Conservation and entropy-inspired Lyapunov functions for positive polynomial systems

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Dedicated to A.N. Gorban on the occasion of his 60th birthday

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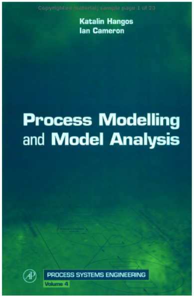
Systems and control theory – Process systems



state equations : $\frac{dx}{dt} = f(x) + g(x)u$

conservation balances

overall mass, energy $\mapsto$ *temperature*

component masses $\mapsto$ *concentrations*

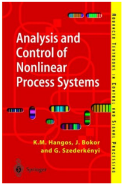
chemical reaction networks (CRNs) with MAL

class of positive polynomial systems, autonomous

constant overall mass (closed) $\mapsto$ **conservation**

only component mass balances

Stability of process systems – Lyapunov functions



state equations of **CRNs** : $\frac{dx}{dt} = P(x)$

Positive polynomial systems

structural $\approx$ *parameter – independent (robust)*

Structural properties of CRNs

structural descriptor $\mapsto$ *reaction graph*

structural properties $\mapsto$ *reaction graph properties*

Lyapunov function of CRNs

entropy – motivated

Markov chains and their relative entropies

Continuous time Markov chains with positive equilibrium probabilities p_j^*. The dynamics of the probability distribution $p_i, i = 1, ..., N$ with $q_{ij} \geq 0, (i \neq j)$:

$$\frac{dp_i}{dt} = \sum_{j,j\neq i} q_{ij} p_j - q_{ji} p_i \quad , \quad \sum_i p_i = 1 \quad , \quad 0 \leq p_i \leq 1 \tag{1}$$

Relative entropies from the Csiszár-Morimoto function: level-set equivalent Lyapunov functions

- Kullback-Leibner divergence (relative BGS entropy):
  $H_{\tilde{h}}(p) = H_{\tilde{h}}(p||p^*) = -\sum_i p_i \ln\left(\frac{p_i}{p_i^*}\right) \quad \simeq \quad$ reversible CRNs
- relative Burg entropy: $H_h(p) = H_h(p||p^*) = -\sum_i p_i^* \ln\left(\frac{p_i}{p_i^*}\right) \simeq V_{linCRN}(p)$
- normalized relative Burg entropy:
  $H_{\bar{h}}(p) = H_{\bar{h}}(p||p^*) = -\sum_i p_i^* \left(\ln\left(\frac{p_i}{p_i^*}\right) + (\frac{p_i}{p_1^*} - 1)\right) \simeq V_{LV}(p)$

A. N. Gorban, P. A. Gorban, G. Judge: Entropy: the Markov ordering approach. Entropy, 2010, 12, 1145-1193

Positive polynomial systems and their entropy-inspired Lyapunov functions

System dynamics with a given positive equilibrium point x^*

LV | **linCRN**

$$\frac{dx}{dt} = \mathrm{diag}(x) \cdot M \cdot (x - x^*) \qquad \frac{dx}{dt} = A_k \cdot (x - x^*)$$

Lyapunov functions $V(x)$

$$V_{LV}(x) = \sum_{i=1}^{m} c_i \left(x_i - x_i^* - x_i^* \ln \frac{x_i}{x_i^*} \right) \qquad V_{linCRN}(x) = -\sum_{i=1}^{n} x_i^* \ln \left(\frac{x_i}{x_i^*} \right)$$

Stability conditions: negative definiteness of

$$\left(\mathrm{diag}(c) \cdot M + M^T \cdot \mathrm{diag}(c) \right)$$

Deficiency Zero Theorem

MAL-CRN models

MAL-CRN - formal description

Irreversible reactions: elementary reaction step

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

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
$x = [x_1, ..., x_L]^T$, $x_s = [\mathrm{A}_s]$, $Y_{sj} = \alpha_{sj}$

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

$k_j > 0$ 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

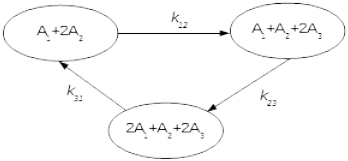
The Kirchhoff-matrix A_k determines the reaction graph.

Example: nonlinear MAL-CRN

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

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

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



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

$$YA_k = TYA_k'(\mathrm{diag}(\varphi(c)))^{-1} \qquad (2)$$

Properties of the LD transformation

- 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.

