
\lim_{x \to \bar{x}} \sum_{\text{supp } v_i \subseteq \text{ supp } \bar{x}} k_i x^{v_i} = \lim_{x \to \bar{x}} \sum_{\text{supp } v_i \subseteq \text{ supp } \bar{x}} k_i x^{v_i} \exp\left[(v'_j - v_j)^T \nabla f(x)\right] + \lim_{x \to \bar{x}} \sum_{\text{supp } v_j \not\subseteq \text{ supp } \bar{x}} k_j x^{v_j} \exp\left[(v'_j - v_j)^T \nabla f(x)\right].
\]

If the value of (a) is zero, for each \(R_i\) such that \(\text{supp } v_i \subseteq \text{ supp } \bar{x}\) and \(\text{supp } v'_j \subseteq \text{ supp } \bar{x}\) there exist \((v'_j - v_j)^T \nabla f(x) = -\infty\). Then:

\[
\lim_{x \to \bar{x}} \sum_{\text{supp } v_i \subseteq \text{ supp } \bar{x}} k_i x^{v_i} (v'_j - v_j)^T \nabla f(x) = -\infty.
\]

From the proof of 4.6, we know \(\ast 3, \ast 4\) is bounded. So:

\[
\lim f(x) = -\infty.
\]

From 4.3, we know \(\bar{x}\) is not an \(\omega\)-limit point. If there exist one of reaction \(R_i\) doesn’t satisfy above property, the value of (a) is strictly positive because \(k_i x^{v_i}\) is bigger than zero. Meanwhile
there exist at least one reaction satisfies \( \text{supp } v_j \not\subseteq \text{supp } x \) and \( \text{supp } v'_j \subseteq \text{supp } x \) that makes \( x^{v_i} \) and \( \exp[-(v'_j - v_j)^T \nabla f(x)] \) the same order infinitesimal, so 

\[
\lim_{x \to \bar{x}} \sum_{\text{supp } v_j \subseteq \text{supp } x} k_j x^{v_j} \exp[(v'_j - v_j)^T \nabla f(x)] = M < \lim_{x \to \bar{x}} \sum_{\text{supp } v_j \subseteq \text{supp } x} k_j x^{v_j}
\]

In this case, we have:

\[
\lim_{x \to \bar{x}} \sum_{\text{supp } v_j \subseteq \text{supp } x} k_j x^{v_j} \exp[(v'_j - v_j)^T \nabla f(x)] = \lim_{x \to \bar{x}} \sum_{\text{supp } v_j \subseteq \text{supp } x} k_j x^{v_j} - M \\
\leq \lim_{x \to \bar{x}} \sum_{\text{supp } v_j \subseteq \text{supp } x} k_j x^{v_j} - (M - \eta)
\]

where \( \eta < M \) is a positive constant.

And further use the inequation \( e^\delta > a + 1 \), we obtain:

\[
\lim_{x \to \bar{x}} \sum_{\text{supp } v_j \subseteq \text{supp } x} k_j x^{v_j} (v'_j - v_j)^T \nabla f(x) + \lim_{x \to \bar{x}} \sum_{\text{supp } v_j \subseteq \text{supp } x} k_j x^{v_j} \\
\leq \lim_{x \to \bar{x}} \sum_{\text{supp } v_j \subseteq \text{supp } x} k_j x^{v_j} - (M - \eta) \\
= \lim_{x \to \bar{x}} \sum_{\text{supp } v_j \subseteq \text{supp } x} k_j x^{v_j} - (M - \eta)
\]

As a consequence, we can easily get:

\[
*1 \leq -(M - \eta) = -M'
\]

where \( M \) and \( M' \) are positive constants. For all reactions satisfy \( \text{supp } v_j \not\subseteq \text{supp } \bar{x} \) and \( \text{supp } v'_j \subseteq \text{supp } \bar{x} \), we can divide the \( (v'_j - v_j)^T \nabla f(x) \) into three classes:

1. If \( \lim_{x \to \bar{x}} (v'_j - v_j)^T \nabla f(x) = -\infty \), then from the non-negativity of \( k_j x^{v_j} \), we obtain that
   \[
   \lim_{x \to \bar{x}} k_j x^{v_j} (v'_j - v_j)^T \nabla f(x) \leq 0.
   \]

2. If \( \lim_{x \to \bar{x}} (v'_j - v_j)^T \nabla f(x) = A \) where \( A \) is a constant, from \( \lim_{x \to \bar{x}} k_j x^{v_j} = 0 \), we can easily get:
   \[
   \lim_{x \to \bar{x}} k_j x^{v_j} (v'_j - v_j)^T \nabla f(x) = 0.
   \]

3. If \( \lim_{x \to \bar{x}} (v'_j - v_j)^T \nabla f(x) = +\infty \), from the boundedness of \( \lim_{x \to \bar{x}} k_j x^{v_j} \exp[(v'_j - v_j)^T \nabla f(x)] \), we can get
   \[
   \lim_{x \to \bar{x}} k_j x^{v_j} (v'_j - v_j)^T \nabla f(x) = 0.
   \]
From (1)-(3), \( *3 \leq 0 \) has proved. Now we use the same way in 4.6 and get that \( *4 \leq 0 \). So \( \lim_{x \to \bar{x}} f(\tilde{x}) = 1 + *3 + *4 \leq -M' \). Thus, from 4.3 we have proved that \( \tilde{x} \) is not an \( \omega \)-limit point in this case.

5. Some applications on chemical reaction network

In this section we will take the non-equilibrium of complex-balanced and 1d \( W_l \)-endotactic network as research objects to derive the property about \( \omega \)-limit.

