

ON THE PARAMETRIC UNCERTAINTY OF WEAKLY REVERSIBLE REALIZATIONS OF KINETIC SYSTEMS

GYÖRGY LIPTÁK ^{✉1}, GÁBOR SZEDERKÉNYI^{1,2} AND KATALIN M. HANGOS^{1,3}

¹Process Control Research Group, MTA SZTAKI, Kende u. 13-17, Budapest, 1111, HUNGARY

²Faculty of Information Technology, Péter Pázmány Catholic University, Práter u. 50/a, Budapest, 1083, HUNGARY

³Department of Electrical Engineering and Information Systems, University of Pannonia, Egyetem u. 10,
Veszprém, 8200, HUNGARY

[✉]E-mail: lipgyorgy@gmail.com

The existence of weakly reversible realizations within a given convex domain is investigated. It is shown that the domain of weakly reversible realizations is convex in the parameter space. A LP-based method of testing if every element of a convex domain admits weakly reversible realizations is proposed. A linear programming method is also presented to compute a stabilizing kinetic feedback controller for polynomial systems with parametric uncertainty. The proposed methods are illustrated using simple examples.

Keywords: parametric uncertainty; computational methods; optimization; kinetic systems

Introduction

The notion of parametric robustness is well-known and central in linear and nonlinear systems and control theory [1]. It is used for ensuring a desirable property, such as stability, in a given domain in the parameter space around a nominal realization having the desired property.

The aim of the paper is to extend the notions and tools of parametric robustness for a class of positive polynomial systems, namely a class of kinetic systems. Only the very first steps are reported here that offer a computationally efficient method for checking one of the many important properties of kinetic systems, their weak reversibility.

Basic Notions and Methods

The basic notions and tools related to reaction kinetic systems and their realizations are briefly summarized in this section.

Kinetic Systems, their Dynamics and Structure

Deterministic kinetic systems with mass action kinetics or simply chemical reaction networks (CRNs) form a wide class of non-negative polynomial systems, that are able to produce all the important qualitative phenomena (e.g. stable/unstable equilibria, oscillations, limit cycles, multiplicity of equilibrium points and even chaotic behaviour) present in the dynamics of nonlinear processes [2].

The general form of dynamic models studied in this paper is the following

$$\dot{x} = M \cdot \psi(x), \quad (1)$$

where $x \in \mathbb{R}^n$ is the state variable and $M \in \mathbb{R}^{n \times m}$. The monomial vector function $\psi : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is defined as

$$\psi_j(x) = \prod_{i=1}^n x_i^{Y_{ij}}, \quad j = 1, \dots, m \quad (2)$$

where $Y \in \mathbb{N}_0^{n \times m}$. The system Eq.(1) is kinetic if and only if the matrix M has a factorization

$$M = Y \cdot A_k. \quad (3)$$

The Kirchhoff-matrix A_k has non-positive diagonal and non-negative off-diagonal elements and zero column sums. The matrix pair (Y, A_k) is called the realization of the system Eq.(1).

The chemically originated notions: The chemically originated notions of kinetic systems are as follows: the *species* of the system are denoted by X_1, \dots, X_n , and the concentrations of the species are the state variables of Eq.(1), i.e. $x_i = [X_i] \geq 0$ for $i = 1, \dots, n$. The structure of kinetic systems is given in terms of its *complexes* C_i , $i = 1, \dots, m$ that are non-negative linear combinations of the species i.e. $C_i = \sum_{j=1}^n [Y]_{ji} X_j$ for $i = 1, \dots, m$, and therefore Y is also called the *complex composition matrix*.

The reaction graph: The weighted directed graph (or reaction graph) of kinetic systems is $G = (V, E)$, where

$V = \{C_1, C_2, \dots, C_m\}$ and E denote the set of vertices and directed edges, respectively. The directed edge (C_i, C_j) (also denoted by $C_i \rightarrow C_j$) belongs to the reaction graph if and only if $[A_k]_{j,i} > 0$. In this case, the weight assigned to the directed edge is $C_i \rightarrow C_j$ is $[A_k]_{j,i}$.

Stoichiometric subspace: Stoichiometric subspace S is given by the span of the reaction vectors

$$S = \{[Y]_{\cdot i} - [Y]_{\cdot j} \mid [A_k]_{ij} > 0\}. \quad (4)$$

The stoichiometric compatibility classes of a kinetic system are the affine translations of the stoichiometric subspace: $(x_0 + S) \cap \mathbb{R}_{\geq 0}^n$.

