Design of a global stabilizing dynamic feedback structure for positive polynomial systems

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1 Introduction

The field of feedback controller design for nonlinear systems has been continuously developing in recent decades, because of its practical importance and challenging theoretical nature. It is well-known that the utilization of the physical and/or structural specialties of different nonlinear system classes greatly helps in obtaining theoretically well-grounded, powerful and practically still feasible control methods: e.g. we have sound methods of nonlinear feedback design for smooth input-affine systems [1], flat systems [2], Hamiltonian or port-Hamiltonian systems [3, 4], or that for Euler-Lagrange systems [5].

Deterministic kinetic systems with mass action kinetics or simply chemical reaction networks (CRNs) form a wide class of nonnegative polynomial systems. CRNs are able to produce all the important qualitative phenomena present in nonlinear systems, so they form a rich-enough sub-class there. A recent survey shows [6] that CRNs are also widely used in other areas than chemical reaction kinetics or process systems that include biological applications, such as to model the dynamics of intracellular processes and metabolic or cell signalling pathways [7].

The theory of chemical reaction networks has significant results relating network structure and the qualitative properties of the corresponding dynamics [8, 9]. However, the network structure corresponding to a given dynamics is generally not unique [10]. Recently, optimization-based computational methods were proposed for dynamically equivalent network structures with given preferred properties (see, e.g. [11–14]).

Therefore, the general purpose of our work is to construct polynomial feedback controllers to polynomial systems to achieve a kinetic closed loop system with given advantageous structural properties. These properties will ensure the global asymptotic stability of the closed loop system even for non-kinetic and unstable polynomial open loop systems.

The known basic notions and tools of positive kinetic systems will be shortly reviewed first, then the optimization methods that enable to construct kinetic realizations with given preferred properties will be described. Thereafter we show how these methods can be used for static and dynamic polynomial feedback design. The developed methods and tools are illustrated with several examples.

2 Underlying notions and methods

Polynomial systems form a wide and well-studied class of smooth nonlinear systems that have important applications in diverse engineering fields, such as (bio)chemical engineering, process systems engineering, transportation engineering, etc. Within these fields, *positive (or nonnegative) polynomial systems* are often considered that is dictated by the physical meaning (e.g. pressure, concentration or the vehicle number/density) of the signals.

The notion of positive systems builds upon the *essential nonnegativity* of a function $f = [f_1 \ \dots \ f_n]^T : [0,\infty)^n \to \mathbb{R}^n$, that holds if, for all $i = 1,\dots,n$, $f_i(x) \geq 0$ for all $x \in [0,\infty)^n$, whenever $x_i = 0$ [15].

An autonomous nonlinear system defined on the nonnegative orthant $[0,\infty)^n = \overline{\mathbb{R}}^n_+ \subset \mathcal{X}$

$$\dot{x} = f(x),\ x(0) = x_0 \tag{2.1}$$

where $f : \mathcal{X} \to \mathbb{R}^n$ is locally Lipschitz, $\mathcal{X}$ is an open subset of $\mathbb{R}^n$ and $x_0 \in \mathcal{X}$ is nonnegative (or positive) when the nonnegative (or positive) orthant is invariant for the dynamics (2.1). This property holds if and only if f is essentially nonnegative.

2.1 Kinetic systems, their dynamics and structure

Deterministic kinetic systems with mass action kinetics or simply chemical reaction networks (CRNs) form a wide class of nonnegative 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 behavior) present in the dynamics of nonlinear processes [6]. The structure of CRNs is well characterized by a weighted directed graph, called the *reaction graph*, and by their *complex composition matrix*.

The problem of kinetic realizability of polynomial vector fields was first examined and solved in [16] where it was shown, that the necessary and sufficient condition for kinetic realizability of a polynomial vector field is that all coordinates functions of f in (2.1) must have the form

$$f_i(x) = -x_i g_i(x) + h_i(x),\ i = 1,\dots,n \tag{2.2}$$

where g_i and h_i are polynomials with nonnegative coefficients. It's easy to prove that kinetic systems are nonnegative.

2.1.1 The ODE form

If the condition (2.2) is fulfilled for a polynomial dynamical system, then it can always be written into the form

$$\dot{x} = Y \cdot A_k \cdot \psi(x), \tag{2.3}$$

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). As it will be visible later, the generally non-unique factorization (2.3) is particularly useful for prescribing structural constraints using optimization. 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. $x_i = conc[X_i]$ for $i = 1, \ldots, n$. Moreover, $\psi : \mathbb{R}^n \mapsto \mathbb{R}^m$ is a mapping given by

$$\psi_j(x) = \prod_{i=1}^{n} x_i^{[Y]_{ij}}, \quad j = 1, \ldots, m. \tag{2.4}$$

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

$$[A_k]_{ij} = \begin{cases} -\sum_{l=1, l \neq i}^{m} k_{il}, & \text{if} \quad i = j \\ k_{ji}, & \text{if} \quad i \neq j. \end{cases} \tag{2.5}$$

Note that A_k is also called as the *Kirchhoff matrix* of the network.

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

$$C_i = \sum_{j=1}^{n} [Y]_{ji} X_j, \ i = 1, \ldots, n \tag{2.6}$$

Note, that a column (let's say column i) of the matrix Y may be equal to the zero vector. In such a case, node C_i is called the *zero complex*.

2.1.2 Reaction graph and its properties

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 $[A_k]_{j,i}$.

The dynamic properties of a CRN depend on some of the structural properties of the reaction graph. 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.

2.1.2.1 Incidence matrix of the reaction graph

The incidence matrix of a reaction graph with r reaction is denoted by the matrix $B_G \in \{-1, 0, 1\}^{m \times r}$. Each reaction is represented as follows: B_G has a column vector v where $v_i = 1$, $v_j = -1$ and the other elements are 0 iff there exists a reaction from the jth to the ith complex.

2.1.3 Stability of kinetic systems

The deficiency [9] is a fundamental property of a CRN. Its notion depends on the notion of a reaction vector corresponding to $C_i \to C_j$, and denoted by e_k:

$$e_k = [Y]_{\cdot,j} - [Y]_{\cdot,i}, \ k = 1, \ldots, r, \tag{2.7}$$

where $[Y]_{\cdot,i}$ denotes the ith column of Y and r is the number of reactions. The *rank* of a reaction network denoted by s is the rank of the set of vectors $H = \{e_1, e_2 \ldots, e_r\}$. The *stoichiometric subspace*, denoted by S, is defined as $S = \text{span}\{e_1, \ldots, e_r\}$.

The deficiency d of a reaction network is defined as [9]:

$$d = m_{ni} - l - s, \tag{2.8}$$

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.

The *Deficiency Zero Theorem* [9] 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. as long as the positive elements of the A_k matrix remain positive) they are at least locally stable with a known logarithmic Lyapunov function that is also independent of the system parameters. According to the so-called Global Attractor Conjecture (to which no counterexample has been found), weakly reversible deficiency zero CRNs are globally stable (within the positive orthant). This conjecture has been proved for CRNs containing one linkage class [17]. Moreover, weakly reversible deficiency zero models are input-to-state stable with respect to the off-diagonal elements of A_k as inputs [18], it is straightforward to asymptotically stabilize them by additional feedback [19], and it is possible to construct efficient state observers for them [20].

2.2 Optimization methods

In mathematics optimization is the selection of the best element from the set of the possible solutions. We are going to deal with only the case of the finding the extremum of a real-valued function. The general form of this problem:

$$\min_{x \in \mathbb{X}} f(x) \tag{2.9}$$

where the function $f(x)$ is called the cost or object function of the optimization problem. Variables of the function $f(x)$ is called the decision variables. $\mathbb{X}$ is the set of the available decision variables.

