Kinetic nonlinear feedback design for polynomial systems

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joint work with
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Contents

Positive systems

Essential non-negativity of a function $f = [f_1 \ \ldots \ f_n]^T : [0, \infty)^n \to \mathbb{R}^n$, holds if, for all $i = 1, \ldots, n$, $f_i(x) \geq 0$ for all $x \in [0, \infty)^n$, whenever $x_i = 0$.

Definition (Positive systems)

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

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

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* (1).

This property holds if and only if f is essentially nonnegative.

Positive polynomial systems

Kinetic systems: positive polynomial systems

A positive polynomial vector field with all coordinates functions of f in (1) must have the form

$$f_i(x) = -x_i g_i(x) + h_i(x),\ i = 1, \ldots, n \tag{2}$$

where g_i and h_i are polynomials with nonnegative coefficients.

Kinetic systems always have a MAL-CRN (chemical reaction networks with mass action law) realization.

MAL-CRN models

MAL-CRN - formal description

Irreversible reactions: elementary reaction step

$$\sum_{s=1}^{L} \alpha_{sj} \mathrm{A}_s \to \sum_{s=1}^{L} \beta_{sl} \mathrm{A}_s$$

the stoichiometric coefficients α_{sj} *and* β_{sl} *are always non-negative integers*
Complexes C_k $(k = 1, ..., m)$ associated to the LHS of the reaction steps

Dynamic model: an autonomous ODE with polynomial RHS on the positive orthant
$x = [x_1, ..., x_L]^T$, $x_s = [\mathrm{A}_s]$, $Y_{sj} = \alpha_{sj}$

$$\dot{x} = Y \cdot A_k \cdot \varphi(x) \ \ , \ \ \varphi_j(x) = \prod_{s=1}^{L} x_s^{\alpha_{sj}}, \quad j = 1, \ldots, m$$

$k_j > 0$ is the *reaction rate constant* of the jth reaction, *always positive*

$$A_{k,lj} = \begin{cases} -\sum_{\ell=1}^{m} k_{l,\ell}, & \text{if} \quad l = j \\ k_{jl}, & \text{if} \quad l \neq j \end{cases}$$

A_k is a *Kirchhoff matrix* with zero column sum.

MAL-CRN - reaction graph

The reaction graph: weighted directed graph

- vertexes correspond to the complexes
- edges describe reactions

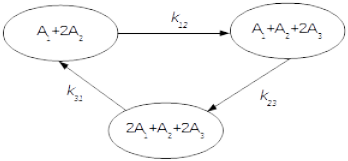
The Kirchhoff-matrix A_k determines the reaction graph.

Example: nonlinear MAL-CRN

$$\mathrm{A}_1 + 2\mathrm{A}_2 \xrightarrow{k_{12}} \mathrm{A}_1 + \mathrm{A}_2 + 2\mathrm{A}_3\ ,\ \mathrm{A}_1 + \mathrm{A}_2 + 2\mathrm{A}_3 \xrightarrow{k_{23}} 2\mathrm{A}_1 + \mathrm{A}_2 + 2\mathrm{A}_3\ ,$$

$$2\mathrm{A}_1 + \mathrm{A}_2 + 2\mathrm{A}_3 \xrightarrow{k_{31}} \mathrm{A}_1 + 2\mathrm{A}_2$$

$$Y = \begin{bmatrix} 1 & 1 & 2 \\ 2 & 1 & 1 \\ 0 & 2 & 2 \end{bmatrix},\ A_k = \begin{bmatrix} -k_{12} & 0 & k_{31} \\ k_{12} & -k_{23} & 0 \\ 0 & k_{23} & -k_{31} \end{bmatrix}$$



Structural properties

Structural properties hold irrespectively of the actual value of the reaction kinetic parameters $k_i > 0$

Reaction vector corresponding to $C_i \rightarrow C_j$:

$$e_k = [Y]_{\cdot,j} - [Y]_{\cdot,i}, \;\; k = 1, \ldots, r, \tag{3}$$

The *rank* of a reaction network s: the rank of the set of vectors $H = \{e_1, e_2 \ldots, e_r\}$

- **Deficiency**: $d = m - s - l$, where l is the number of linkage classes
- **Weak reversibility**
  whenever exists a directed path from C_i to C_j, then there exists a directed path from C_j to C_i (the reaction graph consists of strongly connected components)

Realizations of MAL-CRN models

Dynamic equivalence, LD transformation

Two MAL-CRNs with **realizations** $(Y^{(1)}, A_k^{(1)})$ and $(Y^{(2)}, A_k^{(2)})$ of the form

$$\dot{x} = M\varphi(x)$$

are **dynamically equivalent** if $M = Y^{(1)}A_k^{(1)} = Y^{(2)}A_k^{(2)}$. Most often $Y^{(1)} = Y^{(2)} = Y$ is given.

