Optimization-based design of kinetic feedbacks for nonnegative polynomial systems

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***Abstract*—Motivated by the strong results on the relation between the dynamics and graph structure of kinetic systems, static and dynamic feedbacks for polynomial nonlinear systems are proposed in this paper that render the open loop system into weakly reversible kinetic form. The solution of the problem is based on optimization, and uses earlier results on computing different realizations of kinetic systems. The operation of the method is shown through illustrative example.**

I. Introduction

Nonnegative dynamical systems are characterized by the property that the state variables always remain nonnegative during the operation, i.e. the nonnegative orthant is invariant for the dynamics. These systems appear primarily in such applications where nonnegative physical variables (e.g. concentrations, pressures, number of items in a set etc.) describe the state of the studied systems. Therefore the main application areas of nonnegative systems are chemistry, biology, thermodynamics, population and epidemic modeling or even certain transportation processes. It is important to note that any bounded operation domain of a general non-positive system can be easily shifted into the nonnegative orthant.

Deterministic kinetic systems with mass action kinetics or simply chemical reaction networks (CRNs) form a wide class of nonnegative systems. CRNs are able to produce all the important qualitative phenomena (e.g. stable/unstable equilibria, oscillations, limit cycles, multiplicity of equilibrium points and even chaotic behavior) that are important for the study and better understanding of nonlinear processes. Therefore, we can agree with the claim that CRNs can be regarded as a possible "prototype of nonlinear systems" [25]. The theory of chemical reaction networks has significant results relating network structure and the qualitative properties of the corresponding dynamics [10], [12](some relevant details will be summarized in subsection II-D). However, the network structure corresponding to a given dynamics is generally not unique [7]. Recently, optimization-based computational methods were proposed for dynamically equivalent network structures with given preferred properties (see, e.g. [15], [20], [22], [24] and other references in the first paragraph of section II). Therefore, a straightforward extension of our earlier results on autonomous kinetic systems is to study control systems and the possibility of the application of feedback to achieve a kinetic closed loop system with given advantageous structural properties. The aim of this paper is to present the first results in this area considering polynomial nonlinear systems with a simple linear input structure. The structure of the paper is the following. Section II summarizes the basic notions and known results about the optimization-based computation of dynamically equivalent kinetic systems. The new contribution of the paper can be found in sections III and IV, where a MILP-based controller design procedure is proposed and an illustrative example is shown, respectively. Finally, the most important conclusions are drawn in section V.

II. Basic notions and tools

This section summarizes the basic system properties and computation tools used later in feedback design. This introductory section is based on the thesis [21] that summarizes the notions and results of the authors published originally in [8], [11], [14], [18], [20], [23], [24].

A. Nonnegative systems

The notions and results of this subsection section are based on [6]. A function $f = [f_1 \ \dots \ f_n]^T : [0,\infty)^n \to \mathbb{R}^n$ is called *essentially nonnegative* if, for all $i = 1,\dots,n$, $f_i(x) \geq 0$ for all $x \in [0,\infty)^n$, whenever $x_i = 0$. In the linear case, when $f(x) = Ax$, the necessary and sufficient condition for essential nonnegativity is that the off-diagonal entries of A are nonnegative (such a matrix is also called a *Metzler-matrix*).

Consider an autonomous nonlinear system

$$\dot{x} = f(x),\ x(0) = x_0 \tag{1}$$

where $f : \mathcal{X} \to \mathbb{R}^n$ is locally Lipschitz, $\mathcal{X}$ is an open subset of $\mathbb{R}^n$ and $x_0 \in \mathcal{X}$. Suppose that the nonnegative orthant $[0,\infty)^n = \overline{\mathbb{R}}^n_+ \subset \mathcal{X}$. Then the nonnegative orthant is invariant for the dynamics (1) if and only if f is essentially nonnegative.

It is easy to prove that kinetic systems are essentially nonnegative.