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

- weakly reversible: 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)
- 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.

Conservation of MAL-CRNs

Definition (Conservation property)

The mass conservation property of a MAL-CRN model $\frac{dx}{dt} = M\varphi(x) = YA_k\varphi(x)$ *holds if a strictly element-wise positive row vector* $\underline{\mathbf{m}} = [m_1, ..., m_n]$ *exists in the left kernel of* M*, i.e.*

$$\underline{\mathbf{m}}M = \underline{\mathbf{0}} \tag{3}$$

with $\underline{\mathbf{0}} = [0, 0, ..., 0]$*, that shows the rank-deficient nature of* M *in a MAL-CRN with mass conservation.*

Conservation and the Kirchhoff property

The zero column-sums within the Kirchhoff property of A_k can be expressed as

$$\underline{\mathbf{1}}A_k = \underline{\mathbf{0}}$$

where $\underline{\mathbf{1}} = [1, 1, ..., 1]$, $\quad \Rightarrow rank(A_k) \leq m - 1$.

$\Rightarrow \quad A_k$ has the conservation property with $\underline{\mathbf{m}} = \underline{\mathbf{1}}$

Linear MAL-CRNs

A linear MAL-CRN (with $Y = I, M = A_k$) has a unique realization with **zero deficiency**

$$\frac{dx}{dt} = A_k x$$

where A_k is a Kirchhoff and therefore **Metzler** matrix

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

with $k_{ij} \geq 0$. This implies

$$[A_k]_{ii} < 0 \;\; ; \;\; [A_k]_{ij} \geq 0 \; , \; i \neq j \;\; ; \;\; \underline{1} A_k = \underline{0}$$

where $\underline{1} = [1, ..., 1]$ a row vector.
A MAL-CRN is **weakly reversible**, if and only if there exists a positive vector p

$$A_k p = 0$$

LD transformation of linear MAL-CRNs

The LD transformed form A_k' of a linear MAL-CRN (with $Y = I, M = A_k$) satisfies

$$A_k = TA_k' T^{-1}$$

$\Rightarrow$ a **linear variable transformation**

Properties

- leaves the reaction graph unchanged
- leaves all structural properties unchanged
- the equilibrium point is rescaled

Stability of weakly reversible linear MAL-CRNs

Global stability of the equilibrium point x^* follows from the Deficiency Zero theorem.

Lyapunov functions:

1. Quadratic:

$$V_2(x) = (x - x^*)^T P(x - x^*) \quad \Rightarrow \quad A_k^T P + PA_k \preceq 0$$

with a positive definite **diagonal** P (A_k is a Metzler matrix).

2. Entropy-motivated

$$V_{\ln}(x) = -\sum_{i=1}^{n} x_i^* \ln\left(\frac{x_i}{x_i^*}\right)$$

Linear kinetic systems and their MAL-CRN realizations

Non-degenerate linear kinetic systems

A set of polynomial ODEs of the form $\dot{x} = f(x)$, where $x \in \mathbb{R}^n$, is kinetic if and only if all coordinates functions of f can be written in the form

$$f_i(x) = -x_i g_i(x) + h_i(x), \quad i = 1, \dots, n$$

where g_i and h_i are polynomials with nonnegative coefficients.
$\Rightarrow$ positivity

Linear kinetic systems

$$\frac{dx}{dt} = \overline{M}x \tag{4}$$

where the following **sign pattern** holds:

$$m_{ij} \geq 0, \; i \neq j \quad , \quad m_{ii} \leq 0 \tag{5}$$

Properties:

- **non-degenerate**: each row and also column of the coefficient matrix $\overline{M}$ contains at least one non-zero element
- **variable-structure graph**: the non-weighted version of the reaction graph for A_k in a CRN

Conservation

$\overline{M}$ is a conservation matrix if $\underline{\mathbf{m}}\overline{M} = \underline{\mathbf{0}}$ holds with $\underline{\mathbf{0}} = [0, ..., 0]$.

Theorem

The coefficient matrix $\overline{M}$ of a non-degenerate linear kinetic system (4) is a conservation matrix if and only if there exists a positive diagonal matrix $T = \mathrm{diag}(c_1, ..., c_n),\ c_i > 0$ such that $T\overline{M} = A_k$ where A_k is a Kirchhoff matrix.