5.1. boundary non-equilibrium of Complex balanced network

The complex balanced network is an important class of network. And from [19] we have known that the pseudo-Helmholtz free energy function:

\[
G(x) = \sum_{j=1}^{n} x_j (\ln x_j - \ln x_j^* - 1) + x_j^*, \quad x, x^* \in \mathbb{R}^n_+.
\]  

is a solution of PDE and its boundary condition, where \( x^* \) is a positive equilibrium in the same stoichiometric compatibility class as \( x \).

**Theorem 5.1.** Let \( (S, C, R, k) \) be a complex-balanced chemical reaction system with mass action kinetics. \( k \in \mathbb{R}^r_+ \) is the vector of reaction rate constant. \( \bar{x} \) is boundary non-equilibrium point of this network. Then \( \bar{x} \) is not an \( \omega \)-limit point.

**Proof.** If the mass action system is complex balanced, then pseudo-Helmholtz free energy \( G \) is a solution of Lyapunov Function PDE. And further there exists the only one complex-balanced equilibrium \( x^* \in \mathbb{R}^n_+ \cap (\bar{x} + S) \). Apparently, \( G(x) \) is twice differentiable, and its Hessian matrix can be written as:

\[
\nabla^2 G(x) = \begin{pmatrix}
\frac{1}{x_1} & \cdots \\
\vdots & \ddots \\
\frac{1}{x_n}
\end{pmatrix}
\]

For any \( x \in \mathbb{R}^n_+ \cap (\bar{x} + S) \), \( \nabla^2 G(x) \) is obviously positive definite and diagonally. And as we all known, \( G(x) \) is non-negative and \( \dot{G}(x) \) is strictly negative for non-equilibrium. So from 4.10 \( \bar{x} \) is not an \( \omega \)-limit point. \( \square \)

The complex-balanced network can be an example which applied the above theories. Next, we will further given an example — the 1d \( w \)-endotactic network which PDE’s solution has displayed in [19].
5.2. The Persistence of 1d $W_I$-endotactic network

The 1d network is the network with one-dimensional chemical stoichiometric subspace. $w$ is the basis of this 1d network. Then we stipulate that each $k \in S$, $w_k$ can not be zero. If $w_k$ is zero, the concentration $x_k$ will never changed, then we can remove this species out of our network. We will study persistence of this network by using the solution of the Lyapunov PDE.

As discussed before, we just need to consider the case that $I$ is a semilocking set.

**Proposition 5.2.** Let $(S, C, R, k)$ be a 1d reaction system. $k \in \mathbb{R}_{\geq 0}^r$ is the vector of reaction rate constant. If $W$ is a semilocking set, the corresponding $\bar{x}$ is a boundary equilibrium point.

**Proof.** When the dimension of chemical stoichiometric subspace is one, each element of $S$ can be expressed linearly by another element. So there exists one $w$ in $\mathbb{R}^n \setminus \{0\}$ which is the basis of $\mathcal{S}$. In this case, each reaction vector can be expressed by:

$$v'_{ij} - v_{ij} = m_i w, \forall i = 1, \ldots, r, m_i \in \mathbb{Z} \setminus \{0\}$$

If network has reaction vector $v'_{ij} \rightarrow v_{ij}$ such that $\text{supp } v_{ij} \subseteq \text{supp } \bar{x}$ and $\text{supp } v'_{ij} \subseteq \text{supp } \bar{x}$. Then:

$$w_k = 0, \forall k \in W$$

Therefore, $v'_{k_j} - v_{k_j}$ is equal to zero whenever $k$ belongs to $I$ for each reaction $R_j$. We assume that every species $k$ at least appears in one reaction $R_j$ and there must exist one reaction $R_j$ that can change the concentration of $k$. In this case, there can not have reaction that $\text{supp } v_{ij} \subseteq \text{supp } \bar{x}$ and $\text{supp } v'_{ij} \subseteq \text{supp } \bar{x}$. $I$ is a semilocking set, so there does not exist a reaction vector which satisfies $\text{supp } v_{ij} \subseteq \text{supp } \bar{x}$ and $\text{supp } v'_{ij} \not\subseteq \text{supp } \bar{x}$. As a consequence, for each reaction $R_i$, there is $\text{supp } v_{ij} \not\subseteq \text{supp } \bar{x}$. So $W$ is not only semilocking but also a locking set. In this way, $\bar{x}$ is an equilibrium point. \hfill \Box

From 5.2 we can see it is common that boundary point $\bar{x}$ is an equilibrium when $W$ is a semilocking set. So we want to derive the persistence of 1d $W_I$-endotactic network by proving each $\bar{x}$ is a local maximal point of $f(x)$. First we give the definition of $W_I$-endotactic network.

**Definition 5.3.** Consider the network $(S, C, R, k)$, $I$ is a semilocking set of this system, then we define $w_I$ as:

$$w_I = \begin{cases} 
1, & i \in I, \\
0, & i \notin I.
\end{cases}$$
Then $W_I$ is the set of $w_I$ for all semilocking set $I$ of this network. Then a network is called 1d $W_I$-endotactic network if the network is $w_I$-endotactic network for any semilocking set $I$.

**Lemma 5.4.** $\text{MAS} (S, C, R, k)$ with 1d stoichiometric compatibility class. For arbitrary trajectory $x(t)$ with a positive initial point $x(0)$, there can not exist two species that the one tends to zero and the other one goes to infinity when $t \to \infty$.

