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Entropy-inspired Lyapunov Functions and Linear First Integrals for Positive Polynomial Systems

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Abstract. Two partially overlapping classes of positive polynomial systems, chemical reaction networks with mass action law (MAL-CRNs) and quasi-polynomial systems (QP systems) are considered. Both of them have an entropy-like Lyapunov function associated to them which are similar but not the same. Inspired by the work of Prof. Gorban [12] on the entropy-functionals for Markov chains, and using results on MAL-CRN and QP-systems theory we characterize MAL-CRNs and QP systems that enable both types of entropy-like Lyapunov functions.

The starting point of the analysis is the class of linear weakly reversible MAL-CRNs that are mathematically equivalent to Markov chains with an equilibrium point where various entropy level set equivalent Lyapunov functions are available. We show that non-degenerate linear kinetic systems with a linear first integral (that corresponds to conservation) can be transformed to linear weakly reversible MAL-CRNs using linear diagonal transformation, and the coefficient matrix of this system is diagonally stable. This implies the existence of the weighted version of the various entropy level set equivalent Lyapunov functions for non-degenerate linear kinetic systems with a linear first integral.

Using translated X-factorable phase space transformations and nonlinear variable transformations a dynamically similar linear ODE model is associated to the QP system models with a positive equilibrium point. The non-degenerate kinetic property together with the existence of positive equilibrium point form a sufficient condition of the existence of the weighted version of the various entropy level set equivalent Lyapunov functions in this case. Further extension has been obtained by using the time re-parametrization transformation defined for QP models.

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1. Introduction

The class of positive polynomial ordinary differential equations (ODEs) plays an important role in describing the dynamics of various physical, chemical and ecological systems, where the positivity of the variables is dictated and ensured by the physical meaning, as certain quantities - such as concentrations, pressures, population numbers etc. - cannot take negative values. At the same time, the underlying physics and chemistry of these systems often ensure certain advantageous dynamic properties, such as stability or bounded trajectories by construction. Physically meaningful Lyapunov function candidates are also available for certain classes of positive polynomial systems.

Lyapunov functions play a central role in stability analysis of dynamical systems, see e.g. [14]. Besides of the well-known quadratic Lyapunov function candidate for linear systems, however, there is unfortunately no unified way to construct a suitable Lyapunov function to an arbitrary nonlinear system, but one can utilize the special structure of a given nonlinear system class or look for a physical interpretation to find one. In the field of process systems, for example, the entropy and other entropy-related physical quantities can be used for constructing Lyapunov or storage functions for stability or passivity analysis, see e.g. [31], [15]. Entropy-inspired Lyapunov functions are also common in information science, where Markov chains describe the dynamics in the simplest case, see [12] and the references therein.

Chemical reaction networks (abbreviated as CRNs in this paper) [1] and quasi-polynomial systems (or QP systems in short) [3] are partially overlapping classes of positive polynomial systems, that are the subject of this paper. Both have an entropy-inspired natural Lyapunov function candidate associated with it (see [8] for CRNs and [9] for QP systems), but these are not exactly in the same functional form.

The presence of first integrals is another important joint property of CRNs, and the canonical Lotka-Volterra forms of QP systems. In the case of CRNs, the presence of a linear first integral is the consequence of mass conservation in closed systems, while other nonlinear first integrals may also exist in both system classes. This property presents an additional difficulty when one applies Lyapunov method for stability analysis, that is well recognized and solved under certain conditions, see e.g. [2].

The aim of this paper is to understand the difference of the functional form of the natural Lyapunov functions of CRNs and QP systems, and to develop different level-set equivalent Lyapunov functions that can be used for both classes. The idea is to use the level-set equivalent entropy-inspired Lyapunov functions described by Gorban [12] and use them for both the linear CRN case and to a special subclass of Lotka-Volterra systems.

2. Basic notions and properties of positive polynomial systems

A frequent and simple form of smooth nonlinear autonomous systems described by a set of ODEs is when all the right hand sides are in the form of multivariate polynomials. This section is devoted to describing the positivity and positivity-related properties of such dynamic systems, and to a brief overview on the notion and basic properties of the two considered class of positive polynomial systems: the CRN and QP system classes.