Corollary

A non-degenerate kinetic matrix $\overline{M}$ with the conservation property is a stability matrix.

Lemma

If the coefficient matrix $\overline{M}$ of a non-degenerate linear kinetic system (4) is a conservation matrix and its variable-structure graph consists of strongly connected components, then there exists a linear weakly reversible MAL-CRN that can be obtained from (4) by using a suitable LD transformation.

Positive equilibrium points and conservation

Definition

*A kinetic matrix $\overline{M}$ has the **p-property**, if it has at least one positive (off-diagonal) element in each of its rows.*

Theorem

Let the coefficient matrix $\overline{M}$ of a non-degenerate linear kinetic system be a conservation matrix that has the p-property. Then its variable structure graph $\vec{G}_{\overline{M}}$ consists of strongly connected components.

Corollary

The existence of positive equilibrium points follows from Theorem 2.

Theorem

Consider a non-degenerate kinetic matrix $\overline{M}$ with the p-property, that has an element-wise positive vector p in its kernel. Then $\overline{M}$ is a conservation matrix.

Diagonal stability

Theorem

Consider a non-degenerate kinetic matrix $\overline{M}$ with the p-property, that has an element-wise positive vector p in its kernel, i.e. $\overline{M}p = 0$. Then $\overline{M}$ is diagonally stable, i.e. there exists an element-wise positive diagonal matrix $Q \in \mathcal{D}_+$ such that

$$\overline{M}^T Q + Q\overline{M} \preceq 0 \qquad (6)$$

Lyapunov functions for non-degenerate linear kinetic systems 1

Theorem (LinearKinetic)

*Assume that the coefficient matrix $\overline{M}$ of a non-degenerate kinetic system has variable structure graph $\vec{G}_M$ consisting of strongly connected components. Then this system allows to have **suitable scaled** Lyapunov functions*

- $V_2 = (x - x^*)^T P (x - x^*)$ *with a positive definite diagonal* $P = \mathrm{diag}(p_1, ..., p_n)$
- $V_{CRN} = -\sum_{i=1}^{n} t_i x_i^* \ln\left(\frac{x_i}{x_i^*}\right)$
- $V_{LV}(x) = \sum_{i=1}^{m} c_i \left(x_i - x_i^* - x_i^* \ln \frac{x_i}{x_i^*}\right)$

that are level set equivalent.

Lyapunov functions for non-degenerate linear kinetic systems 2

Proof:

1. there exists a positive diagonal matrix $T = \mathrm{diag}(t_1, ..., t_n) \in \mathcal{D}_+$, such that $A_k = T\overline{M}$ is a Kirchhoff matrix
2. apply state transformation $x_i' = t_i x_i$ to the ODE $\frac{dx}{dt} = \overline{M}x$ of the original system to obtain $\frac{dx'}{dt} = (T\overline{M})T^{-1}x' = A_k T^{-1}x' = A_k' x'$ where A_k' is also a Kirchhoff matrix
3. $\frac{x_i}{x_i^*} = \frac{x_i'}{x_i'^*}$, therefore the CRN-type Lyapunov function of the transformed system in the original coordinates is

$$V_{CRN} = \sum_{i=1}^{n} t_i x_i^* \ln(\frac{x_i}{x_i^*})$$

that is a **weighted version** (with the positive weights t_i) of the original CRN-type Lyapunov function V_{linCRN}.

Generalization to nonlinear cases

Lotka-Volterra models

Quasi-polynomial (QP) ODE models

Variables: $z_i, i = 1, ..., n$ and quasi-monomials (QMs) $q_j, j = 1, ..., m$
System dynamics: an autonomous ODE with quasi-polynomial RHS on the positive orthant

$$\frac{dz_i}{dt} = z_i \left(\Lambda_i + \sum_{j=1}^{m} A_{ij} q_j \right)$$

QM (output) relationships: $q_j = \prod_{i=1}^{m} z_i^{B_{ji}}$
Algebraic characterization: (Λ, A, B),