**Proof.** We assume $x_i \to \infty$ and $x_j \to 0$ when $t \to \infty$ in order to find a contradiction. We know

$$x(t) - x(0) = mw$$

(21)

for arbitrary $t$. In this case,

$$x(t)_i - x(0)_i = mw_i$$

and $m$ can be arbitrary large when $t$ is enough large. But

$$0 - x(0)_j = mw_j$$

where $m$ is a constant. Then when $t \to \infty$, there doesn’t exist a $m$ such that (21) holds. So our assumption is wrong. □

Above lemma tells us a significant characteristic of 1d network and will help us to obtain that the boundedness of each trajectory in 1d $W_I$-endotactic network which starts at any positive initial point $x(0)$.

**Lemma 5.5.** $(S, C, R, k)$ is a 1d $W_I$-endotactic chemical reaction system with reaction rate constant $k \in \mathbb{R}_{\geq 0}$. Then every trajectory is bounded.

**Proof.** Supposing there exist an initial point $x(0)$ whose trajectory is unbounded, we let $H$ be the set of the species $S_k$ whose concentration $x_k$ can be infinity. Without loss of generality, we suppose $H = \{S_1, \cdot \cdot \cdot, S_{n_1}\}$ with $n_1 \leq n$ is a subset of $S$. [5,4] tells us that there can not exist a species $k_1 \not\in H$ such that $x_{k_1}$ tends to zero. There must exist a point $x(T) \in \mathbb{R}_{\geq 0}^n \cap (x(0) + S)$ such that:

$$x_k(T) - x_k(0) > 0, k = S_1, \cdot \cdot \cdot, S_{n_1}$$

(22)

In addition, $x(T) - x(0) \in \mathcal{S}$. In that case, it can be expressed as:

$$x(T) - x(0) = mw$$

(23)
where $m$ is a constant. $\text{22}$ and $\text{23}$ indicate that

$$mw_k > 0, \ S_k \in H$$

In that case, $w_k$, for all $S_k \in H$ have the same sign. The index set of positive and negative entries of $w$ are denoted by $P_w$ and $N_w$, then either $H \subset P_w$ or $H \subset N_w$.

If $H \subset N_w$, then we can choose $-w$ as the basis of this 1d network. So without loss of generality, let $H \subset P_w$. From our assumption, $x_k$ can trends to infinity. In this case, $m$ trends to infinity. For any $S_{k_3} \in P_w$, $x_{k_3}(T)$ goes to infinity, thus $S_{k_3} \in H$. So we can conclude that $H = P_w$.

And if there exist one $k_3 \in N_w$, when $m \to \infty$, $x_{k_3}(T) < 0$. This is obvious contradiction. So we just need to consider the situation that $H = S$ as the situation of $H \neq S$ is impossible. In this case, $w_k > 0$ for any $k$ in $S$ as $H \subset P_w$. And we can easily learn about that for any $T$ and $k \in S$, $x_k(T)$ can be expressed by:

$$x_k(T) = mw_k + x_k(0).$$

Then for each $k$, there exists:

$$\lim_{m \to \infty} \frac{x_k(T)}{x_k(T)} = \lim_{m \to \infty} \frac{x_k(0) + mw_k}{x_k(0) + mw_1} = \frac{w_k}{w_1} = b'_k$$

$b'_k$ is obvious a positive constant. Then we can choose a constant $m_1$ which is large enough such that when $m > m_1$ for each $k$ there exists

$$b_k \leq \lim_{m \to \infty} \frac{x_k(0) + mw_k}{x_k(0) + mw_1} \leq B_k$$

where $b_k$ and $B_k$ is a positive constant. And further define $Y$ is the set of all $\preceq_{w,s}$-maximal reactant complexes. Then the following equations are satisfied for any $v, j \in Y$.

$$(v_j - v_i)w_S \geq 0 \quad (24)$$

for arbitrary $i \neq j$ where $w_S = (1, 1, ..., 1)^T$. Because any $x \in x(0) + \mathcal{S}$, it can be expressed as $x - x(0) = mw$. So when $m > m_1$

$$b^{v_i,x_1^{v_i,w,S}} = \prod b^{v_i}(x_1(0) + mw_1)^{v_i} < x^{v_i} = \prod_{i \in S} (x_i(0) + mw_k)^{v_i} < B^{v_i,x_1^{v_i,w,S}}$$

Where $b^{v_i}$ and $B^{v_i}$ is constant. Then from explosiveness of exponential function of $x_1$ and $\text{24}$, there exist a constant $m_2$ which is bigger enough such that $m > \max(m_1,m_2)$,namely, $x_1 > \max[x_0 + m_1w_1, x_0 + m_2w_1]$ can indicates

$$x^{v_j} = \prod_{i \in S} (x_i(0) + mw_k)^{v_j} \geq b^{v_i,x_1^{v_i,w,S}} > B^{v_i,x_1^{v_i,w,S}} \geq x^{v_i}, \forall v_j \in Y \text{ and } v_j \notin Y.$$
Combining this with constant reaction rate vector $k$, there exist a constant $m_3$ such that when $m > \max\{m_1, m_3\}$, we can obtain:

$$k_jx^{v_j} > k_ix^{v_i}, \forall v_j \in Y \text{ and } v_j \notin Y.$$

Because the explosion of exponent function about $x_1$, we can find a constant $m_4$ large enough that can get when $m > \max\{m_1, m_4\}$, namely, when $x_1 > \max\{x_k(0) + m_1w_1, x_k(0) + m_4w_1\}$:

$$\sum_{v_j \in Y} k_jx^{v_j} > \sum_{v_i < Y} k_ix^{v_i}.$$  \hspace{1cm} (25)