2.1. Positivity and kinetic property of polynomial systems

2.1.1. Positive systems

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 $x_i = 0$ [5, 13]. Consider an autonomous nonlinear system

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

where $f : \mathcal{X} \to \mathbb{R}^n$ is locally Lipschitz, and $\mathcal{X}$ is an open subset of $\mathbb{R}^n$. Then the nonnegative orthant is invariant for the dynamics of (2.1) if and only if f is essentially nonnegative [13].

2.1.2. Polynomial and quasi-polynomial ODEs

Among the smooth nonlinear functions, multivariate polynomials play an important role. An autonomous nonlinear system (2.1) defined on the nonnegative orthant is called polynomial, if its right-hand function $f : \mathcal{X} \to \mathbb{R}^n$ is a multivariate polynomial in each of its coordinate functions f_i.

A generalization of polynomial systems is the class of quasi-polynomial systems (QP systems in short), where one allows real numbers in the exponents [3]. A brief overview of QP systems will follow in subsection 2.3.

2.1.3. Kinetic property

A necessary and sufficient condition for the kinetic property for a polynomial ODE model was first given in [17]. According to this result, a set of polynomial ODEs of the form (2.1) is kinetic if and only if all coordinates functions of f can be written in the form

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

where g_i and h_i are polynomials with nonnegative coefficients. It is easy to check that the kinetic property implies the essential nonnegativity of f, i.e. kinetic systems are *nonnegative systems* [13].

2.2. Chemical reaction networks with mass action law (MAL-CRNs)

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 behaviour) present in the dynamics of nonlinear processes [1]. The importance of the CRN system class with mass action law (abbreviated as MAL-CRNs) lies in the fact that strong structural (i.e. parameter-independent) stability results exist for the deficiency zero weakly reversible case [8], and recently for the detailed balanced case, when each of the chemical reactions are assumed to be reversible (see [4], [11], [14], [27] and recently [29]).

2.2.1. Basic description

Consider a CRN that obeys the mass action law (MAL), that will be called MAL-CRN. The structure of the MAL-CRN is given in terms of its complexes $C_i,\ i = 1, ..., m$ that are linear combinations of its species $X_j,\ j = 1, ..., n$ with nonnegative integer coefficients, i.e. $C_i = \sum_{j=1}^{n} \alpha_{ji} X_j$, where $\alpha_{ji} \in \mathbb{N}_0$, $\forall i, j$. The chemical reactions $C_i \mapsto C_j$ with the reaction rate coefficient $k_{ij} \in \mathbb{R}$, $k_{ij} > 0$ transform the complexes into each other with the reaction rate

$$r_{ij} = k_{ij}\varphi_i(x) = k_{ij} \prod_{l=1}^{n} x_l^{\alpha_{li}}. \tag{2.3}$$

We form two matrices, the complex composition matrix $Y \in \mathbb{N}_0^{n \times m}$ with non-negative integer elements, the columns of which describe the composition of the complexes, and the Kirchhoff matrix $A_k \in \mathbb{R}^{m \times m}$, that describes the structure of chemical reactions for the description such that

$$[Y]_{ij} = \alpha_{ij} \quad , \quad [A_k]_{ij} = \begin{cases} -\sum_{l=1, l \neq i}^{m} k_{il} & \text{if } i = j \\ k_{ji} & \text{if } i \neq j \end{cases} \tag{2.4}$$

The vertices $\mathbf{V}$ of the *reaction graph* $G = (\mathbf{V}, \mathbf{E})$ correspond to the complexes, and the edges $\mathbf{E}$ to the reactions. Two complexes C_k and C_l are connected by a directed edge (C_k, C_l), if a reaction in the form of $C_k \mapsto C_l$ exists. Edge weights are associated to the edges that are the reaction rate constants $k_{kl} > 0$, thus he reaction graph is a weighted directed graph.