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B. Mixed integer linear programming and propositional calculus

A mixed integer linear program is the maximization or minimization of a linear function subject to linear constraints. A mixed integer linear program with k variables (denoted by $y \in \mathbb{R}^k$) and p constraints can be written as [16]:

$$\begin{aligned} &\text{minimize } c^T y \\ &\text{subject to:} \\ &A_1 y = b_1 \\ &A_2 y \leq b_2 \\ &l_i \leq y_i \leq u_i \text{ for } i = 1, \ldots, k \\ &y_j \text{ is integer for } j \in I,\ I \subseteq \{1, \ldots, k\} \end{aligned} \tag{2}$$

where $c \in \mathbb{R}^k$, $A_1 \in \mathbb{R}^{p_1 \times k}$, $A_2 \in \mathbb{R}^{p_2 \times k}$, and $p_1 + p_2 = p$.

A very useful result is that statements in propositional calculus can be transformed into linear inequalities (see, e.g. [3]). Therefore, a propositional logic problem, where a statement must be proved to be true given a set of compound statements can be solved by means of a linear integer program. For this, logical variables must be introduced. Then the original compound statements can be translated to linear inequalities involving the logical variables.

C. Dynamics and structure of kinetic systems

The problem of kinetic realizability of polynomial vector fields was first examined and solved in [13] where the constructive proof contains a realization algorithm that produces the weighted directed graph of a possible associated kinetic mechanism (called the *canonical mechanism*). According to [13], the necessary and sufficient condition for kinetic realizability of a polynomial vector field is that all coordinates functions of f in (1) must have the form

$$f_i(x) = -x_i g_i(x) + h_i(x),\ i = 1, \ldots, n \tag{3}$$

where g_i and h_i are polynomials with nonnegative coefficients.

Now we introduce a representation of kinetic systems that transparently shows the relation between the graph structure and the dynamics and that is suitable to put structure-related computations into an optimization framework. If the condition (3) is fulfilled for a polynomial dynamical system, then it can always be written into the form

$$\dot{x} = Y \cdot A_k \cdot \psi(x), \tag{4}$$

where $x \in \mathbb{R}^n$ is the vector of state variables, $Y \in \mathbb{Z}_{\geq 0}^{n \times m}$ with distinct columns is the so-called *complex composition matrix*, $A_k \in \mathbb{R}^{m \times m}$ contains the information corresponding to the weighted directed graph of the reaction network (see below). According to the original chemical meaning of this system class, the state variables represent the concentrations of the chemical *species* denoted by X_i, i.e. $x_i = [X_i]$ for $i = 1, \ldots, n$. Moreover, $\psi : \mathbb{R}^n \mapsto \mathbb{R}^m$ is a mapping given by

$$\psi_j(x) = \prod_{i=1}^{n} x_i^{Y_{ij}}, \quad j = 1, \ldots, m. \tag{5}$$

A_k is a column conservation matrix (i.e. the sum of the elements in each column is zero) defined as

$$[A_k]_{ij} = \begin{cases} -\sum_{l=1, l \neq i}^{m} k_{il}, & \text{if} \quad i = j \\ k_{ji}, & \text{if} \quad i \neq j. \end{cases} \tag{6}$$

The *complexes* are formally defined as nonnegative linear combinations of the species in the following way:

$$C_i = \sum_{j=1}^{n} Y_{ji} X_j,\ i = 1, \ldots, n \tag{7}$$

The weighted directed graph (or reaction graph) of kinetic systems is $G = (V, E)$, where $V = \{C_1, C_2, \ldots, C_m\}$ and E denote the set of vertices and directed edges, respectively. The directed edge (C_i, C_j) (also denoted by $C_i \to C_j$) belongs to the reaction graph if and only if $[A_k]_{j,i} > 0$. In this case, the weight assigned to the directed edge $C_i \to C_j$ is $[A_k]_{j,i}$. Loops (i.e. edges starting from and leading to the same vertex) are not allowed in reaction graph. Thus, it can be seen that A_k is the negative transpose of the weighted Laplacian matrix of G. The diagonal elements $[A_k]_{ii}$ contain the negative sum of the weights of the edges starting from the node C_i, while the off-diagonal elements $[A_k]_{ij}$, $i \neq j$ contain the weights of the directed edges (C_j, C_i) coming into C_i. Therefore, we can call A_k the *Kirchhoff matrix*. 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. We remark, that it is allowed that a column (let's say column i) of the matrix Y is the zero vector. In such a case, node C_i is called the *zero complex*. Without going into the details, we mention that for biochemical models, the zero-complex was originally introduced to handle the exchange of materials between the environment and the system [9]. From a systems theoretic point of view, the zero complex simply allows constant positive terms on the right hand sides of kinetic ODEs.