Because the network is 1d $W_I$-endotactic network and the $v_j \in Y$ is $\leq S$-maximal. And $w_S$ is not orthogonal to the stoichmetric subspace, then any reaction $R_i$ is not orthogonal to $w_S$ for the network is 1d. So there exists

$$(v'_j - v_j) \cdot w_S < 0, \forall v_j \in Y.$$

Combining with

$$v'_j - v_j = mjw$$

where $m_j$ is a constant, we can easily know:

$$-mjw \cdot w_S > 0 \iff m_j < 0$$

as all the elements in $w$ and $w_S$ is positive. At the consequence, $k_j x^{v_j} mj < 0$. The dynamics of the network can be rewritten to:

$$\dot{x} = \sum_{i=1}^{r} k_i x^{v_i}(v'_i - v_i)$$

$$= \sum_{|m_i| > 0} k_i x^{v_i} |m_i| w - \sum_{|m_i| < 0} k_i x^{v_i} |m_i| w$$

where $m_i$ satisfies $v'_i - v_i = mjw$.

So using (25) the above equation implies there exists a constant $m_4$ that $i_k < 0$ when $m > \max\{m_1, m_4\}$, namely $x_k > x_k(0) + mw$. This is contradiction to $x_k$ trends to infinity. So the assumption is wrong, then each $x_k$ is bounded for any $k$. \hfill \square

Above theories have given some related properties about MAS with $\dim S = 1$. Especially, [5, 3] reveals that 1d $W_I$-endotactic network is bounded. In this case, we can use $\omega$-limit point to describe persistent. Now we will use the solution of Lyapunov PDE to get the persistence of 1d $W_I$-endotactic network.
Proposition 5.6. For an $\dim \mathcal{F} = 1 W_1$-endotactic MAS $(S, C, \mathcal{R}, k)$, Firstly, we can see that the Lyapunov Function PDEs can be rewritten as:

$$\sum_{\{l| m_l > 0\}} (k_l x^v) (\sum_{j=0}^{m_l-1} u^j + \sum_{j=m_l}^{r-1} u^j) = 0 \quad (26)$$

where $u = \exp[w^T \nabla f]$, $w \in \mathbb{R}^n \setminus \{0\}$ and $m_l \in \mathbb{Z} \setminus \{0\}$, $l = 1, \cdots, r, \text{satisfying}$

$$v'_l - v_l = -m_l w.$$  

Then we define a scalar function $g(x, u)$ as:

$$g(x, u) = \sum_{\{l| m_l > 0\}} (k_l x^v) (\sum_{j=0}^{m_l-1} u^j + \sum_{j=m_l}^{r-1} u^j).$$  

(27)

it exists a unique $\tilde{u}(x) \in C^2$ such that $g(x, \tilde{u}(x)) = 0$.

In this way, the solution of the PDE above [24] can be defined as:

$$f(x) = \int_0^x \ln \tilde{u}(y_t(x) + \tau w) d\tau \quad (28)$$

where $y_t(x) = C^2(\mathbb{R}_{>0}; \mathbb{R}_n)$ is a twice continuous differential function with respect to $x$. In addition, there also exists another twice continuous differential function $\gamma(x) \in C^2(\mathbb{R}_{>0}; \mathbb{R})$, which together with $y_t(x)$ satisfies

$$x = y_t(x) + \gamma(x) w \quad \text{and} \quad \gamma(x + \delta w) = \gamma(x) + \delta, \forall \delta \in \mathbb{R},$$

where $w$ is a set of bases of $S$.

Proof. The 1-\textit{d} network is $W_1$-endotactic, then neither $\{|m_l| > 0\}$ nor $\{|m_l| < 0\}$ is empty. Combining this with the proof of Proposition 15 in our preceding article [19]. From the first part of the proof of Theorem 18 [19], $f(x)$ satisfies [26] and the boundary condition, obviously. What’s more, the proof reveals $f(x)$ satisfies PDE must have

$$\dot{f}(x) \leq 0$$

for each chemical reaction network. In this case, it is also true for 1d network. \hfill \square

Theorem 5.7. Each 1d $W_1$-endotactic MAS $(S, C, \mathcal{R}, k)$ with $\dim \mathcal{F} = 1$ is persistence.
Proof. Since \( \dim \mathcal{S} = 1 \), let \( w \) denote a set of bases of the network. For arbitrary boundary point \( \bar{x} \), \( f(x) \) is obviously a twice continuous differentiable function defined on \( \mathbb{R}^n_{>0} \) as \( \bar{u}(x), \bar{v}(x), \gamma(x) \in C^2 \). Supposing boundary point \( \bar{x} \) is an \( \omega \)-limit point in order to find a contradiction, and the complement of supp \( \bar{x} \) is denoted by \( W \). Without loss out of generality, let \( W = \{S_1, \cdots, S_m\} \) with \( m \leq n \). In this case, \( \bar{x} \), \( i = S_1, \cdots, S_m \) is zero.