Solving the general problem is hard, so the solution methods have compromises (e.g. long computing time, the solution is only a local extremum, etc.). Specializations of the optimization problem could result in more effective methods. In the following subsections we are going to present two specialization of the original problem.

2.2.1 Linear programming

Linear programming (LP) is a special case of the optimization problems where the object function is linear and the set of the feasible decision variables is a convex polyhedron which is defined by linear inequalities. The form of LP problems that will be used in this report is the following (this from is equivalent with the standard form)

$$\min_x c^T x \tag{2.10}$$

subject to

$$A_1 x \leq b_1 \tag{2.11}$$
$$A_2 x = b_2 \tag{2.12}$$

where $x \in \mathbb{R}^n$ is the vector of decision variables, $c \in \mathbb{R}^n$, $b_1 \in \mathbb{R}^{p_1}$ and $b_2 \in \mathbb{R}^{p_2}$ are known vectors, $A_1 \in \mathbb{R}^{p_1 \times n}$ and $A_2 \in \mathbb{R}^{p_2 \times n}$ are known matrices. '=' and '$\leq$' in (2.11) and (2.12) means elementwise comparison. For a long time the complexity of the LP problem has been an open problem, but nowadays number of polynomial time algorithm exist (e.g. interior point method, ellipsoid method).

2.2.2 Mixed integer linear programming

Mixed integer linear programming (MILP) is an optimization technique which lies between the linear programming and the combinatorial optimization. It differs from the linear programming that decision variables can also be integer ones. Due to this difference the solvable problem set is much larger than in the LP case. The form of MILP problems that will be used in this report is the following (this from is equivalent with the standard form)

$$\min_x c^T x \tag{2.13}$$

subject to

$$A_1 x \leq b_1 \tag{2.14}$$
$$A_2 x = b_2 \tag{2.15}$$
$$x_i \text{ is interger for } i \in I,\ I \subseteq \{1, \ldots, n\} \tag{2.16}$$

where x is the n dimensional vector of decision variables with real and integer elements, $c \in \mathbb{R}^n$, $b_1 \in \mathbb{R}^{p_1}$ and $b_2 \in \mathbb{R}^{p_2}$ are known vectors, $A_1 \in \mathbb{R}^{p_1 \times n}$ and $A_2 \in \mathbb{R}^{p_2 \times n}$ are known matrices. '=' and '$\leq$' in (2.15) and (2.14) means elementwise comparison.

Generally the mixed integer linear programming is NP-hard. In spite of this, there exist a number of effective free (e.g. GLPK [21], lpsolve [22]) and commercial (e.g. CPLEX [23]) solver.

2.2.2.1 Propositional expressions as mixed integer linear inequalities

This section is based on the article [24]. Let X_i be a propositional variable which can either be true or false. One can associate variables logical variables: $\delta_i \in \{0, 1\}$ to the propositional ones where $\delta_i = 0$ when X_i is false and $\delta_i = 1$ when X_i is true. In Boolean algebra, propositional variables can be combined by the following operation: $\wedge$ (and), $\vee$ (or), $\neg$ (not), $\oplus$ (exclusive or), $\rightarrow$ (implies), $\leftrightarrow$ (iff). With these notations the connection between the propositional expressions and integer linear inequalities is the following

$$\begin{aligned} X_1 \vee X_2 &\Leftrightarrow \delta_1 + \delta_2 \geq 1 \\ X_1 \wedge X_2 &\Leftrightarrow \delta_1 = 1,\, \delta_2 = 1 \\ \neg X_1 &\Leftrightarrow \delta_1 = 0 \\ X_1 \rightarrow X_2 &\Leftrightarrow \delta_1 - \delta_2 \leq 0 \\ X_1 \leftrightarrow X_2 &\Leftrightarrow \delta_1 - \delta_2 = 0 \\ X_1 \oplus X_2 &\Leftrightarrow \delta_1 + \delta_2 = 1. \end{aligned} \tag{2.17}$$

Furthermore we are going to give the connection between the continuous and logical variables. Consider the following logical expression: $X = [f(x) \leq 0]$, where f is a linear function, $x \in \mathbb{X}$ and $\mathbb{X}$ is bounded. The following linear inequality system is equivalent to the logical expression X:

$$[f(x) \leq 0] \leftrightarrow [\delta = 1] \Leftrightarrow \begin{cases} f(x) \leq M(1 - \delta) \\ f(x) \geq \epsilon + (m - \epsilon)\delta \end{cases} \tag{2.18}$$

where m is the lower, M is the upper bound of f and ϵ is a small positive constant.

3 Different realizations of CRNs

It was shown in e.g. [11] that key properties such as the number of directed edges or non-isolated vertices in the reaction graph, the number of linkage classes, deficiency or (weak) reversibility 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 [12–14].

In this chapter we are going to shortly summarize the constraint sets to dynamically equivalent realizations, weakly reversible realizations and weakly reversible realizations with minimal deficiency. The integration of these constraints into an optimization framework in order to compute dynamically equivalent realizations with these properties is also presented.

We are going to give a new method to compute deficiency zero realizations. Determining the minimal complex set to compute a weakly reversible realization would be a new result, too.

3.1 Dynamical equivalence of CRNs

It is a known result of chemical reaction network theory that a reaction graph corresponding to a given set of kinetic ODEs is generally not unique. We will use the degree of freedom given by this phenomenon for feedback design. Using the notation $M = Y \cdot A_k$, equation (2.3) can be written in the form

$$\dot{x} = M \cdot \psi(x), \tag{3.1}$$

where M contains the coefficients of the monomials in the polynomial ODE (2.3) describing the time-evolution of the state variables. We call two reaction networks given by the matrix pairs $(Y^{(1)}, A_k^{(1)})$ and $(Y^{(2)}, A_k^{(2)})$ *dynamically equivalent*, if

$$Y^{(1)} A_k^{(1)} \psi^{(1)}(x) = Y^{(2)} A_k^{(2)} \psi^{(2)}(x) = f(x), \quad \forall x \in \overline{\mathbb{R}}_+^n \tag{3.2}$$

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

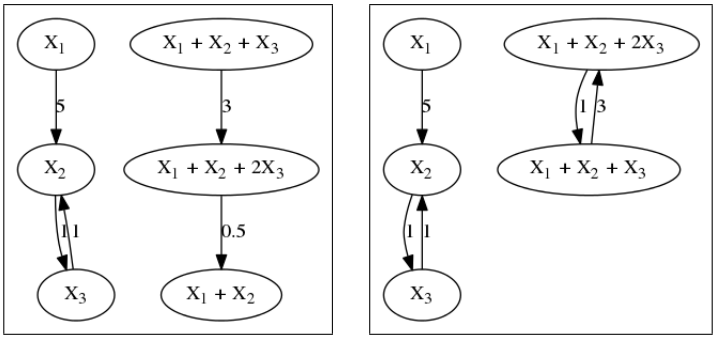
$$\psi_j^{(i)}(x) = \prod_{k=1}^{n} x_k^{[Y^{(i)}]_{kj}}, \quad i = 1, 2, \ j = 1, \ldots, m_i. \tag{3.3}$$

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.

Example 1. Let us consider the following differential equation system:

$$\begin{aligned} \dot{x}_1 &= -5x_1 \\ \dot{x}_2 &= 5x_1 - x_2 + x_3 \\ \dot{x}_3 &= x_2 - x_3 - x_1x_2x_3^2 + 3x_1x_2x_3 \end{aligned} \tag{3.4}$$

You can see two different realization of this differential equation system in Fig. 3.1. These two realizations are example for the different complex set and reaction network structure.