The reaction vector corresponding to $C_i \to C_j$, and denoted by e_k is defined as

$$e_k = [Y]_{\cdot,j} - [Y]_{\cdot,i},\ k = 1, \ldots, r, \tag{8}$$

where $[Y]_{\cdot,i}$ denotes the ith column of Y. The *rank* of a reaction network denoted by s is the rank of the set of vectors $H = \{e_1, e_2 \ldots, e_r\}$ where r is the number of reactions. The *stoichiometric subspace*, denoted by S, is defined as $S = \text{span}\{e_1, \ldots, e_r\}$. The positive *stoichiometric compatibility class* containing a $x_0 \in \mathbb{R}^n$ is the following set [10]:

$$(x_0 + S) \cap \mathbb{R}_+^n,$$

where $\mathbb{R}_+^n$ denotes the positive orthant in $\mathbb{R}^n$. The deficiency d of a reaction network is defined as [9], [10]:

$d = m_{ni} - l - s$, where m_{ni} is the number of non-isolated (i.e. reacting) vertices in the reaction graph, l is the number of linkage classes (graph components) and s is the rank of the reaction network. The deficiency is a very useful measure for studying the dynamical properties of reaction networks and for establishing parameter-independent global stability conditions.

Using the notation

$$M = Y \cdot A_k, \tag{9}$$

equation (4) can be written in the form

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

where M contains the coefficients of the monomials in the polynomial ODE (4) describing the time-evolution of the state variables. It is clear from the above description that the system's reaction graph and the corresponding dynamics can be fully characterized by the matrix pair (Y, A_k).

As it has been mentioned before, in [13], the authors give a procedure for generating a possible reaction graph for a given kinetic ODE system. (As we will see in subsection II-E, this reaction graph is generally not unique) It is worth sketching this algorithm in the same form as it was given in [19]. Let us write the right hand side of a kinetic system (1) as

$$f_i(x) = \sum_{j=1}^{r_i} m_{ij} \prod_{k=1}^{n} x_k^{b_{jk}}, \tag{11}$$

where r_i is the number of monomial terms in f_i. Let us denote the transpose of the ith standard basis vector in $\mathbb{R}^n$ as e_i and let $B_j = [b_{j1} \ \dots \ b_{jn}]$.

Procedure 1 for constructing the canonical mechanism [13]
For each $i = 1, \dots, n$ and for each $j = 1, \dots, r_i$ do:

1) $C_j = B_j + \text{sign}(m_{ij}) \cdot e_i$
2) Add the following reaction to the graph of the realization

$$\sum_{k=1}^{n} b_{jk} X_k \longrightarrow \sum_{k=1}^{n} c_{jk} X_k \tag{12}$$

with weight $|m_{ij}|$, where $C_j = [c_{j1} \ \dots \ c_{jn}]$.

The main significance of the above procedure is that through defining and adding graph nodes and directed edges in (12), it generates the Y matrix for a kinetic system. We will use the principle of this procedure for generating the complex composition matrix for a closed loop kinetic system in section III.

D. Relations between graph structure and dynamical properties

The following results and conjectures illustrate the potential of applying the theory of kinetic systems in nonlinear control.

The *Deficiency Zero Theorem* [10] shows a very robust stability property of a certain class of kinetic systems. It says that deficiency zero weakly reversible networks possess well-characterizable equilibrium points, and independently of the weights of the reaction graph (i.e. that of the system parameters) they are at least locally stable with a known logarithmic Lyapunov function that is also independent of the system parameters. Moreover, they are input-to-state stable with respect to the off-diagonal elements of A_k as inputs [4], it is straightforward to asymptotically stabilize them by additional feedback [17], and it is possible to construct efficient state observers for them [5].