The following part proves that \( \bar{x} \) whose corresponding \( W \) is a semilocking set is a local maximum point in its stoichiometric subspace. For every point \( x \in \mathbb{R}^n_{>0} \cap (\bar{x} + S) \), it can be expressed by \( \bar{x} + \delta w \). From \([?]\) we know either \( W \subset P_w \) or \( W \subset N_w \). Without loss of generality, we let \( W \subset P_w \), otherwise, we can choose \(-w\) as the basis of this 1d network. In this way, \( \delta \) is bigger than zero. So we define \( \bar{u}(\bar{x}) = \lim_{\delta \to 0^+} u(\bar{x} + \delta w) \) and \( f(\bar{x}) = \lim_{\delta \to 0^+} f(\bar{x} + \delta w) \). Now we consider a point \( x \in \mathbb{R}^n_{>0} \cap (\bar{x} + S) \) that \( x \) can be expressed by \( x = \bar{x} + \delta w \) where \( \delta \) is a enough small positive number, then we have:

\[
\lim_{\delta \to 0^+} \frac{f(\bar{x} + \delta w) - f(\bar{x})}{\delta} = \lim_{\delta \to 0^+} \frac{1}{\delta} \int_{\gamma(\bar{x})}^{\gamma(\bar{x} + \delta w)} \ln \bar{u}(y) \gamma(y) w dy \\
= \lim_{\delta \to 0^+} \frac{1}{\delta} \int_{\gamma(\bar{x})}^{\gamma(\bar{x} + \delta w)} \ln \bar{u}(y) \gamma(y) w dy \\
= \lim_{\delta \to 0^+} \frac{1}{\delta} \int_{\gamma(\bar{x})}^{\gamma(\bar{x} + \delta w)} \ln \bar{u}(y) \gamma(y) w dy \\
= \ln \bar{u}(x) + \gamma(x) w
\]

where \( \bar{u}(x) \) is a solution of \( g(x, u) = 0 \).

Further defining \( g(\bar{x}, u) = \lim_{x \to \bar{x}} g(x, u) \), thus \( \bar{u}(\bar{x}) \) satisfies \( g(\bar{x}, \bar{u}(\bar{x})) = 0 \). Now we have known that:

\[
g(\bar{x}, \bar{u}(\bar{x})) = \lim_{x \to \bar{x}} g(x, \bar{u}(x)) \\
= \lim_{x \to \bar{x}} \left( \sum_{|l| > 0} (k_j x^l) \left( \sum_{j=0}^{m-1} u_j^l - \sum_{|l| < 0} (k_j x^l) \left( \sum_{j=m_0}^{m-1} u_j^l \right) \right) \right)
\]

What’s more, let \( Y \) be the set of \( \leq_{w} \)-minimal reactant complexes. Namely, for any \( v \), \( j \in Y \)

\[
(v_j - v) w _{w} \leq 0, \quad i \in W
\]

for any \( i \neq j \) and \( w_w = (1, ..., 1, 0, ..., 0)^T \). Now we choose any \( x(0) \in (\bar{x} + \mathcal{S}) \cup \mathbb{R}^n_{>0} \). Then any \( x \in \bar{x} + \mathcal{S} \) near \( \bar{x} \), it can be expressed as: \( x = x(0) - mw \). And we know each element \( k \in W \) must have one \( m_0 \) that makes \( x_k(0) - m_0 w_k = 0 \) and for \( k \notin W \), \( x_k(0) - m_0 w_k = \bar{x}_k \) where \( \bar{x}_k \) is a positive
constant. In this case, there exists:

\[
\lim_{m \to m_1} \frac{x_k}{x_1} = \lim_{m \to m_1} \frac{x_k(0) - mw_k}{x_1(0) - mw_1} = \frac{w_k}{w_1} = u'_k, k = S_1, \ldots, S_n
\]

\[
\lim_{m \to m_1} x_k = \bar{x}_k, k = S_{m+1}, \ldots, S_n.
\]

We can see that \(u'_k\) is a constant.

So we can choose a positive constant \(\tau_1\) which is small enough such that when \(m_0 - m < \tau_1\) there exists:

\[
u_k \leq \frac{x_k(0) - mw_k}{x_1(0) - mw_1} \leq U_k, k = S_1, \ldots, S_n.
\]

We can write \(x^{v_i}\) as:

\[
x^{v_i} = \prod_{i \in W} x_{k_i}^{v_i} = \prod_{i \in W} (x_k(0) - mw_k)^{v_i} \prod_{i \in W} x_{k_i}^{v_i}.
\]

And for \(m - m_0 < \tau_1\) and any reaction \(R_j\):

\[
u_k x^{v_i, w_i} \triangleq (\prod_{i \in W} u_k^{v_i}) x^{v_i, w_i} = (\prod_{i \in W} u_k^{v_i})(x_k(0) - mw_k)^{v_i + w_i}
\]

\[
\leq \prod_{i \in W} x_k^{w_i} = \prod_{i \in W} (x_k(0) - mw_k)^{v_i} \leq (\prod_{i \in W} U_k^{v_i}) x_k^{v_i} \triangleq U x_k^{v_i, w_i}
\]

Where \(u\) and \(U\) is constant. Then from the property of exponential function when \(x_1\) is small enough and \(v_j \cdot w_i\) is smaller than \(v_i \cdot w_i\) for any \(v_j \in Y\) and \(v_i \notin Y\). Then there exist a constant \(\tau_2\) which is small enough such that \(m_0 - m < \min(\tau_1, \tau_2)\), namely, \(x_1 < \min(x_1(0) - (m_0 - \tau_1)w_i, x_1(0) - (m_0 - \tau_2)w_1)\) can indicates

\[
\prod_{i \in W} x_k^{v_i} \geq \nu_k x^{v_i, w_i} \geq U \prod_{i \in W} x_k^{v_i}
\]

for arbitrary \(v_j \in Y\) and \(v_i \notin Y\). In addition, \(x_0\) is a positive bounded constant with \(k \notin W\). So that means: \(\prod_{i \in W} x_k^{v_i}\) for each reactant complex \(v_i\). Combining this with constant reaction rate vector \(k\), there exist a constant \(\tau_3\) such that when \(m_0 - m < \min(\tau_1, \tau_3)\), we can obtain:

\[
k_j x^{v_i} > k_i x^{v_i}
\]