The MAL-CRN model with a realization (Y, A_k) can be transformed to another MAL-CRN model with a realization (Y, A'_k) using a **linear diagonal (LD) transformation** matrix $T = \mathrm{diag}(c)$, where $c \in \mathbb{R}_+^n$ is an element-wise positive vector

$$YA_k = TYA'_k(\mathrm{diag}(\varphi(c)))^{-1} \tag{4}$$

Properties of the LD transformation - linear conjugacy

- the LD transformation is an invertible variable transformation, that is also called **variable rescaling**,
- under an LD transformation, the kinetic property and the **qualitative dynamical properties** of MAL-CRNs are preserved.

Szederkényi G (2013). *Computational Methods for the Analysis of Nonnegative Polynomial Systems*. thesis for the title: Doctor

Computing dynamically equivalent realizations

- Problem statement
  - given the ODE model of a CRN with its matrices M (coefficients) and Y (monomials)
  - compute a realization (possibly with a given set of properties), i.e. a Kirchhoff matrix A_k such that $M = Y \cdot A_k$
- Useful desired properties
  - maximal realization (maximal number of edges in the reaction graph): unique
  - minimal realization: not unique
  - weakly reversible realizations
- Solution: a ***linear (LP or MILP) optimization problem***

The linear programming problem of computing dynamically equivalent realizations

Dynamic equivalence and Kirchhoff properties: linear constraint set

$$\begin{cases} M = Y \cdot A_k \\ \mathbf{1}^T \cdot A_k = \mathbf{0}^T \\ [A_k]_{ij} \geq 0 \quad i,j = 1,\ldots,m, \; i \neq j, \end{cases}$$

Weak reversibility: linear constraint set

$$\sum_{i=1}^{m} [\tilde{A}_k]_{i,j} = 0, \quad j = 1,\ldots,m \quad (\tilde{A}_k)\mathbf{1} = \mathbf{0})$$

$$\sum_{i=1}^{m} [\tilde{A}_k]_{j,i} = 0, \quad j = 1,\ldots,m \quad [\tilde{A}_k]_{i,j} \geq 0, \quad i,j = 1,\ldots,m, \; i \neq j,$$

where A_k and $\tilde{A}_k$ are structurally equal.
Decision variables: the elements of matrices A_k and $\tilde{A}_k$
Objective function: e.g. $f_{obj} = \sum [A_k]_{ij}$, for $i,j = 1,\ldots,m, \; i \neq j$

MAL-CRN structural stability

Structural stability of an ODE $\frac{dz}{dt} = F(z, P)$ with parameters P:
stability for a set of parameters P

Important CRN properties: ***realization properties*** (!!)

- weakly reversible: determined by the reaction graph
- deficiency zero property: determined by $M = YA_k$

Deficiency Zero theorem
For a ***weakly reversible MAL CRN of deficiency zero*** - but *regardless of the positive values the reaction rate coefficients take* - the differential equations of the corresponding reaction system have the following properties: There exists within each positive stoichiometric compatibility class *precisely one steady state; that steady state is asymptotically stable*; and there is no nontrivial cyclic composition trajectory along which all species concentrations are positive.

Polynomial feedback design

Open loop system model, static state feedback

Polynomial system with linear input structure

$$\dot{x} = M \cdot \psi_1(x) + Bu, \tag{5}$$

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

Static state feedback: **polynomial**

- feedback equation

$$u = K \cdot \overline{\psi}(x), \tag{6}$$

  where $\overline{\psi}(x) = [\psi_1^T(x) \ \psi_2^T(x)]^T$ with $\psi_2 \in \mathbb{R}^n \rightarrow \mathbb{R}^{m_2}$ containing possible additional monomials for the feedback, $B \in \mathbb{R}^{n \times p}$, and $K \in \mathbb{R}^{p \times (m_1 + m_2)}$.

- closed loop system model

$$\dot{x} = \underbrace{\left[\begin{array}{cc} M + BK_1 & BK_2 \end{array} \right]}_{\overline{M}} \left[\begin{array}{c} \psi_1(x) \\ \psi_2(x) \end{array} \right] = \overline{M} \cdot \overline{\psi}(x) \tag{7}$$

Dynamic state feedback

- state equations

$$\dot{x}^{(1)} = M_{11}\psi_1(x^{(1)}) + Bu, \tag{8}$$

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 $u \in \mathbb{R}^p$

- dynamic extension

$$\dot{x}^{(2)} = M_{21}\psi_1(x^{(1)}) + M_{22}\psi_2(x), \tag{9}$$

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

- monomial feedback: $u = K\overline{\psi}(x) = K_1\psi_1 + K_2\psi_2$
- closed loop system

$$\dot{x} = \begin{bmatrix} M_{11} + BK_1 & BK_2 \\ M_{21} & M_{22} \end{bmatrix} \overline{\psi}(x) = \overline{M} \cdot \overline{\psi}(x), x = \begin{bmatrix} x^{(1)} \\ x^{(2)} \end{bmatrix}, \overline{\psi}(x) = \begin{bmatrix} \psi_1(x^{(1)}) \\ \psi_2(x) \end{bmatrix}$$