The *Global Attractor Conjecture* says that for any complex balanced CRN (i.e. there exists a strictly positive equilibrium point x^* such that $A_k\psi(x^*) = 0$) and any initial condition $x(0) \in \mathbb{R}^n_+$, the equilibrium point x^* is a global attractor in the corresponding positive stoichiometric compatibility class.

The *Boundedness Conjecture* says that any weakly reversible reaction network with mass-action kinetics has bounded trajectories.

Recently, both the Global Attractor Conjecture and the Boundedness Conjecture were successfully proved for one linkage class kinetic systems [1], [2].

The Deficiency Zero Theorem together with the Boundedness Conjecture underline the importance of weak reversibility. Therefore, we will concentrate on this property in section III.

E. Dynamical equivalence and searching for preferred realizations

It has been known since at least the 1970s that reaction graphs with different structure and/or with different weighting can induce exactly the same kinetic differential equations. Therefore, we call two reaction networks given by the matrix pairs $(Y^{(1)}, A_k^{(1)})$ and $(Y^{(2)}, A_k^{(2)})$ *dynamically equivalent*, if

$$Y^{(1)} A_k^{(1)} \psi^{(1)}(x) = Y^{(2)} A_k^{(2)} \psi^{(2)}(x) = f(x), \quad \forall x \in \overline{\mathbb{R}}^n_+ \tag{13}$$

where for $i = 1, 2$, $Y^{(i)} \in \mathbb{R}^{n \times m_i}$ have nonnegative integer entries, $A_k^{(i)}$ are valid Kirchhoff matrices, and

$$\psi_j^{(i)}(x) = \prod_{k=1}^{n} x_k^{[Y^{(i)}]_{kj}}, \quad i = 1, 2, \ j = 1, \dots, m_i. \tag{14}$$

In this case, $(Y^{(i)} A_k^{(i)})$ for $i = 1, 2$ are called *dynamically equivalent realization*s of the corresponding kinetic vector field f. It is also appropriate to call $(Y^{(1)}, A_k^{(1)})$ a *(dynamically equivalent) realization* of $(Y^{(2)}, A_k^{(2)})$ and vice versa.

It was shown in e.g. [20] that key properties such as the number of directed edges or non-isolated vertices in the reaction graph, the number of linkage classes, deficiency, (weak) reversibility or complex balance are realization-dependent properties. Therefore, optimization- (LP and MILP) based computational procedures have been proposed to decide the existence of and compute kinetic realizations with preferred structural properties [15], [22], [24]. The optimization framework for this is shortly summarized below. We assume that we have a kinetic polynomial system of the form (10). Then, dynamical equivalence and the Kirchhoff property of A_k can be expressed using the following linear constraints:

$$Y \cdot A_k = M \tag{15}$$

$$\sum_{i=1}^{m} [A_k]_{ij} = 0, \quad j = 1, \ldots, m \tag{16}$$

$$[A_k]_{ij} \geq 0, \quad i, j = 1, \ldots, m, \quad i \neq j \tag{17}$$

$$[A_k]_{ii} \leq 0, \quad i = 1, \ldots, m, \tag{18}$$

where A_k is the decision variable.

The constraints for weak reversibility can be constructed as follows. We use the fact known from the literature that 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 $A_k \cdot b = 0$. Since b is unknown, too, this constraint in this form is not linear. Therefore, we introduce a scaled matrix $\tilde{A}_k$ with entries

$$[\tilde{A}_k]_{ij} = [A_k]_{ij} \cdot b_j. \tag{19}$$

It is clear from (19) 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 $\ker(\tilde{A}_k)$. 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. Therefore, the following constraints have to be fulfilled for $\tilde{A}_k$

$$\begin{aligned}
&\sum_{i=1}^{m} [\tilde{A}_k]_{ij} = 0, \quad j = 1, \ldots, m \\
&\sum_{i=1}^{m} [\tilde{A}_k]_{ji} = 0, \quad j = 1, \ldots, m \\
&[\tilde{A}_k]_{ij} \geq 0, \quad i, j = 1, \ldots, m, \; i \neq j \\
&[\tilde{A}_k]_{ii} \leq 0, \quad i = 1, \ldots, m.
\end{aligned} \tag{20}$$