(a) (b)

Figure 3.1: Two different dynamically equivalent realization of (3.4). Figures use of the notations of the subsection 2.1.2

3.2 Computing dynamically equivalent realizations using optimization

. In this section we are going to present how one can solve the problem of computing dynamically equivalent realizations with optimization methods. For this we choose the problem of computing of the sparse and dense realizations [11]. Sparse realizations have minimal number of edges and a dense realization has maximal number of edges.

3.2.1 The constraints

In the optimization problems we will use a fixed complex composition matrix Y to the dynamical equivalence constraint (3.2) that remains linear. We are going to use a decision variable A_k to represents the Kirchhoff matrix of the realization. Firstly we have to guarantee the dynamical equivalence:

$$M = Y \cdot A_k \tag{3.5}$$

where M contains the coefficients of the monomials in the polynomial ODE (2.3). Constraints of the Kirchhoff property are the following:

$$\begin{aligned} &\sum_{i=1}^{m}[A_k]_{ij} = 0, \quad j = 1, \dots, m \\ &[A_k]_{ij} \geq 0, \quad i, j = 1, \dots, m,\ i \neq j \\ &[A_k]_{ii} \leq 0, \quad i = 1, \dots, m. \end{aligned} \tag{3.6}$$

We can introduce a binary matrix variable $\Theta \in \{0,1\}^{m \times m}$. $[\Theta]_{ij}$ is 0 when $[A_k]_{ij} = 0$ otherwise $[\Theta]_{ij}$ is 1. We can give this property with the following linear inequalities:

$$\epsilon \cdot [\Theta]_{ij} \leq [A_k]_{ij} \leq U \cdot [\Theta]_{ij} \tag{3.7}$$

where ϵ is a small positive constant and U is the upper bound of values $[A_k]_{ij}$. To reach the maximal (minimal) number of edges we have to maximize (minimize) the following object function:

$$V(\Theta) = \sum_{i,j} [\Theta]_{ij} \tag{3.8}$$

It is visible that constraints (3.5)-(3.7) together with the objective function in (3.8) form a standard mixed integer linear programming (MILP) problem.

Example 2. Let us consider a CRN which is given with its reaction graph: Fig. 3.2a. Now, by using the proposed method we are able to determine a sparse and a dense realizations which are dynamically equivalent to (Y, A_k). The reaction graph of the sparse realization is depicted in Fig. 3.2b and the reaction graph of the dense realization is depicted in Fig. 3.2c.

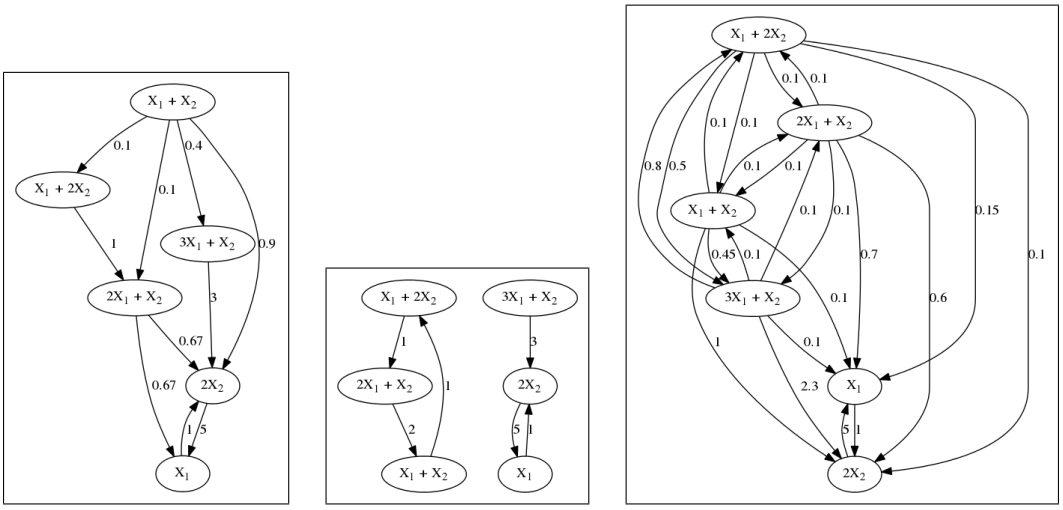
3.3 Computing weakly reversible realizations

In this section, a method for computing weakly reversible realization based on results of [12] will be presented.

The constraints for weak reversibility can be constructed as follows. 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 $A_k \cdot b = 0$ [25]. Since b is unknown, too, this constraint in this form is not linear. Therefore, we introduce a scaled matrix $\tilde{A}_k$ with entries

$$\tilde{A}_k = A_k \cdot diag(b). \tag{3.9}$$

where $diag(b)$ is a diagonal matrix with elements of b. It is clear from (3.9) 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



(a) Reaction graph of the original realization.

(b) Reaction graph of the sparse realization.

(c) Reaction graph of the dense realization.

Figure 3.2: Three CRNs which are dynamically equivalent with each other.

network if and only if A_k corresponds to a weakly reversible network. Therefore, the following constraints have to be fulfilled for $\tilde{A}_k$

$$\begin{aligned}
&\sum_{i=1}^{m}[\tilde{A}_k]_{ij} = 0, \quad j = 1, \dots, m \\
&\sum_{i=1}^{m}[\tilde{A}_k]_{ji} = 0, \quad j = 1, \dots, m \\
&[\tilde{A}_k]_{ij} \geq 0, \quad i, j = 1, \dots, m,\ i \neq j \\
&[\tilde{A}_k]_{ii} \leq 0, \quad i = 1, \dots, m.
\end{aligned} \tag{3.10}$$

Moreover, we transform the original equivalence equation (3.2) by $diag(b)$ (we can do this, because $diag(b)$ is invertable):

$$M \cdot diag(b) = Y \cdot \underbrace{A_k \cdot diag(b)}_{\tilde{A}_k} \tag{3.11}$$

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 a LP framework using the linear constraints (3.11) and (3.10).

3.3.1 Determining the necessary complexes in weakly reversible realizations

In this section we are going to show that a weakly reversible realization has a dynamically equivalent one without *pseudo complexes* and this realization is weakly reversible.

Definition 1. Consider a CRN having the complex composition matrix Y and the Kirchhoff matrix A_k. The kth complex is called *pseudo complex*, if its monomial does not appear in the differential equation system of the CRN i.e. kth column of the matrix $Y \cdot A_k$. is zero.

Theorem 1. *Consider a CRN having the complex composition matrix Y and the Kirchhoff matrix A_k. If the kth complex is a pseudo source complex then there exists a dynamically equivalent realization (Y, A'_k) where the kth complex is isolated.*

Proof. Consider the kth column m_k of matrix $M = Y \cdot A_k$:

$$0 = m_k = -\sum_{i \neq k} [A_k]_{ik} [Y]_{\cdot k} + \sum_{i \neq k} [A_k]_{ik} [Y]_{\cdot i} \tag{3.12}$$

We can divide both sides of the equation with $\sum_{i \neq k} [A_k]_{ik}$ because the kth complex is a source complex so $\sum_{i \neq k} [A_k]_{ik} > 0$:

$$[Y]_{\cdot k} = \sum_{i \neq k} \frac{[A_k]_{ik}}{\sum_{j \neq k} [A_k]_{jk}} [Y]_{\cdot i} \tag{3.13}$$

Consider the lth column m_l of matrix M:

$$m_l = -\sum_{i \neq l} [A_k]_{il} [Y]_{\cdot l} + \sum_{i \neq l} [A_k]_{il} [Y]_{\cdot i} \tag{3.14}$$