Structural Properties and Dynamical Behaviour

It is possible to utilize certain structural properties of kinetic systems that enable us to effectively analyze the stability of the system.

Deficiency: There are several equivalent ways to define deficiency. We will use the following definition

$$\delta = \dim(\ker(Y) \cap \text{Im}(B_G)), \quad (5)$$

where B_G is the incidence matrix of the reaction graph. It is easy to see that deficiency is zero if $\ker(Y) = \{0\}$ or equivalently $\text{rank}(Y) = m$.

Weak reversibility: A CRN is called *weakly reversible* if whenever there exists a directed path from C_i to C_j in its reaction graph, then there exists a directed path from C_j to C_i . In graph theoretic terms, this means that all components of the reaction graph are strongly connected components.

Deficiency zero theorem: A weakly reversible kinetic system with zero deficiency has precisely one equilibrium point in each positive stoichiometric compatibility class that is locally asymptotically stable (conjecture: globally asymptotically stable).

Computing Weakly Reversible Realizations Formulated as an Optimization Problem

In this section, first a method for computing weakly reversible realization based on Ref.[3] is briefly presented. We assume that we have a kinetic polynomial system of the form Eq.(1).

We use the fact known from the literature that a realization of a CRN is weakly reversible if and only if there exists a vector with strictly positive elements in the kernel of A_k , i.e. there exists $b \in \mathbb{R}_+^n$ such that $A_k \cdot b = 0$ [4]. Since b is unknown, too, this condition in this form is not linear. Therefore, we introduce a scaled matrix \tilde{A}_k

$$\tilde{A}_k = A_k \cdot \text{diag}(b) \quad (6)$$

where $\text{diag}(b)$ is a diagonal matrix with elements of b . It is clear from Eq.(6) that \tilde{A}_k is also a Kirchhoff matrix

and that $\mathbf{1} \in \mathbb{R}^m$ (the m -dimensional vector containing only ones) lies in kernel of \tilde{A}_k . Moreover, it is easy to see that \tilde{A}_k defines a weakly reversible network if and only if A_k corresponds to a weakly reversible network. Then, the weak reversibility and the Kirchhoff property of \tilde{A}_k can be expressed using the following linear constraints

$$\begin{aligned} \sum_{i=1}^m [\tilde{A}_k]_{ij} &= 0, \quad j = 1, \dots, m \\ \sum_{i=1}^m [\tilde{A}_k]_{ji} &= 0, \quad j = 1, \dots, m \\ [\tilde{A}_k]_{ij} &\geq 0, \quad i, j = 1, \dots, m, \quad i \neq j \\ [\tilde{A}_k]_{ii} &\leq 0, \quad i = 1, \dots, m. \end{aligned} \quad (7)$$

Moreover, the equation Eq.(3) is transformed by $\text{diag}(b)$ (we can do this, because $\text{diag}(b)$ is invertible):

$$M \cdot \text{diag}(b) = Y \cdot \underbrace{A_k}_{\tilde{A}_k} \cdot \text{diag}(b) \quad (8)$$

Finally, by choosing an arbitrary linear objective function of the decision variables \tilde{A}_k and b , weakly reversible realizations of the studied kinetic system can be computed (if any exist) in a LP framework using the linear constraints Eq.(7) and (8).

Weakly Reversible CRN Realizations

In this section, first the convexity of the weakly reversible Kirchhoff matrix will be shown. After that the practical benefits of this property will be demonstrated in the field of system analysis and robust feedback design.

Convexity of the Weak Reversibility in the Parameter Space

Theorem 1. Let $A_k^{(1)}$ and $A_k^{(2)}$ be $m \times m$ weakly reversible Kirchhoff matrices. Then the convex combination of the two matrices remains weakly reversible.