$M = BA$ is a **descriptor**, it is invariant under **QM-transformation**

$$z_j' = \prod_{i=1}^{n} x_i^{\Gamma_{ji}}$$

Equivalence transformation: $B' = B\Gamma \quad , \quad A' = \Gamma^{-1} A$

Lotka-Volterra models

From any QP-model with parameters (A, B, λ) of an equivalence class, the LV model form can be obtained **by QM-transformation and variable extension** such that $B' = I$ with $z' = q := x$. Then the transformed matrix A' becomes

$$A' = M = B \cdot A \tag{7}$$

The resulting transformed ODE in LV form

$$\frac{dx_l}{dt} = x_l \left(\Lambda_l + \sum_{j=1}^{m} M_{ij} x_j \right) \ , \quad l = 1, ..., m \tag{8}$$

is a homogeneous bi-linear ODE that describes the dynamics in the space $\mathcal{X} \subseteq \mathbb{R}_+^m$. However, because of the variable extension and the relationship $m \geq n$, the dynamics lives in a lower n-dimensional manifold of the monomial space $\mathcal{X}$.

Lyapunov function, stability conditions

Abstract form:

$$\frac{dx}{dt} = \mathrm{diag}(x) \cdot M \cdot (x - x^*)$$
$$0 = \Lambda + M \cdot x^*$$

Lyapunov function

$$V(x) = \sum_{i=1}^{m} c_i \left(x_i - x_i^* - x_i^* \ln \frac{x_i}{x_i^*} \right)$$

Stability condition:
A QP system with a positive equilibrium point x^* is globally stable if the linear matrix inequality

$$M^T C + CM \leq 0 \tag{9}$$

is solvable for a positive diagonal matrix $C = \mathrm{diag}(c_1, .., c_m)$, with $M = BA$.

Dynamically similar ODE model

Given an ODE

$$\frac{dz}{dt} = F(z)$$

on the positive orthant with $F(z) = 0$.

The **nonlinear translated X-factorable transformation** transforms it to

$$\frac{dz}{dt} = \mathrm{diag}(z)F(z - z^*)$$

where $z^* = [z_1^*, \ldots, z_n^*]^T$ are positive real numbers, and $z = [z_1, ..., z_n]^T$.

If $F(z)$ is composed of polynomial-type functions with a finite number of singular solutions, then the above transformation can move the singular solutions into the positive orthant, and **leaves the geometry of the state (or phase) space unchanged** within it (but not at or near the boundary).

The underlying dynamically similar linear ODE model By using the nonlinear translated X-factorable transformation to the LV model with a positive equilibrium point x^*, the following **linear** transformed model is obtained

$$\frac{dx}{dt} = M \cdot (x - x^*)$$

Lyapunov functions of kinetic Lotka-Volterra systems 1

Theorem

Consider the special case of Lotka-Volterra systems

$$\frac{dx}{dt} = \mathrm{diag}(x) \cdot M \cdot (x - x^*)$$

with a non-degenerate kinetic matrix M having a variable structure graph with strongly connected components. Then this system also admits ***suitably scaled*** *Lyapunov functions*

- $V_2 = (x - x^*)^T P (x - x^*)$ *with a positive definite diagonal* $P = \mathrm{diag}(p_1, ..., p_n)$
- $V_{CRN} = -\sum_{i=1}^{n} t_i x_i^* \ln \left(\frac{x_i}{x_i^*} \right)$

besides of the usual $V_{LV}(x) = \sum_{i=1}^{m} c_i \left(x_i - x_i^* - x_i^* \ln \frac{x_i}{x_i^*} \right)$.

Lyapunov functions of kinetic Lotka-Volterra systems 2

Proof:

1. apply nonlinear translated X-factorable transformation to the Lotka-Volterra ODE model to obtain the dynamically similar linear ODE model $\frac{dx}{dt} = Mx$ with the same non-degenerate kinetic coefficient matrix M.
2. the statement follows directly from **Theorem LinearKinetic**.

Conclusion and Future Work

The basis of the results is the level set equivalence of entropy-inspired Lyapunov functions for continuous Markov chains (Gorban et al, 2010).

Non-degenerate linear kinetic systems with a variable structure graph consisting of strongly connected components

- re-scalability to linear weakly reversible MAL-CRNs
- equivalence of conservation and the existence of positive equilibrium points
- existence and equivalence of suitably scaled Lyapunov functions (quadratic, CRN, LV)

Kinetic Lotka-Volterra systems with positive equilibrium points

- using a dynamically similar linear kinetic model
- suitably scaled Lyapunov functions (quadratic, CRN, LV)

Future work

- extensions to nonlinear MAL-CRNs
- extension to the case of non-diagonal positive linear variable transformations