We can substitute (3.13) into (3.14):

$$m_l = -\sum_{i \neq l} [A_k]_{il} [Y]_{\cdot l} + \sum_{i \neq l \neq k} [A_k]_{il} [Y]_{\cdot i} + [A_k]_{kl} \sum_{i \neq k} \frac{[A_k]_{ik}}{\sum_{j \neq k} [A_k]_{jk}} [Y]_{\cdot i} \tag{3.15}$$

Let $[A'_k]_{il}$ $\forall i, k \neq l$ the following:

$$[A'_k]_{il} = [A_k]_{il} + [A_k]_{kl} \frac{[A_k]_{ik}}{\sum_{j \neq k} [A_k]_{jk}} \tag{3.16}$$

A'_k remains Kirchhoff matrix, because

$$\sum_{i \neq k} ([A_k]_{il} + [A_k]_{kl} \frac{[A_k]_{ik}}{\sum_{j \neq k} [A_k]_{jk}}) = \underbrace{\sum_{i \neq k} [A_k]_{il}}_{0} + \underbrace{\sum_{i \neq k} [A_k]_{kl} \frac{[A_k]_{ik}}{\sum_{j \neq k} [A_k]_{jk}}}_{0} = 0 \tag{3.17}$$

and the case of $i = k$:

$$[A_k]_{kl} = [A_k]_{kl} + [A_k]_{kl} \frac{-\sum_{j \neq k} [A_k]_{jk}}{\sum_{j \neq k} [A_k]_{jk}} = 0 \tag{3.18}$$

The other elements of the off-diagonal of matrix $[A'_k]$ are greater or equal than 0. □

Theorem 2. *Every weakly reversible CRN has a realization (Y, A_k) which is weakly reversible and all of its pseudo complexes are isolated.*

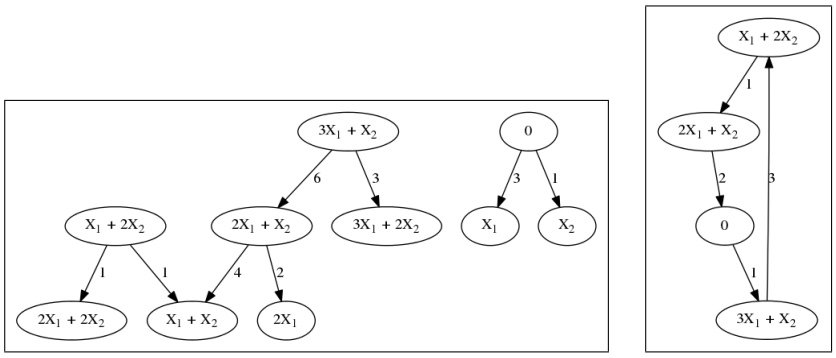
Proof. All of the pseudo complexes in a weakly reversible realization are either source complexes or isolated ones. The source pseudo complexes could be be converted into isolated ones by using of the previously presented Theorem. □

Example 3. Let us consider a CRN having the complex composition matrix Y as follows:

$$Y = \begin{bmatrix} 1 & 2 & 2 & 1 & 0 & 1 & 3 & 2 & 0 & 3 \\ 2 & 2 & 1 & 1 & 0 & 0 & 1 & 0 & 1 & 2 \end{bmatrix}$$

and a Kirchhoff-matrix A_k containing the following non-zero off-diagonal elements: $[A_k]_{2,1} = 1$, $[A_k]_{4,1} = 1$, $[A_k]_{4,3} = 4$, $[A_k]_{8,3} = 2$, $[A_k]_{6,5} = 3$, $[A_k]_{9,5} = 1$, $[A_k]_{3,7} = 6$, $[A_k]_{10,7} = 3$. The reaction graph of this system can be found in Fig. 3.3a. It is easy to see that this realization is not weakly reversible and contain number of non-isolated pseudo complexes.

Now, by using the proposed method we are able to determine an alternative realization (Y, A'_k) which is dynamically equivalent to (Y, A_k), weakly reversible and it does not contain any pseudo complex. The complex set remains unchanged but the number of "active" (i.e. non-isolated) complexes decreased by 6. The non-zero off-diagonal elements of the matrix A'_k are the following: $[A'_k]_{3,1} = 0.6154$, $[A'_k]_{5,1} = 0.0769$, $[A'_k]_{7,1} = 0.2308$, $[A'_k]_{5,3} = 2$, $[A'_k]_{7,5} = 1$, $[A'_k]_{1,7} = 3$. This reaction graph is depicted in Fig. 3.3b.



(a) Reaction graph of the realization (Y, A_k).

(b) Reaction graph of the realization (Y, A'_k).

Figure 3.3: Two CRNs which are dynamically equivalent with each other. The second one is weakly reversible. Isolated complexes are omitted from the figure.

3.4 Computing realizations with zero deficiency

In this section we are going to give a new method to compute dynamically equivalent realizations with zero deficiency. For this we are going to show some new results in

the topic of deficiency of CRNs. The integration of these methods into a optimization framework in order to compute dynamically equivalent realizations with zero deficiency is also presented.

3.4.1 Zero deficiency as a rank constraint

We can reformulate the definition from eq. (2.8) by using the incidence matrix of the reaction graph denoted by B_G:

$$d = rank(B_G) - rank(Y \cdot B_G) \tag{3.19}$$

Theorem 3. *The deficiency definition eq.* (2.8) *and that of eq.* (3.19) *are equivalent.*

Proof. The rank of the incidence matrix of a directed graph is $m - l$ where m is the number of vertices and l is the number of connected components in the graph [26]. As $Y \cdot B_G$ spans the stoichiometric subspace, the rank of $Y \cdot B_G$ is the rank of the stoichiometric subspace. □

Now it can be seen that zero deficiency holds if the following rank constraint is fulfilled:

$$rank(B_G) = rank(Y \cdot B_G) \tag{3.20}$$

3.4.2 Reformulation of the rank constraint as linear constraint

Theorem 4. *Let m be the number of complexes in a CRN having the complex composition matrix Y and the Kirchhoff matrix A_k. Then zero deficiency is fulfilled if and only if there exist vectors $\eta^1 \in \mathbb{R}^m, \eta^2 \in \mathbb{R}^m, \ldots, \eta^{m-rank(Y)} \in \mathbb{R}^m$ so that $m = rank(Y^T, \eta^1, \eta^2, \ldots, \eta^{m-rank(Y)})$ and $[A_k]_{ij} > 0 \implies \eta_i^l = \eta_j^l$.*

Proof. We can rewrite the rank of a matrix product as [27]:

$$rank(B_G^T \cdot Y^T) = rank(B_G^T) + rank(Y^T, \eta^1, \eta^2, \ldots, \eta^{m-rank(B_G)}) - m \tag{3.21}$$

where η^l is the solution of the following homogeneous linear equation system:

$$B_G^T \cdot x = 0 \tag{3.22}$$

If we apply eq. (3.20) to eq. (3.21) we obtain the following criteria to zero deficiency:

$$m = r(Y^T, \eta^1, \eta^2, \ldots, \eta^{m-r(Y)}). \tag{3.23}$$

The reaction graph has an edge from the jth complex to the ith iff $[A_k]_{ij} > 0$, so the relationship between B_G and A_k can be formulated as

$$[A_k]_{ij} > 0 \iff v \in B_G \tag{3.24}$$

where v is a column vector in the incidence matrix B_G. By using the structure of v eq. (3.22) can be converted into the following logical expression:

$$[A_k]_{ij} > 0 \implies x_i = x_j \tag{3.25}$$

□

Theorem 5. *$m = r(Y^T, \eta^1, \eta^2, \ldots, \eta^{m-r(Y)})$ is fulfilled if and only if there exists a $[Y^\perp]_i \; \forall i = 1 \ldots m - r(Y)$ constructed the following way: $[Y^\perp]_i = \beta_1^i \cdot \eta^1 + \ldots + \beta_{m-r(Y)}^i \cdot \eta^{m-r(Y)} + \alpha_1^i \cdot [Y^T]_1 + \ldots + \alpha_n^i \cdot [Y^T]_n$ where $Y^\perp$ is the orthogonal complement of Y, β_j^i and α_j^i are real coefficients and $[Y]_i$ is the ith column of matrix Y.*

Proof. **First direction:** If $m = r(Y^T, \eta^1, \eta^2, \ldots, \eta^{m-r(Y)})$, then $[Y^\perp]_i = \beta_1^i \cdot \eta^1 + \ldots + \beta_{m-r(Y)}^i \cdot \eta^{m-r(Y)} + \alpha_1^i \cdot [Y^T]_1 + \ldots + \alpha_n^i \cdot [Y^T]_n$.