Moreover, we set the following logical constraint for the structural identity (i.e. the position of zero and non-zero elements) of A_k and $\tilde{A}_k$:

$$[A_k]_{ij} > \epsilon \leftrightarrow [\tilde{A}]_{ij} > \epsilon, \quad i, j = 1, \ldots, m, \quad i \neq j, \tag{21}$$

where '$\leftrightarrow$' means 'if and only if', and ϵ is a sufficiently small positive threshold for distinguishing practically zero and nonzero elements. The propositional logic expression (21) can be translated into the following linear inequalities

$$\begin{aligned}
&0 \leq [A_k]_{ij} - \epsilon\delta_{ij}, \quad i, j = 1, \ldots, m, \quad i \neq j, \\
&0 \leq -[A_k]_{ij} + u_{ij}\delta_{ij}, \quad i, j = 1, \ldots, m, \quad i \neq j. \\
&0 \leq [\tilde{A}_k]_{ij} - \epsilon\delta_{ij}, \quad i, j = 1, \ldots, m, \quad i \neq j \\
&0 \leq -[\tilde{A}_k]_{ij} + u_{ij}\delta_{ij}, \quad i, j = 1, \ldots, m, \quad i \neq j,
\end{aligned} \tag{22}$$

where $\delta_{ij}, i, j = 1, \ldots, m, \; i \neq j$ are boolean variables, and u_{ij} are uniform upper bounds for the off-diagonal elements of A_k and $\tilde{A}_k$. Thus, the final set of decision variables in this case is $[A_k]_{ij}$, $[\tilde{A}_k]_{ij}$ and δ_{ij} for $i, j = 1, \ldots, m$, $i \neq j$.

Finally, by choosing an arbitrary linear objective function of the decision variables, weakly reversible realizations of the studied kinetic system can be computed (if any exists) in an MILP framework using the linear constraints (15)-(18), (20) and (22).

III. Kinetic feedback design using optimization

In this section, the optimization problems for the design of static and dynamic kinetic feedbacks will be presented.

A. Open loop model form

We assume that the equations of the open loop polynomial system with linear input structure are given as

$$\dot{x} = M \cdot \psi_1(x) + Bu, \tag{23}$$

where $x \in \mathbb{R}^n$, is the state vector, $u \in \mathbb{R}^p$ is the input, $\psi_1 \in \mathbb{R}^n \to \mathbb{R}^{m_1}$ contains the monomials of the open-loop system, $B \in \mathbb{R}^{n \times p}$and $M \in \mathbb{R}^{n \times m_1}$.

The problem that we will study is to design a static or dynamic monomial feedback such that the closed loop system is kinetic, and there exists a realization that fulfills a required property (in this particular case, weak reversibility).

B. Static feedback design

We assume a polynomial feedback of the form

$$u = K \cdot \overline{\psi}(x), \tag{24}$$

where $\overline{\psi}(x) = [\psi_1^T(x) \; \psi_2^T(x)]^T$ with $\psi_2 \in \mathbb{R}^n \to \mathbb{R}^{m_2}$ containing possible additional monomials for the feedback, $B \in \mathbb{R}^{n \times m}$, and $K \in \mathbb{R}^{p \times (m_1 + m_2)}$. The closed-loop system can be written as

$$\dot{x} = M \cdot \psi_1(x) + BK \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \end{bmatrix}. \tag{25}$$

We can partition K into two blocks as

$$K = [K_1 \; K_2], \tag{26}$$

where $K_1 \in \mathbb{R}^{p \times m_1}$ and $K_2 \in \mathbb{R}^{p \times m_2}$. Using this notation, the closed loop dynamics is given by

$$\dot{x} = \underbrace{\begin{bmatrix} M + BK_1 & BK_2 \end{bmatrix}}_{\overline{M}} \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \end{bmatrix} = \overline{M} \cdot \overline{\psi}(x). \tag{27}$$

The aim is to set the closed loop coefficient matrix $\overline{M}$ such that it defines a kinetic system with $\overline{\psi}$. It is clear

from subsection II-C that this is possible if and only if $\overline{M}$ can be factorized as $\overline{M} = \overline{Y} \cdot \overline{A}_k$ where $\overline{Y} \in \mathbb{Z}_{\geq 0}^{n \times (m_1+m_2)}$, and $\overline{A}_k \in \mathbb{R}^{(m_1+m_2)\times(m_1+m_2)}$ is a valid Kirchhoff matrix.