Proof. The idea behind the proof is based on Ref.[5]. A Kirchhoff matrix is weakly reversible if and only if there is a strictly positive vector in its kernel. Therefore strictly positive vectors p_1, p_2 exist such as $A_k^{(1)} \cdot p_1 = 0$ and $A_k^{(2)} \cdot p_2 = 0$. Let us define the following scaled Kirchhoff matrix: $\hat{A}_k^{(1)} = A_k^{(1)} \cdot \text{diag}(p_1)$ and $\hat{A}_k^{(2)} = A_k^{(2)} \cdot \text{diag}(p_2)$. These scaled matrices have identical structures to the original ones. Moreover, $\hat{A}_k^{(1)} \cdot \mathbf{1}^{(m)} = 0$ and $\hat{A}_k^{(2)} \cdot \mathbf{1}^{(m)} = 0$ where the vector $\mathbf{1}^{(m)}$ denotes the m dimensional column vector composed of ones. For that

$$(\lambda \hat{A}_k^{(1)} + (1 - \lambda) \hat{A}_k^{(2)}) \cdot \mathbf{1}^{(m)} = 0. \quad (9)$$

for any $\lambda \in [0, 1]$. Therefore the convex combination of the original two realizations has to be weakly reversible. \square

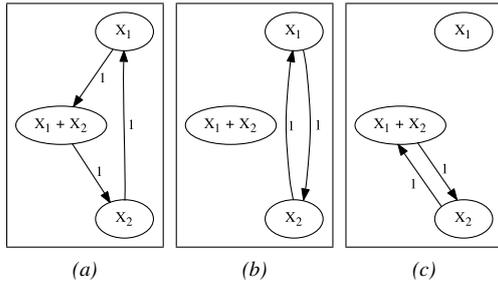


Figure 1: A weakly reversible reaction graphs of the three realizations $(Y, A_k^{(1)})$, $(Y, A_k^{(2)})$ and $(Y, A_k^{(3)})$

Weak Reversibility of CRN Realizations with Parametric Uncertainty

We assume that a CRN with parametric uncertainty is given as

$$\dot{x} = M \cdot \psi(x), \quad (10)$$

where $x \in \mathbb{R}^n$ is the state variable, $\psi \in \mathbb{R}^n \rightarrow \mathbb{R}^m$ contains the monomials and the matrix $M \in \mathbb{R}^{n \times m}$ is an element of the following set

$$\mathcal{M} = \left\{ \sum_{i=1}^l \alpha_i M_i \mid (\forall i : \alpha_i \geq 0) \wedge \sum_{i=1}^l \alpha_i = 1 \right\}. \quad (11)$$

The goal is to find a method for checking the weak reversibility of the system Eq.(10) for all matrices $M \in \mathcal{M}$.

When all vertices M_i have a weakly reversible realization $(Y, A_k^{(i)})$ then any element of the set \mathcal{M} has a realization (Y, A_k) such that A_k is the convex combination of the Kirchhoff matrices $A_k^{(i)}$. The obtained realization A_k will be weakly reversible due to Theorem 1. Therefore, it is enough to compute a weakly reversible realization for each matrix M_i by using the previously presented LP-based method.

A Simple Example

Let us consider the following polynomial system

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = M \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{bmatrix}, \quad (12)$$

where M is an arbitrary convex combination of the following three matrices

$$M_1 = \begin{bmatrix} 0 & 1 & -1 \\ 1 & -1 & 0 \end{bmatrix},$$

$$M_2 = \begin{bmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \end{bmatrix}, \text{ and}$$

$$M_3 = \begin{bmatrix} 0 & 1 & -1 \\ 0 & 0 & 0 \end{bmatrix}.$$

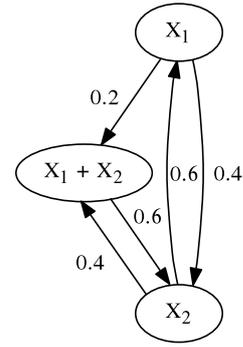


Figure 2: A weakly reversible realization of the convex combination $M = 0.2M_1 + 0.4M_2 + 0.4M_3$

In order to show weak reversibility for all possible convex combinations, we have to find a weakly reversible realization for each matrix M_1 , M_2 and M_3 . The resulting weakly reversible reaction graphs are depicted in Fig.1, while Fig.2 illustrates an inner point realization which is weakly reversible too.

Computing Kinetic Feedback for a Polynomial System with Parametric Uncertainty

Besides the possible application of the above described LP-based method for robust stability analysis, it can also be used for stabilizing feedback controller design. For this purpose, a generalized version of our preliminary work on kinetic feedback computation for polynomial systems to achieve weak reversibility and minimal deficiency [6] is used here.