$[Y^T]_1, \ldots, [Y^T]_n, \eta^1, \eta^2, \ldots, \eta^{m-r(Y)}$ is a generator system in $\mathbb{R}^m$ because it has a rank m. Hence, an arbitrary vector in $\mathbb{R}^m$ can be described by the linear combinations of the elements of this generator system.
Second direction: If $[Y^\perp]_i = \beta_1^i \cdot \eta^1 + \ldots + \beta_{m-r(Y)}^i \cdot \eta^{m-r(Y)} + \alpha_1^i \cdot [Y^T]_1 + \ldots + \alpha_n^i \cdot [Y^T]_n$, then $m = r(Y^T, \eta^1, \eta^2, \ldots, \eta^{m-r(Y)})$.

$[Y^T]_1, \ldots, [Y^T]_n, [Y^\perp]_1, \ldots, [Y^\perp]_{m-r(Y)}$ has a rank m. Let us consider the vector space generated by these vectors. If it can be given by the linear combinations of the vectors $[Y^T]_1, \ldots, [Y^T]_n, \eta^1, \eta^2, \ldots, \eta^{m-r(Y)}$, then this vector set also have to have rank m.
We chose the following set of vectors as generator system: $[Y^T]_1, \ldots, [Y^T]_n, [Y^\perp]_1, \ldots, [Y^\perp]_{m-r(Y)}$, because by using this only $m - r(Y)$ conditions will be obtained in the optimization problem. □

In order to use these results in a MILP framework we have to reformulate them to linear ones. Firstly we are going to give a linear inequality system which is equivalent with the kernel constraint eq. (3.22). For this we are going to apply the result of the section 2.2.2.1. We can introduce a binary matrix $\Theta \in \{0,1\}^{m \times m}$. $[\Theta]_{ij}$ is 0 when $[A_k]_{ij} = 0$ otherwise $[\Theta]_{ij}$ is 1. We can give this property of Θ with the following inequalities:

$$\epsilon \cdot [\Theta]_{ij} \leq [A_k]_{ij} \leq U \cdot [\Theta]_{ij} \tag{3.26}$$

where ϵ is a small positive constant and U is the upper bound of $[A_k]_{ij}$. By using of variable Θ the logical version of the kernel constraint (3.25) can be written as follows:

$$-(1 - [\Theta]_{ij}) \cdot 2 \cdot U \leq x_i - x_j \leq (1 - [\Theta]_{ij}) \cdot 2 \cdot U \tag{3.27}$$

where ϵ is a small positive constant and U is the upper bound of $|x_i|$.

The presented bilinear constraint in Theorem 5 can be simplified to a linear one:

$$[Y^\perp]_i = \bar{\eta}^i + \alpha_1^i \cdot [Y^T]_1 + \ldots + \alpha_n^i \cdot [Y^T]_n \tag{3.28}$$

considering that the linear combination $\beta_1^i \cdot \eta^1 + \ldots + \beta_{m-r(Y)}^i \cdot \eta^{m-r(Y)}$ is a solution of eq. (3.22):

$$B_G^T(\beta_1^i \cdot \eta^1 + \ldots + \beta_{m-r(Y)}^i \cdot \eta^{m-r(Y)}) = 0 \tag{3.29}$$

since any η^l is a solution of eq. (3.22):

$$B_G^T \cdot \beta_l^i \cdot \eta^l = \beta_l^i \cdot B_G^T \cdot \eta^l = 0. \tag{3.30}$$

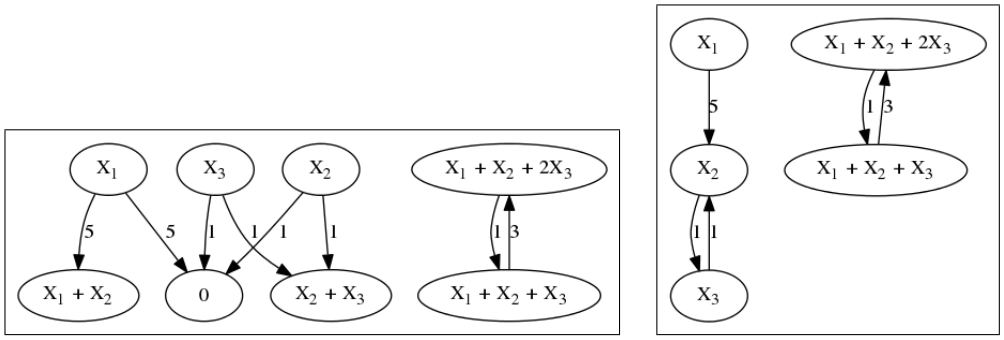
Finally, by choosing an arbitrary linear objective function of the decision variables, realizations with zero deficiency of the studied kinetic system can be computed (if any exists) in a MILP framework using the linear constraints (3.5) and (3.26)-(3.28).

Example 4. Let us consider a CRN having the complex composition matrix Y as follows:

$$Y = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 2 & 1 \end{bmatrix}$$

and a non-reversible Kirchhoff-matrix A_k containing the following non-zero off-diagonal elements: $[A_k]_{2,1} = 5$, $[A_k]_{3,1} = 5$, $[A_k]_{2,4} = 1$, $[A_k]_{6,4} = 1$, $[A_k]_{2,5} = 1$, $[A_k]_{6,5} = 1$, $[A_k]_{8,7} = 1$, $[A_k]_{7,8} = 3$. The deficiency of this realization: $d = 3$. The reaction graph of this system can be found in Fig. 3.4a where the complex described by the ith column of Y is denoted as C_i.

Now, by using the proposed method we are able to determine an alternative realization (Y, A'_k) which is dynamically equivalent to (Y, A_k) and has zero deficiency. The complex set remains unchanged and the non-zero off-diagonal elements of the matrix A'_k are the following: $[A'_k]_{4,1} = 5$, $[A'_k]_{5,4} = 1$, $[A'_k]_{4,5} = 1$, $[A'_k]_{8,7} = 1$, $[A'_k]_{7,8} = 3$. This reaction graph is depicted in Fig. 3.4b.



(a) Reaction graph of the realization (Y, A_k).

(b) Reaction graph of the realization (Y, A'_k).

Figure 3.4: Two CRNs which are dynamically equivalent with each other and have different deficiency values. This system has no weakly reversible realization. Isolated complexes are omitted from the figure.

3.5 Computing weakly reversible realizations with minimal deficiency

In this section, the results of [14] are briefly summarized. The basis of the method is the recognition that for weakly reversible networks, it is enough to maximize the number of linkage classes (i.e. graph components) to minimize deficiency. An additional applied known result is that a reaction graph is weakly reversible if and only if there

is a strictly positive vector in the kernel of the Kirchhoff matrix A_k. Then, the goal of the optimization task is to allocate complexes between the possible maximal number of linkage classes while maintaining dynamical equivalence.