Based on **Procedure 1** summarized in subsection II-C, we can give a simple method to generate matrix $\overline{Y}$ (and thus ψ_2 given by such monomials that do not appear in (23)) using the monomials of the open loop system as follows. Let $col(A)$ denote the set of columns in a matrix A. Moreover, let the monomials of (23)) given by

$$\psi_1(x) = \prod_{i=1}^{n} x_i^{b_{ij}}, \quad j = 1, \ldots, m_1, \tag{28}$$

and let e_i denote the ith standard basis vector in $\mathbb{R}^n$. Then, we can build $\overline{Y}$ as follows

Procedure 2 for generating $\overline{Y}$
Let $col(\overline{Y}) = \emptyset$
For each $j = 1, \ldots, m_1$ do:
  Let $v^{(j)} := [b_{1j}\ b_{2j}\ \ldots\ b_{nj}]^T$
  For each $i = 1, \ldots, n$ do:
    Let $col(\overline{Y}) := col(\overline{Y}) \cup v^{(j)}$
    Let $col(\overline{Y}) := col(\overline{Y}) \cup (v^{(j)} + e_i)$
    If $v_i^j > 0$ then let $col(\overline{Y}) := col(\overline{Y}) \cup (v^{(j)} - e_i)$

We remark that the above procedure gives only one feasible set of monomials, and $\overline{Y}$ (and therefore ψ_2) can be further extended by additional column vectors (monomials), if necessary. After constructing $\overline{Y}$, the kinetic property of the closed loop system can be given as a set of linear constraints:

$$\overline{Y} \cdot \overline{A}_k = \overline{M} \tag{29}$$

$$\sum_{i=1}^{m_1+m_2} [\overline{A}_k]_{ij} = 0, \quad j = 1, \ldots, m_1 + m_2 \tag{30}$$

$$[\overline{A}_k]_{ij} \geq 0, \quad i, j = 1, \ldots, m_1 + m_2, \quad i \neq j \tag{31}$$

$$[\overline{A}_k]_{ii} \leq 0, \quad i = 1, \ldots, m_1 + m_2, \tag{32}$$

where the unknowns are the controller parameter matrix K contained in $\overline{M}$ and the Kirchhoff matrix $\overline{A}_k$. Finally, the weak reversibility of the reaction graph of the closed loop system can be prescribed by setting the constraints (20) and (22) for $\overline{A}_k$. Thus, the feedback gain computation and the search for weakly reversible realizations of the closed loop system has been integrated into one MILP optimization problem.

C. Computation of dynamic feedbacks

To increase the degree of freedom in transforming a polynomial system to kinetic form via feedback, it is a straightforward idea to apply a dynamic extension. In this case, let us write the equations of the open-loop system as

$$\dot{x}^{(1)} = M_{11}\psi_1(x^{(1)}) + Bu, \tag{33}$$

where $x^{(1)} \in \mathbb{R}^n$, $M_{11 \in \mathbb{R}^{n\times m_1}}$, $\psi_1 : \mathbb{R}^n \to \mathbb{R}^{m_1}$, $B \in \mathbb{R}^{n\times p}$, and $u \in \mathbb{R}^p$. Let us give the equations of the dynamic extension as

$$\dot{x}^{(2)} = M_{21}\psi_1(x^{(1)}) + M_{22}\psi_2(x), \tag{34}$$

where $x^{(2)} \in \mathbb{R}^k$, $M_{21} \in \mathbb{R}^{k\times m_1}$, $M_{22} \in \mathbb{R}^{k\times m_2}$. Moreover,

$$x = \begin{bmatrix} x^{(1)} \\ x^{(2)} \end{bmatrix} \in \mathbb{R}^{n+k}, \ \overline{\psi}(x) = \begin{bmatrix} \psi_1(x^{(1)}) \\ \psi_2(x) \end{bmatrix}, \tag{35}$$