For the same reason, we can find a constant \(\tau_4\) small enough that can get when \(m_0 - m < \min(\tau_1, \tau_4)\):

\[
\sum_{v_i \in Y} k_j x^{v_j} > \sum_{v_i \notin Y} k_i x^{v_i}
\]

(29)
Because the network is 1d $W_I$-endotactic network and $W$ is a semilocking set so it is $w_W$-endotactic network. Then $v_j \in Y$ is $\leq_{w_W}$-minimal. And $w_W$ is not orthogonal to the stoichiometric subspace, then any reaction $R_i$ is not orthogonal to $w_W$ for the network is 1d. So there exists

$$(v'_j - v_j) \cdot w_W > 0, \forall v_j \in Y.$$ Combining with

$v'_j - v_j = h_j w$

where $h_j$ is a constant, we can easily know:

$$h_j w \cdot w_W > 0. \quad (30)$$

And as $W \in P_u$, we can know $w_k > 0, k \in W$. Thus

$$w \cdot w_W = \sum_{k=1}^{n} w_k > 0.$$ So from (30) we obtain $h_j > 0$. In this case $\sum_{|h| > 0} k_i x^{|i|}$ can be arbitrary large compared with $\sum_{|h| < 0} k_i x^{|i|}$ when $x \to \bar{x}$. Thus from $g(\bar{x}, \tilde{u} (\bar{x})) = 0$ we can obtain

$$\lim_{x \to \bar{x}} \sum_{|h| > 0} k_i x^{|i|} (\sum_{j=h} \tilde{u}_j) = \lim_{x \to \bar{x}} \sum_{|h| < 0} k_i x^{|i|} (\sum_{j=h} (-1)^{|j|} \tilde{u}_j).$$

Thus we can find only $\tilde{u}(\bar{x}) << 1$ that this equality holds. This can indicates that:

$$\lim_{\delta \to 0} \frac{f(\bar{x} + \delta w) - f(\bar{x})}{\delta} = \ln \tilde{u}(\bar{x}) < 0. \quad (31)$$

Thus, $\bar{x}$ is a local maximum point if the corresponding $W$ is a semilocking set. But 4.4 and 5.6 implies that $\bar{x}$ is not an $\omega$-limit point. Since each boundary point which semilocking set corresponding to is not $\omega$-limit point, we obtain 1d $W_I$-endotactic network is persistent. $\square$

6. Examples and Conclusion

This section we will present some examples to help us understand above theories.
Example 4. First we consider the following network:

\[ 2S_1 \rightleftharpoons S_1 + S_2 \rightarrow 2S_2 \]

The reaction rate constant \( k \) of \( R = \{ 2S_1 \rightarrow S_1 + S_2, S_1 + S_2 \rightarrow 2S_1, S_1 + S_2 \rightarrow 2S_2 \} \) is \( k = (k_1, k_2, k_3)^T \). And reaction vectors constitute the matrix \( S \):

\[
S = \begin{pmatrix}
-1 & 1 & -1 \\
1 & -1 & 1
\end{pmatrix}
\]

The dynamical equation has the following form:

\[
\dot{x} = S v = k_1 x_1^2 + \begin{pmatrix}
-k_1 x_1^2 + (k_1 - k_3) x_1 x_2 \\
-k_1 x_1^2 - (k_1 - k_3) x_1 x_2
\end{pmatrix}
\]

And we can easily see this is an 1-d network but it is not endotactic. At the same time, \cite{19} tells us that the solution of the Lyapunov PDE of 1-d network is:

\[
f(x) = \int_0^{\gamma(x)} \ln \tilde{u}(y^\top(x) + \tau w) d\tau.
\]

Now we consider two specific boundary points.

(1) \( \bar{x} = (l_1, 0)^T \) where \( l_1 > 0 \) is a constant and \( W = \{ S_2 \} \). We can get \( W \) is not a semilocking set. Choose \( w = (-1, 1)^T \) as a set of basis for \( W \). In this case, \( m_1 = 1, m_2 = -1, \) and \( m_3 = 1 \).

Thus:

\[
P_w = \{ 2 \}, N_w = \{ 1 \} \text{ and } g(x, u) = k_1 x_1^2 + k_3 x_1 x_2 - k_2 x_1 x_2 u^{-1}.
\]

we can use \( (x_1 - m, x_2 + m)^T \) to express any point in \( (x + \mathcal{M}) \subset \mathbb{R}_2^2 \). In this case,

\[
J(y^\top) = x_2 + m - x_1 + m = 0 \Rightarrow m = \frac{x_1 - x_2}{2} \text{ and } y^\top = \begin{pmatrix}
\frac{x_1 + x_2}{2} \\
\frac{x_1 - x_2}{2}
\end{pmatrix} = \frac{1}{2} \begin{pmatrix}
\mathbb{1}_2^\top \\
\mathbb{1}_2^T
\end{pmatrix} x
\]

Further, setting \( g(x, u) = 0 \) we can obtain:

\[
\gamma(x) = \frac{w^\top x}{2} \text{ and } \tilde{u}^{-1}(x) = \frac{k_1 x_1^2 + k_3 x_1 x_2}{k_2 x_1 x_2} \Rightarrow \tilde{u}(x) = \frac{k_3 x_2}{k_1 x_1 + k_3 x_2}
\]

In this case, \( f(x) \) can be written as:

\[
f(x) = \int_0^{\gamma(x)} \ln \frac{1}{2} \left( \begin{array}{cc}
1 & 1 \\
1 & 1
\end{array} \right) x + \tau w d\tau.
\]
Then let \( f(x) \) express the derivative of \( f(x) \) about \( t \) we obtain:

\[
\lim_{x \to \bar{x}} \dot{f}(x) = \lim_{x \to \bar{x}} \left( k_1 x_1^2 w^\top \nabla f(x) + k_3 x_1 x_2 w^\top \nabla f(x) - k_2 x_1 x_2 w^\top \nabla f(x) \right)
= \lim_{x \to \bar{x}} \frac{k_2 x_2}{k_1 x_1 + k_3 x_2} = -\infty.
\]

From [4,3] we know \( \bar{x} = (l_1, 0)^\top \) is not an \( \omega \)-limit point for any rate constant \( k \) and any \( l_1 > 0 \).