The constraints for dynamical equivalence are easy to write as follows:

$$\begin{array}{rl} \tilde{Y} \cdot \tilde{A}_k & = \tilde{M} \\ \sum_{i=1}^{m} [\tilde{A}_k]_{ij} & = 0,\ j = 1, \ldots, m \\ 0 \leq [\tilde{A}_k]_{ij} & \leq 1/\epsilon,\ i, j = 1, \ldots, m, i \neq j \end{array} \tag{3.31}$$

where $\tilde{Y}$ and $\tilde{M}$ are the known complex composition matrix and coefficient matrix of the right hand side of the polynomial differential equations, respectively. The off-diagonal elements of the Kirchhoff matrix $\tilde{A}_k$ are unknowns, and ϵ is a sufficiently small number used for bounding the elements of A_k. This bounding is technically needed because the final optimization problem will contain integer variables as well. It can be easily shown that the maximal possible number of linkage classes in any computed realization is $m - s$ [14]. To track the graph nodes among the graph components (linkage classes), binary variables γ_{ik}, for $i = 1, \ldots m$, $k = 1, \ldots m - s$ are introduced: $\gamma_{ik} = 1$ if and only if C_i belongs to the k-th linkage class. We also introduce other auxiliary variables $\theta_k \in [0, 1]$, for $k = 1, \ldots, m - s$, where $\theta_k = 0$ indicates that the k-th linkage class is empty. The complete partitioning of the complexes between linkage classes is expressed by the constraints:

$$\begin{array}{l} \sum_{k=1}^{m-s} \gamma_{ik} = 1, \quad i = 1, \ldots, m \\ \sum_{i=1}^{m} \gamma_{ik} - \epsilon\theta_k \geq 0, \quad k = 1, \ldots, m - s \\ -\sum_{k=1}^{m} \gamma_{ik} + \frac{1}{\epsilon}\theta_k \geq 0, \quad k = 1, \ldots, m - s \\ \gamma_{ik} \in \{0, 1\}, \quad i = 1, \ldots, m, k = 1, \ldots, m - s \\ \theta_k \in [0, 1], \quad k = 1, \ldots, m - s. \end{array} \tag{3.32}$$

To ensure weak reversibility, we use an $m \times m$ Kirchhoff matrix Φ that is a column-scaled version of A_k, i.e. $\Phi = \tilde{A}_k \cdot \mathrm{diag}(b)$, where $b \in \mathbb{R}^m$ is a strictly positive vector in the kernel of $\tilde{A}_k$. It is clear that the positions of zero and non-zero elements in $\tilde{A}_k$ and Φ are the same, and therefore reaction graph encoded by $\tilde{A}_k$ is weakly reversible if and only if the m-dimensional vector containing only ones, i.e. $[1\ 1\ \ldots\ 1]^T \in \mathbb{R}^m$ belongs to the

kernel of Φ. Let us add the following constraint set to the problem:

$$\begin{aligned}
&\sum_{\substack{l=1\\l\neq i}}^{m}\Phi_{il}=\sum_{\substack{l=1\\l\neq i}}^{m}\Phi_{li}\\
&\Phi_{ij}\leq\frac{1}{\epsilon}(\gamma_{ik}-\gamma_{jk}+1)\\
&\Phi_{ij}\geq\epsilon[\tilde{A}_k]_{ij}\\
&\Phi_{ij}\leq\frac{1}{\epsilon}[\tilde{A}_k]_{ij}\\
&i,j=1,\ldots,m,i\neq j,\ \ k=1,\ldots,m-s.
\end{aligned}\tag{3.33}$$

The constraints in (3.33) ensure the following key properties: 1) identical structure of Φ and A_k, 2) weak reversibility of the reaction graph corresponding to Φ and A_k, 3) there cannot be directed edges between different linkage classes. Finally, the uniqueness of solution can be enforced by the following constraint:

$$\begin{aligned}
&\sum_{j=1}^{i-1}\gamma_{jk}\geq\sum_{l=k+1}^{m-s}\gamma_{il},\\
&i=1,\ldots,m,k=1,\ldots,m-s,k\leq i.
\end{aligned}\tag{3.34}$$

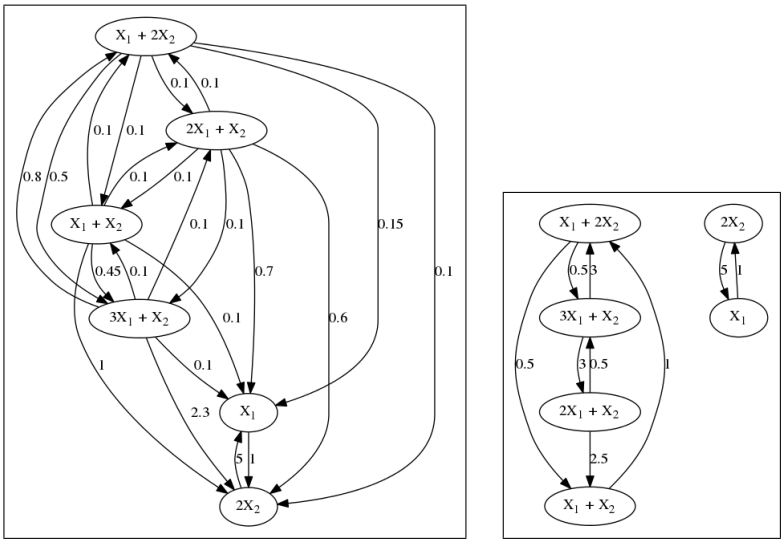
By minimizing the following objective function, the deficiency is also minimized (through maximizing the number of linkage classes):

$$V(\theta)=\sum_{k=1}^{m-s}\theta_k\tag{3.35}$$

It is visible that constraints (3.31)-(3.34) together with the objective function in (3.35) form a standard mixed integer linear programming (MILP) problem.

Example 5. Let us consider a CRN which is given with its reaction graph: Fig. 3.5a. It is easy to see that this realization is not weakly reversible and its deficiency is 3.

Now, by using the proposed method we are able to determine an alternative realization (Y,A'_k) which is dynamically equivalent to (Y,A_k), weakly reversible and it has minimal deficiency: 2. This reaction graph is depicted in Fig. 3.5b.



(a) Reaction graph of the realization (Y, A_k).

(b) Reaction graph of the realization (Y, A'_k).

Figure 3.5: Two CRNs which are dynamically equivalent with each other. The second one is weakly reversible with minimal deficiency.

4 Feedback computation

In this section, the optimization problems for the design of static and dynamic kinetic feedback are described. First, the autonomous system model (3.1) will be extended with a simple linear input structure.

4.1 Open loop model form

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

$$\dot{x} = M \cdot \psi_1(x) + Bu, \tag{4.1}$$

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 with minimal deficiency).

4.2 Static feedback design: structure and parameters

We assume a polynomial feedback of the form

$$u = K \cdot \overline{\psi}(x), \tag{4.2}$$

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, $B \in \mathbb{R}^{n\times p}$, and $K \in \mathbb{R}^{p\times(m_1+m_2)}$. The closed-loop system can be written as

$$\dot{x} = M \cdot \psi_1(x) + BK \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \end{bmatrix}. \tag{4.3}$$

We can partition K into two blocks as $K = [K_1\ K_2]$, 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

$$\dot{x} = \underbrace{\begin{bmatrix} M + BK_1 & BK_2 \end{bmatrix}}_{\overline{M}} \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \end{bmatrix} = \overline{M} \cdot \overline{\psi}(x). \tag{4.4}$$

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 2.1 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 constructing the so-called canonical realization of a kinetic system [16], we can give a simple method to generate matrix $\overline{Y}$ (and thus ψ_2 given by such monomials that do not appear in (4.1)) using the monomials of the open loop system as as described in [28]. After constructing $\overline{Y}$, the kinetic property, minimal deficiency and weak reversibility of the controlled system can be achieved if the MILP problem defined by (3.31)-(3.34) and (3.35) can be solved for $\tilde{A}_k = \overline{A}_k$ substituting $\tilde{Y} = \overline{Y}$ and $\tilde{M} = \overline{M}$.