where $\psi_2 : \mathbb{R}^{n+k} \to \mathbb{R}^{m_2}$. Let us again use a monomial feedback in the form

$$u = K\overline{\psi}(x) = K_1\psi_1 + K_2\psi_2, \tag{36}$$

where $K_1 \in \mathbb{R}^{p\times m_1}$, $K_2 \in \mathbb{R}^{p\times m_2}$, and $K = [K_1\ K_2]$. The equations of the closed loop system are given by

$$\dot{x} = \begin{bmatrix} M_{11} + BK_1 & BK_2 \\ M_{21} & M_{22} \end{bmatrix} \cdot \overline{\psi}(x) = \overline{M} \cdot \overline{\psi}(x) \tag{37}$$

The feedback gain computation and the weak reversibility constraint is completely analogous to the static feedback case described in subsection III-B with the only exception that we have more unknowns (i.e. decision variables) in matrices M_{21} and M_{22} giving generally more degrees of freedom to solve the feedback design problem.

IV. Example

Let us consider the following polynomial system

$$\dot{x}_1 = 1 + x_1x_2 + u \tag{38}$$

$$\dot{x}_2 = 1 - 5x_1x_2 \tag{39}$$

$$\dot{x}_3 = 4x_1x_2 - 3x_3^2 \tag{40}$$

It is easy to see from (38) that for $u = 0$, the system has no equilibrium points in the nonnegative orthant. Using the notations of section III, we have:

$$\psi_1(x^{(1)}) = [1\ x_1x_2\ x_3^2]^T, \tag{41}$$

$$M_{11} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & -5 & 0 \\ 0 & 4 & -3 \end{bmatrix}, \quad B = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{42}$$

For a dynamical feedback, let us introduce one new variable $x^{(2)} = x_4$, and two additional monomials as follows: $\psi_2(x) = [x_1^2\ \ x_4]^T$. Then, after performing the procedure presented in subsection III-C, we find that the MILP optimization problem is feasible, and

$$K = [0\ 0\ 0\ -6\ 4],\ M_{21} = [0\ 0\ 0],\ M_{22} = [3\ -3]. \tag{43}$$

This means that the feedback

$$u = -6x_1^2 + 4x_4 \tag{44}$$

and the dynamic extension

$$\dot{x}_4 = 3x_1^2 - 3x_4 \tag{45}$$

results in a closed loop system that has a weakly reversible realization with zero deficiency. Therefore, the controlled system has bounded trajectories in the positive orthant and moreover, it is globally stable with a known logarithmic Lyapunov function. The resulting weakly reversible reaction graph of the closed loop system is depicted in Fig. 1.

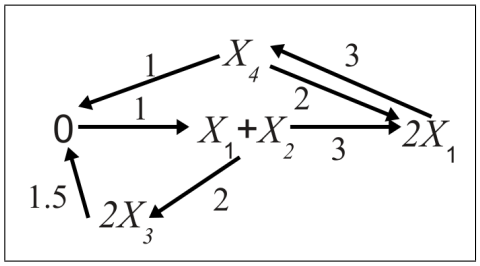

Figure 1. Weakly reversible kinetic structure of the closed loop system

V. Conclusions

Optimization based procedures have been proposed in this paper to transform a polynomial nonlinear system into (weakly reversible) kinetic form using static and dynamic nonlinear feedbacks. The motivations behind the approach were the following: firstly, the application of the known strong results relating the graph structure and dynamics of kinetic systems, and secondly, the utilization of recent results of the authors on determining dynamically equivalent reaction graphs with dynamically relevant structural properties for autonomous kinetic systems. As a first step in kinetic feedback design, we were focusing on weakly reversible closed loop systems in this paper. It was shown that the feedback gain computation and the search for weakly reversible realizations of the closed loop system can be integrated into one MILP optimization step. The main limitation of the approach is the linear input structure of the open loop system. (However, this requirement allows us the direct use of MILP.) Further work will be devoted to the targeted selection of additional monomials in ψ_2 and to robustness with respect to system parameters (i.e. what is the parameter range within which there exists a preferred realization of the closed loop system).

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