(2) \( \bar{x} = (0, l_2)^\top \) and \( W = \{ S_1 \} \) is a semilocking set. In this case,

\[
\lim_{x \to \bar{x}} \dot{f}(x) = 0.
\]

Now we consider if it is the local maximal point of \( f(x) \). So we want find the value of:

\[
w^\top \nabla f(x) = \lim_{\delta \to 0^+} \frac{f(\bar{x} + \delta w) - f(\bar{x})}{\delta} = \ln \tilde{u}(\bar{x})
\]

(32)

\( \delta < 0 \) in above equation because \( W \in N_w \). \( \tilde{u}(x) \) is the solution of \( g(x, u) \):

\[
g(x, u) = k_1 x_1^2 + k_3 x_1 x_2 - k_2 x_1 x_2 u^{-1} = 0
\]

\[
\Rightarrow \ln \tilde{u}(\bar{x}) = \lim_{x \to \bar{x}} \ln \tilde{u}(x) = \lim_{x \to \bar{x}} \frac{k_2 x_2}{k_1 x_1 + k_3 x_2}
\]

So if \( k_2 = 1, k_3 = 2 \), \( \ln \tilde{u}(\bar{x}) = \ln \frac{1}{2} < 0 \). Further with (32) we get \( \bar{x} \) is not the local maximal point of \( f(x) \). But if \( k_2 = 2, k_3 = 1 \), \( \ln \tilde{u}(\bar{x}) = \ln 2 > 0 \). In this case, \( f(\bar{x}) \) is the local maximum of \( f(x) \).

(3) \( \bar{x} = (0, 0)^\top \) and \( W = \{ S_1, S_2 \} \). We can see the dimension of phase space is 2, but the stiochiometric subspace is 1d. So \( (1, 1)^\top \) is a conversation law of this network. Thus if initial point \( x(0) \) is positive, \( x(t) \) can not trend to \( \bar{x} \). In other words, the face \( L_W \) is unattainable.

In conclusion, from (1)-(3), we can see the persistence of this 1-d not endotactic network depends on the reaction rate.

Now we want to introduce an 1d \( W_I \)-endotactic network to see if there exists any differences?

**Example 5.** The mass action system \( (S, C, R, k) \):

\[
2S_1 \rightarrow S_1 + S_2
\]

\[
2S_2 + S_1 \rightarrow 3S_1
\]

This network is obvious not an endotactic network w from [2] The reaction vectors form the matrix \( S \):

\[
S = \begin{pmatrix}
-1 & 2 \\
1 & -2 \\
3 & 5
\end{pmatrix}
\]
And the dynamical equation is

\[ \dot{x} = Sv = \begin{pmatrix} -1 & 2 \\ 1 & -2 \end{pmatrix} \begin{pmatrix} k_1 x_1^3 \\ k_2 x_1 x_2^2 \end{pmatrix} = \begin{pmatrix} -k_1 x_1^3 + 2k_2 x_1 x_2^2 \\ k_1 x_1^3 - 2k_2 x_1 x_2^2 \end{pmatrix} \]  

(33)

We let \( w = (1 - 1)^\top \), thus \( m_1 = -1, m_2 = 2 \). And corresponding \( P_w = \{S_1\} \) and \( N_w = \{S_2\} \). Now we consider the boundary point of this network:

(1) \( \bar{x} = (l_1, 0)^\top \) and \( W = \{S_2\} \). It is obvious that \( W \) is not a semilocking set. Then \( \bar{x} \) can not be \( \omega \)-limit.

(2) \( \bar{x} = (0, l_2)^\top \) and \( W = \{S_1\} \). \( W \) is a semilocking set. Then we let \( w_W = (1, 0)^\top \) and project this network in the line \( w_W \) lies in. From the \( W \) we obtain it is \( w_W \)-endotactic. In this case, we can obtain:

\[ \lim_{x \to \bar{x}} f(x) = 0 \]

So next we judge if \( \bar{x} \) is a local maximal point. Thus we consider:

\[ w^\top \triangledown f(x) = \lim_{\delta \to 0^+} \frac{f(\bar{x} + \delta w) - f(\bar{x})}{\delta} = \ln \bar{u}(\bar{x}) \]  

(34)

\( \delta > 0 \) there because \( W \in P_w \). And:

\[ g(x, u) = k_2 x_1 x_2^2 (1 + u) - k_1 x_1^3 \frac{1}{u} \]
Then we can obtain:
\[ \tilde{u}(x) = \frac{-k_1 x_1 x_2^2 + (k_1^2 x_1^2 x_2^4 + 4k_1 k_2 x_1^3 x_2^2)^{1/2}}{2k_1 x_1 x_2^2} \]
When \( x \to \bar{x} \), namely \( x_1 \to 0 \), we can obtain \( \lim_{x \to \bar{x}} \tilde{u}(x) = 0 \).

\[ \ln \tilde{u}(x) = \lim_{x \to \bar{x}} \ln u(x) = \lim_{x \to \bar{x}} \frac{k_1 x_2^3}{k_2 x_2^2} < 0 \]
for any \( k \). So \( \bar{x} \) is an \( \omega \)-limit point for any \( k \).