Thus, the feedback gain computation and the search for realizations of the closed loop system which is accordance with the requirements has been integrated into one LP or MILP optimization problem. It has to be noted that while $\tilde{M}$ is assumed to be known in (3.31), $\overline{M}$ contains unknowns, namely the feedback parameters K_1 and K_2, but this does not change the linear nature of the constraints and the LP or MILP computation framework is still applicable.

4.3 Dynamic feedback design: structure and parameters

To increase the degrees 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

$$\dot{x}^{(1)} = M_{11}\psi_1(x^{(1)}) + Bu, \tag{4.5}$$

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

$$\dot{x}^{(2)} = M_{21}\psi_1(x^{(1)}) + M_{22}\psi_2(x), \tag{4.6}$$

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,

$$x = \begin{bmatrix} x^{(1)} \\ x^{(2)} \end{bmatrix} \in \mathbb{R}^{n+k},\ \overline{\psi}(x) = \begin{bmatrix} \psi_1(x^{(1)}) \\ \psi_2(x) \end{bmatrix}, \tag{4.7}$$

where $\psi_2 : \mathbb{R}^{n+k} \to \mathbb{R}^{m_2}$. Let us again use a monomial feedback in the form $u = K\overline{\psi}(x) = K_1\psi_1 + K_2\psi_2$, 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

$$\dot{x} = \begin{bmatrix} M_{11} + BK_1 & BK_2 \\ M_{21} & M_{22} \end{bmatrix} \cdot \overline{\psi}(x) = \overline{M} \cdot \overline{\psi}(x) \tag{4.8}$$

The feedback gain computation, constraints of the closed loop are completely analogous to the static feedback case described in subsection 4.2 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.

4.4 Examples with different requirements for the closed loop

In this section we are going to prescribe different requirements for the closed loop system. For computing these closed loops we can use of the results of the section 3.1. The examples with ensuring different structural properties illustrate that useful dynamical properties can be guaranteed to the closed loop system (e.g. bounded trajectories, positive equilibrium points, global stability) using the proposed feedback design method.

4.4.1 Example for weakly reversible closed loop

It was shown in section 3.3 that complexity of computing of a weakly reversible realization is polynomial time in the number of complexes. Hence, when you have a large system with many complexes, the design of the feedback which guarantees bounded trajectory instead of global stability remains computability tractable. With the following example we are going to demostrate this type of feedback.

Example 6. Let us consider the following polynomial system

$$\dot{x} = 0.5y - 16x - x^3 + x^2y + 2 + u \tag{4.9}$$

$$\dot{y} = -0.5y + 16x + x^3 - x^2y \tag{4.10}$$

$$\tag{4.11}$$

You can see in the Fig. 4.2a that for $u = 0$, the system has no equilibrium points in the nonnegative orthant. Using the notations of section 4.1, we have:

$$\psi_1(x, y) = [y \; x \; 1 \; x^3 \; x^2y]^T, \tag{4.12}$$

$$M_{11} = \begin{bmatrix} 0.5 & -16 & 2 & -1 & 1 \\ -0.5 & 16 & 0 & 1 & -1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{4.13}$$

Performing the procedure presented in section 4.2, we find that the LP optimization problem is feasible, and

$$K = \begin{bmatrix} 0 & -2 & 0 & 0 & 0 \end{bmatrix}. \tag{4.14}$$

This means that the feedback: $u = -2x$, results in a closed loop system that has a weakly reversible realization. Therefore, the controlled system has bounded trajectories in the positive orthant but it is not asymptotically stable. The resulting weakly reversible reaction graph of the closed loop system is depicted in Fig. 4.1, while Fig. 4.2b illustrates the bounded trajectories of the controlled system.

4.4.2 Weakly reversible closed loop with minimal and zero deficiency

Previously we showed that a polynomial system which has a weakly reversible realization with zero deficiency can guarantee the global stability of the system. This result is our motivation to design weakly reversible closed loop with zero deficiency. We gave two different methods to compute zero deficiency realization in sections 3.4 and 3.5. With the following examples we are going to demonstrate this type of feedback.

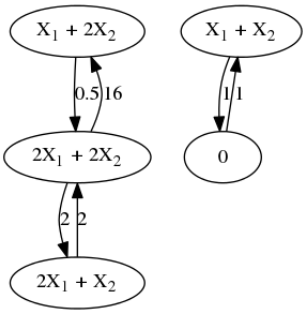
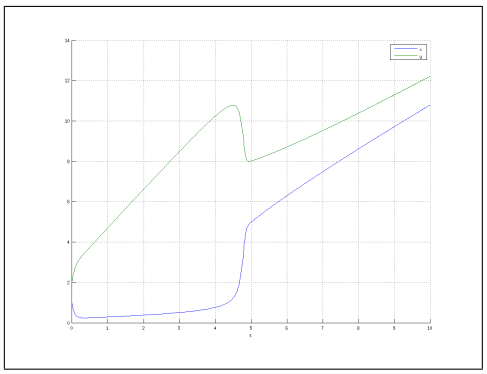
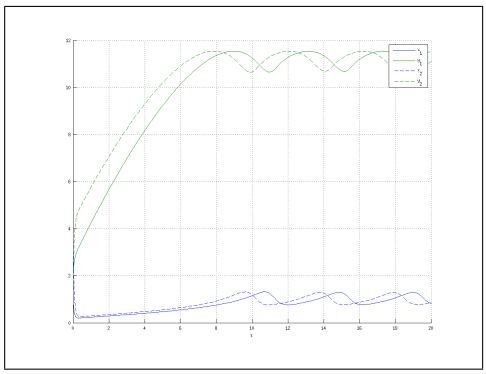


Figure 4.1: Weakly reversible kinetic structure of the closed loop system



(a) Time domain behavior of the open-loop system



(b) Two different trajectories demonstrate the time domain behavior of the closed loop system

Figure 4.2: Time domain behaviour of the open and the closed loop system

Example 7. Let us consider the following polynomial system

$$\dot{x}_1 = -x_1x_2 + 2x_2^2x_3 \tag{4.15}$$

$$\dot{x}_2 = x_1x_2 - 4x_2^2x_3 - x_2x_3^2 + u_1 \tag{4.16}$$

$$\dot{x}_3 = 6 + x_1x_2 - 3x_2^2x_3 + u_2 \tag{4.17}$$

It is easy to see from (4.17) that for $u_1 = 0$, $u_2 = 0$, the system has no equilibrium points in the nonnegative orthant. Using the notations of section 4.1, we have:

$$\psi_1(x^{(1)}) = [1 \; x_1x_2 \; x_2^2x_3 \; x_2x_3^2]^T, \tag{4.18}$$

$$M_{11} = \begin{bmatrix} 0 & -1 & 2 & 0 \\ 0 & 1 & -4 & -1 \\ 6 & 1 & -3 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{4.19}$$

For a dynamical feedback, let us introduce one new variable $x^{(2)} = x_4$, and an additional monomial as follows: $\psi_2(x) = [x_3^2x_4]$. Then, after performing the procedure presented

in section 4.3, we find that the MILP optimization problem is feasible, and

$$K = \begin{bmatrix} 1 & 0 & 2 & 0 & 0 \\ 2 & 0 & 1 & 0 & -10 \end{bmatrix}, \; M_{21} = [3\ 0\ 0\ 1], \; M_{22} = [-5]. \tag{4.20}$$

This means that the feedback: $u_1 = 2x_2^2x_3$, $u_2 = x_2^2x_3 - 10x_3^2x_4$, and the dynamic extension: $\dot{x}_4 = 3 + x_2x_3^2 - 5x_3^2x_4$ 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. 4.3, while Fig. 4.4b illustrates the asymptotically stable trajectories of the controlled system.