Feedback gain calculation

- Closed loop system (in both the static and dynamic feedback cases)

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

  where $\overline{M}(K)$ is ***linear in the feedback gain*** K

- **Problem statement**: given the open loop M and B together with $\overline{Y}$ from $\overline{\psi}(x)$ determine the feedback gain K such that the ***closed loop system has a weakly reversible zero deficiency realization***

- Solution: a MILP problem

Design parameters - open problems

- Input structure: open loop model
  - linear case, dimension and structure of matrix B
  - relationship with nonlinear controllability
- Controller structure
  - monomial selection for the feedback: weakly reversible case
  - static vs. dynamic feedback
- Equilibrium point

1. Szederkényi G, Lipták G, Rudan J and Hangos K (2013), Optimization-based design of kinetic feedbacks for nonnegative polynomial systems, In *IEEE 9th International Conference of Computational Cybernetics*, July 8-10, Tihany, Hungary. , pp. 67-72.
2. Lipták G, Szederkényi G and Hangos KM (2014), Kinetic feedback computation for polynomial systems to achieve weak reversibility and minimal deficiency, In *13th European Control Conference, ECC 2014*, 06. 24 - 06. 27, 2014, Strasbourg, France. , pp. 2691-2696.

Example

Lorenz system

Open loop dynamic model

the extended version of the well-known 3-dimensional Lorenz system by linear input terms as an open loop polynomial system

$$\dot{x} = \sigma(y - x) + u_1 \quad (11)$$
$$\dot{y} = x(\rho - z) - y + u_2 \quad (12)$$
$$\dot{z} = xy - \beta z + u_3 \quad (13)$$

Let the parameter values be $\sigma = 10$, $\rho = 28$, $\beta = 8/3$ that are known to lead to chaotic behaviour for $u = 0$.

The open loop model is not kinetic!

Static feedback structure

Parameters

$$\psi_1(x, y, z) = [x \; y \; z \; xz \; xy]^T, \tag{14}$$

$$M_{11} = \begin{bmatrix} -10 & 10 & 0 & 0 & 0 \\ 28 & -1 & 0 & -1 & 0 \\ 0 & 0 & -2.6667 & 0 & 1 \end{bmatrix}, \tag{15}$$

$$B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{16}$$

Fully actuated case!

Design: using only the original monomials and a static feedback

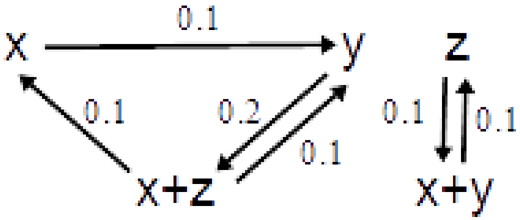
Computing the feedback parameters

Solving the MILP problem: feasible with a gain matrix

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

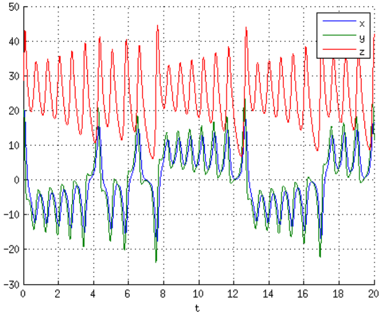
Almost full gain matrix!

Structure graph of the closed loop system

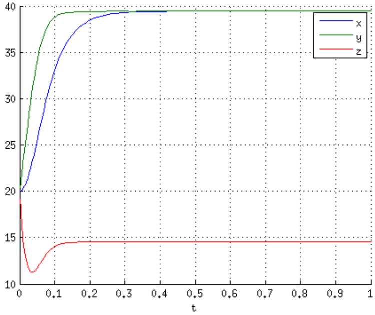


Two linkage classes, deficiency zero
Weakly reversible
All reaction rates were influenced

Time evolution of the solutions



open loop dynamics with $u \equiv 0$



closed loop dynamics

Conclusion and Future Work

A linear optimization based feedback design method is developed for polynomial systems that ensures global structural stability

The design is based on

- properties of MAL-CRNs
- computing dynamically equivalent realizations with MILP
- deficiency zero theorem: searching for a realization of the closed-loop system that is weakly reversible with deficiency zero

Related work

- choice of the feedback monomials for the weakly reversible case
- choice of the equilibrium point
- robustness investigations

Future work

- relationship with controllability
- existence and uniqueness conditions