(3) \( \bar{x} = (0, 0)^\top \) and \( W = \{ S_1, S_2 \} \). \( w_W \) is orthogonal to the stoichiometric subspace. So it is \( w_W \)-endotactic As we know \( W \subset P_{w} \), \( \bar{x} \) can not be the boundary of stoichiometric compatibility class of positive initial point \( x(0) \). So \( \bar{x} \) is unattainable.

So from (1)-(3), we can conclude that this 1d \( W_1 \)-endotactic network is persistent independent of reaction rate \( k \).

Next we want to research another important network—complex balanced network.

**Example 6.**

\[
\begin{align*}
2S_1 & \rightleftharpoons S_1 + S_2 \\
S_2 & \rightleftharpoons S_3
\end{align*}
\]

The reaction rate \( k \) of \( R = \{ 2S_1 \rightarrow S_1 + S_2, S_1 + S_2 \rightarrow 2S_1, S_2 \rightarrow S_3, S_3 \rightarrow S_2 \} \) is: \( k = \{ k_1, k_2, k_3, k_4 \} \). And the matrix of reaction rate vector is:

\[
S = \begin{pmatrix}
-1 & 1 & 0 & 0 \\
1 & -1 & -1 & 1 \\
0 & 0 & 1 & -1
\end{pmatrix}
\]

It is not difficult to verify \( \text{dim} S = 2 \), and the network has two linkage classes. Thus the deficiency of this network is zero, in this case, this network is complex balanced regardless of the \( k \). The dynamical equations:

\[
\dot{x} = S v = \begin{pmatrix}
-1 & 1 & 0 & 0 \\
1 & -1 & -1 & 1 \\
0 & 0 & 1 & -1
\end{pmatrix} \begin{pmatrix}
x_1^2 \\
x_1 x_2 \\
x_2 \\
x_3
\end{pmatrix} = \begin{pmatrix}
-x_1^2 + x_1 x_2 \\
x_1^2 - x_1 x_2 + x_2 - x_3 \\
x_2 - x_3
\end{pmatrix}
\]

37
When $\dot{f}(x) = 0$, the equilibrium is $x^* = (1, 1, 1)^\top$. Then the derivative of the solution of Lyapunov PDE for complex balanced network can be written as:

$$
\dot{f}(x) = \dot{x} \ln \frac{x}{x^*}
= \ln x_1(-x_1^2 + x_1 x_2) + \ln x_2(x_1^2 - x_1 x_2 - x_3) + \ln x_3(x_2 - x_3)
$$

If we choose $\bar{x}$ as:

$$
\begin{pmatrix} l_1 \\ 0 \\ l_3 \end{pmatrix}, \text{ or } \begin{pmatrix} l_1 \\ l_2 \\ 0 \end{pmatrix}, \text{ or } \begin{pmatrix} l_1 \\ 0 \\ l_3 \end{pmatrix}, \text{ or } \begin{pmatrix} 0 \\ l_2 \\ 0 \end{pmatrix},
$$

And the corresponding $W$ are:

$$
W_1 = \{S_2\}, \quad W_2 = \{S_3\}, \quad W_3 = \{S_2, S_3\}, \quad W_4 = \{S_1, S_2\}, \quad W_5 = \{S_1, S_3\}.
$$

respectively. They are all not semilocking set. In this case, we can obtain:

$$
\lim_{x \to \bar{x}} \dot{f}(x) = -\infty
$$

through calculating. From [4, 5], boundary points with above shape are not $\omega$-limit points.

Next we consider the boundary point $\bar{x} = (0, l_2, l_3)^\top$ whose corresponding $W = \{S_1\}$ is a semilocking set. When $x$ trends to $\bar{x}$, there exists:

$$
\lim_{x \to \bar{x}} \dot{f}(x) = \lim_{x \to \bar{x}}(-l_2^2 \ln l_1 + l_1 l_2 \ln l_1 + l_2(-l_2 + l_3) + \ln l_3(l_2 - l_3))
= 0 + (l_2 - l_3)(\ln l_3 - \ln l_2) \leq 0.
$$

If $\bar{x}$ is not an equilibrium of this network, namely, $l_2$ is not equal to $l_3$, $\lim_{x \to \bar{x}} \dot{f}(x) = -M$ where $-M = (l_2 - l_3)(\ln l_3 - \ln l_2)$. If $\bar{x}$ is a boundary equilibrium, $\lim_{x \to \bar{x}} \dot{f}(x) = 0$.

We can also use [4, 10] to obtain all boundary non-equilibrium are not $\omega$-limit points.

Our previous context derives a partial differential equation whose solution can be a Lyapunov function candidate in a microcosmic perspective [19]. Its main purpose is to make some contributions to stability. Our paper devotes to finding that the Lyapunov function PDE not only help to judge the stability but also play an important role in persistence or $\omega$-limit points. We link the PDE with the persistence through the boundary conditions of PDE and the characteristics of PDE’s solution. We give several sufficient conditions to judge whether or not boundary point
is an $\omega$-limit point. As a result, we can use them to help obtain persistence property of some network: such as 1d $W_I$-endotactic network. Next we want to research the relationship between other regions of CRN and PDE such as chemical oscillation and we will further to find more connections of persistence and PDE.

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