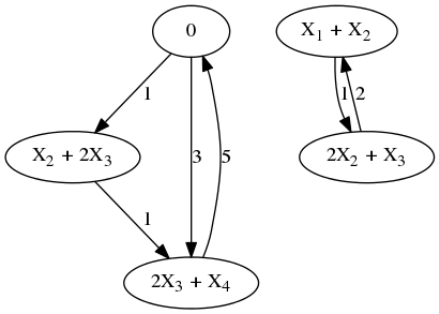
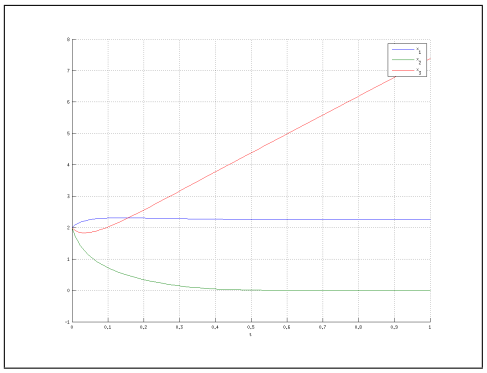
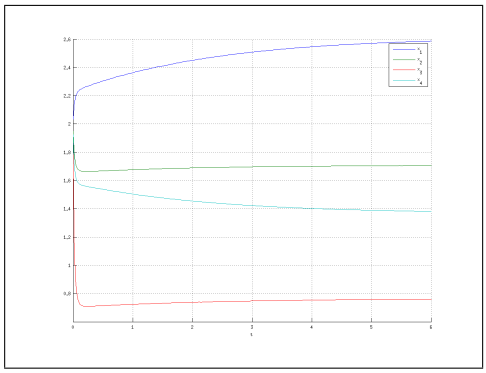


Figure 4.3: Weakly reversible kinetic structure of the closed loop system



(a) Unstable behavior of the open-loop system



(b) Time-domain behaviour of the controlled system

Figure 4.4: Time domain behaviour of the open and the closed loop system

Example 8. Let us consider the extended version of the well-known 3-dimensional

Lorenz system by linear input terms as an open loop polynomial system

$$\dot{x} = \sigma(y - x) + u_1 \tag{4.21}$$
$$\dot{y} = x(\rho - z) - y + u_2 \tag{4.22}$$
$$\dot{z} = xy - \beta z + u_3 \tag{4.23}$$

Let the parameter values be $\sigma = 10$, $\rho = 28$, $\beta = 8/3$ that are known to lead to chaotic behavior for $u = 0$. It is important to note that the above model is not kinetic that is also clearly visible from Fig. 4.6a.

Using the notations of section 4.1, we have:

$$\psi_1(x, y, z) = [x\ y\ z\ xz\ xy]^T, \tag{4.24}$$
$$M_{11} = \begin{bmatrix} -10 & 10 & 0 & 0 & 0 \\ 28 & -1 & 0 & -1 & 0 \\ 0 & 0 & -2.6667 & 0 & 1 \end{bmatrix},\ B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{4.25}$$

In designing the feedback we are going to use the original monomials only and we are not using dynamical extension. Then, after solving the MILP problem described in section 4.2, we find that the problem is feasible, and

$$K = \begin{bmatrix} 9.9 & -9.8 & 0.1 & -0.1 & -0.1 \\ -27.9 & 0.8 & 0.1 & 1.1 & -0.1 \\ 0 & 0.2 & 2.5667 & -0.2 & -0.9 \end{bmatrix}. \tag{4.26}$$

The obtained feedback structure results in a closed loop system that has a weakly reversible realization with zero deficiency. The resulting weakly reversible reaction graph of the closed loop system is depicted in Fig. 4.5, while Fig. 4.6b illustrates the stable behavior of the controlled system. Note that the above feedback completely changes the

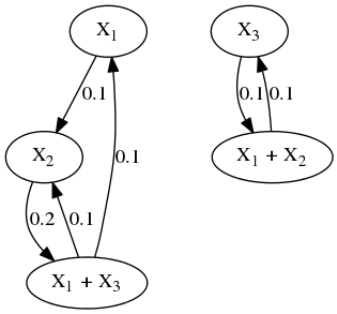
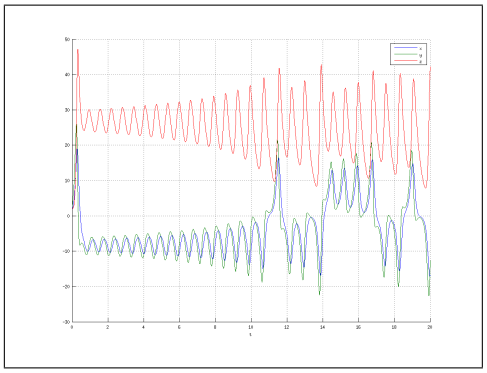
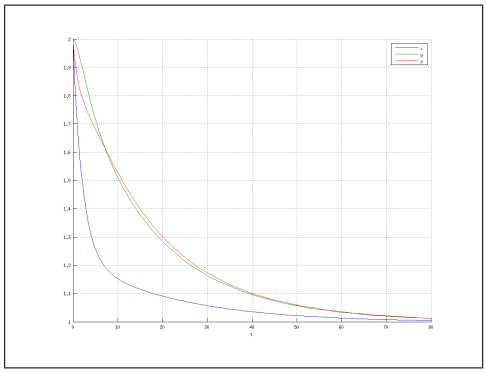


Figure 4.5: Weakly reversible kinetic structure of the closed loop system

coefficients of the nonlinear terms in the model by leaving its monomial terms unchanged.



(a) Chaotic behavior of the open-loop Lorenz system



(b) Time-domain behaviour of the controlled Lorenz system

Figure 4.6: Time domain behaviour of the open and the closed loop Lorenz system

5 Conclusions and future work

Firstly we presented the number of methods to compute different realizations of a CRN. Weakly reversible realizations with zero deficiency guarantee global stability. Hence we gave a new method to computing realizations with zero deficiency. In order to reduce the computational time of computing weakly reversible realizations we determined the minimal set of complexes. This result is useful in choosing of monomials in the feedback computing, too.

Based on our earlier works [28, 29] a novel optimization based state feedback design method was proposed for polynomial systems that transforms the closed loops system into kinetic form with minimal deficiency and weak reversibility. Weak reversibility ensures the boundedness of the trajectories in the positive orthant, while global stability can be achieved in the zero deficiency case. Both static and dynamic feedback designs are considered. The computational method uses optimization for jointly determining the feedback parameters and the preferred dynamically equivalent realization of the closed loop system as a kinetic system. The different requirements request different computational complexity. We gave LP method to compute closed loop with bounded trajectories and MILP methods to reach global stability.

The controller structure assumes a linear input structure of the open loop system, and uses a polynomial feedback constructed from the monomials of the original system possibly extended by new ones.

The proposed methods are illustrated by examples, including a Lorenz system with chaotic behavior in the open-loop case.

Since this report only just presented the first step in the feedback design based on the CRN theory, so a number of open questions remained. Hence we give some possible directions for the future work:

- Choosing of the monomials in the the feedback polynomial.
- Dealing with the robustness of the closed loop.
- Specifying performance requirements in the optimization problems.

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