The Feedback Design Problem

We assume that the equation of the open-loop polynomial system with linear constant parameter input structure is given as

$$\dot{x} = M \cdot \psi(x) + Bu, \quad (13)$$

where $x \in \mathbb{R}^n$ is the state vector, $u \in \mathbb{R}^p$ is the input and $\psi \in \mathbb{R}^n \rightarrow \mathbb{R}^m$ contains the monomials of the open-loop system. The input matrix is $B \in \mathbb{R}^{n \times p}$, the corresponding complex composition matrix is Y with rank m , and $M \in \mathbb{R}^{n \times m}$ is an element of the following set

$$\mathcal{M} = \left\{ \sum_{i=1}^l \alpha_i M_i \mid (\forall i : \alpha_i \geq 0) \wedge \sum_{i=1}^l \alpha_i = 1 \right\}. \quad (14)$$

Moreover, a positive vector $\bar{x} \in \mathbb{R}_{>0}^n$ being the desired equilibrium point is given as a design parameter. Note that the above polynomial system is not necessarily kinetic, i.e. not necessarily positive, and may not have a positive equilibrium point at all.

The aim of the feedback is to set a region in the state space $R \subseteq \mathbb{R}_{\geq 0}^n$ where \bar{x} is (at least) a locally asymptotically stable equilibrium point of the closed-loop system for all $M \in \mathcal{M}$.

For this purpose we are looking for a feedback in the form

$$u = K\psi(x) \quad (15)$$

which transforms the open-loop system into a weakly reversible kinetic system with zero deficiency for all $M \in \mathcal{M}$ with the given equilibrium point \bar{x} .

Feedback Computation

Similarly to the realization computation, the matrix K will be determined by solving an LP problem. The convexity result shows that it is enough to compute one weakly reversible realization $(Y, A_k^{(r)})$ in each vertex M_r to ensure weak reversibility for all possible closed-loop systems. All realizations will have zero deficiency, because of the rank condition $\text{rank}(Y) = m$ [7].

First we note, that the realization $(Y, A_k^{(r)})$ that corresponds to the closed-loop system is

$$M_r + B \cdot K = Y \cdot A_k^{(r)}. \quad (16)$$

where the matrix $A_k^{(r)}$ should be Kirchhoff

$$\begin{aligned} \sum_{i=1}^m [\tilde{A}_k]_{ij} &= 0, \quad j = 1, \dots, m \\ [\tilde{A}_k]_{ij} &\geq 0, \quad i, j = 1, \dots, m, \quad i \neq j \\ [\tilde{A}_k]_{ii} &\leq 0, \quad i = 1, \dots, m. \end{aligned} \quad (17)$$

In order to obtain a weakly reversible closed-loop system with an equilibrium point \bar{x} , the matrix $A_k^{(r)}$ should be weakly reversible and has to have the vector $\psi(\bar{x})$ in its right kernel, i.e.

$$A_k^{(r)} \cdot \psi(\bar{x}) = 0. \quad (18)$$

Finally, by choosing an arbitrary linear objective function of the decision variables $A_k^{(1)}, \dots, A_k^{(l)}$ and K , the feedback gain K can be computed (if it exists) in a LP framework using the linear constraints Eqs.(16-18).

With the resulting feedback gain K , the point \bar{x} will be an equilibrium point of all possible closed-loop systems, and \bar{x} will be locally asymptotically stable in the region $\mathcal{S} = (\bar{x} + S) \cap \mathbb{R}_{\geq 0}^n$, where S is the stoichiometric subspace of the closed-loop system.

Example

Let the open-loop system be given as

$$\dot{x} = M \begin{bmatrix} x_1 x_2 \\ x_2 x_3 \\ x_1 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} u \quad (19)$$

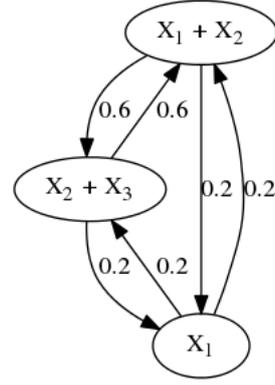


Figure 3: Weakly reversible realization of the closed-loop system, where

$$M = 0.6M_1 + 0.2M_2 + 0.2M_3$$

where M is an arbitrary convex combination of the following three matrices:

$$M_1 = \begin{bmatrix} -1 & 1 & 0 \\ 2 & 1 & 2 \\ 1 & -1 & 0 \end{bmatrix},$$

$$M_2 = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 1 & 3 \\ 0 & 0 & 0 \end{bmatrix}, \text{ and}$$

$$M_3 = \begin{bmatrix} 0 & 1 & -1 \\ 2 & 0 & 3 \\ 0 & -1 & 1 \end{bmatrix}.$$

The desired equilibrium point $\bar{x} = [1 \ 1 \ 1]^T$.

We are looking for a feedback law with gain K which transforms the matrices M_i into weakly reversible kinetic systems with the given equilibrium point.

By solving the feedback design LP optimization problem using the linear constraints Eqs.(16-18), the computed feedback is in the following form:

$$u = [2 \ 1 \ 2] \psi(x). \quad (20)$$

Fig.3 depicts a weakly reversible realization of the closed-loop system. The obtained closed-loop system in an inner point of the convex set \mathcal{M} has the following stoichiometric subspace:

$$S = \text{span} \left(\left(\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} - \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} - \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \right) \right). \quad (21)$$

Therefore, the equilibrium point \bar{x} will be asymptotically stable with the region $\mathcal{S} = (\bar{x} + S) \cap \mathbb{R}_{\geq 0}^n$. Note, that one should choose the initial value of the state variables from \mathcal{S} .

Fig.4 shows the time dependent behaviour of the closed-loop solutions started from different initial points in \mathcal{S} .

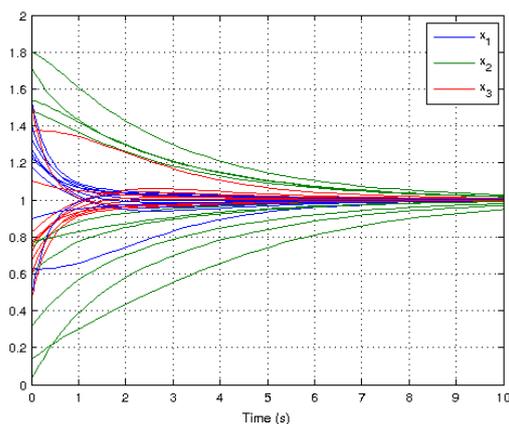


Figure 4: Time-domain simulation of the closed-loop system

Conclusion

It is shown in this paper that the domain of weakly reversible realizations is convex in the parameter space. This property is utilized for developing methods in system analysis and robust control design. An LP-based optimization method is proposed for testing if every element of a convex domain given by its extremal matrices admits a weakly reversible realization. An LP-based feedback design method is also proposed that guarantees stability with a desired equilibrium point. The proposed methods are illustrated with simple examples.

REFERENCES

- [1] SILJAK D.: Parameter space methods for robust control design: a guided tour, *Aut. Contr., IEEE Transactions on*, 1989, 34(7), 674–688
- [2] ANGELI D.: A tutorial on chemical network dynamics, *Eur. J. Contr.*, 2009, 15, 398–406
- [3] SZEDERKÉNYI G., HANGOS K. M., TUZA Z.: Finding weakly reversible realizations of chemical reaction networks using optimization, *MATCH Commun. Math. Comp. Chem.*, 2012, 67, 193–212
- [4] FEINBERG M., HORN F.: Chemical mechanism structure and the coincidence of the stoichiometric and kinetic subspaces, *Arch. Rational Mechanics and Analysis*, 1977, 66(1), 83–97
- [5] RUDAN J., SZEDERKÉNYI G., HANGOS K.M., PÉNI T.: Polynomial time algorithms to determine weakly reversible realizations of chemical reaction networks, *J. Math. Chem.*, 2014, 52(5), 1386–1404
- [6] LIPTÁK G., SZEDERKÉNYI G., HANGOS K.M.: Kinetic feedback computation for polynomial systems to achieve weak reversibility and minimal deficiency, 13th Eur. Control Conf. ECC, Strasbourg, France, 2014, 2691–2696
- [7] ANGELI D., LENHEE, P.D., SONTAG E.D.: On the structural monotonicity of chemical reaction networks, *Proc. 45th IEEE Conf. Decision and Control*, 2006, 7–12