Note that the Kirchhoff matrix A_k of a CRN uniquely determines its reaction graph and vice versa. However, the Kirchhoff matrix of the reaction graph does not uniquely determine the reaction kinetic

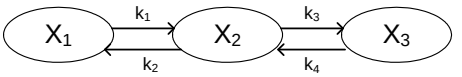

FIGURE 1. The reaction graph of the simple linear example

system itself, since the information on the composition of the complexes is missing from the graph: it is contained in the complex composition matrix Y.

The reaction graph G without its edge weights (i.e. the values of the reaction rate coefficients) describes the *structure of a MAL-CRN*.

The connected components in the reaction graph are called *linkage classes*, their number is denoted by $\ell \geq 1$.

The dynamics of a MAL-CRN is described in the form of the following set of ODEs

$$\frac{dx}{dt} = Y A_k \varphi(x) \tag{2.5}$$

where $x(t) \in \mathbb{R}^n_+$ is the concentration vector for the species, and $\varphi(x) \in \mathbb{R}^m_+$ is the vector formed from the reaction monomials in defined Eq. (2.3). From now, we assume for the studied CRN models that *the number of species is not more than the number of complexes, i.e.* $n \leq m$.

Example 2.1 (A simple linear example)**.** Let us assume a simple reaction kinetic system with two reversible first order steps (i.e. four irreversible elementary reaction steps) and three components

$$\mathbf{X}_1 \rightleftarrows \mathbf{X}_2 \rightleftarrows \mathbf{X}_3$$

The dynamic state equations are linear ODEs

$$\frac{dx_1}{dt} = -k_1 x_1 + k_2 x_2$$

$$\frac{dx_2}{dt} = k_1 x_1 - k_2 x_2 - k_3 x_2 + k_4 x_3$$

$$\frac{dx_3}{dt} = k_3 x_2 - k_4 x_3$$

The stoichiometric and Kirchhoff matrices are

$$Y = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad A_k = \begin{bmatrix} -k_1 & k_2 & 0 \\ k_1 & -(k_2 + k_3) & k_4 \\ 0 & k_3 & -k_4 \end{bmatrix}$$

The reaction graph of this simple linear example can be seen in Fig. 1.

2.2.2. Basic structural properties

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.

It is well-known from the literature [7] that

Lemma 2.2. *a CRN is weakly reversible if and only if there is a strictly (element-wise) positive vector* q^* *in the kernel of* A_k.

Then, the intersection of this kernel and the positive orthant contains (infinitely many) positive equilibrium points for the dynamics (2.5). It is important to remark that the stoichiometric compatibility class can be fixed by selecting the equilibrium point $q^* = \varphi(x^*)$.

The notion of the *deficiency* of a CRN is built on the set of *reaction vectors* that are defined as: $\mathcal{R} = \{\rho^{(l,k)} = \eta^{(l)} - \eta^{(k)} \mid (C_k, C_l) \in \mathbf{E} \text{ in } G\}$, where $\eta^{(i)}$ denotes the ith column of Y. Then, the deficiency δ of a CRN is an integer number that is usually defined as:

$$\delta = m - \ell - s \tag{2.6}$$

where m is the number of complexes and ℓ is the number of connected components in the reaction graph, while s is the dimension of the stoichiometric sub-space, i.e. $s = rank(\mathcal{R})$.

The celebrated *Deficiency Zero Theorem* [8] 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.

2.2.3. Linear diagonal (LD) transformation

It is known that under a positive diagonal state transformation, the kinetic property of a MAL-CRN is preserved [6, 24]. Consider a positive diagonal matrix $T = \text{diag}(c)$, where $c \in \mathbb{R}^n_+$ is an element-wise positive vector. Then one can transform the MAL-CRN model with a realization (Y, A_k) to another MAL-CRN model with a realization (Y, A'_k) (i.e. this transformation does not lead out of the MAL-CRN model class) [25] such that

$$YA_k = TYA'_k(\text{diag}(\varphi(c)))^{-1} \tag{2.7}$$

It is important to note that the LD transformation is an invertible variable transformation, that is also called variable rescaling. Therefore, the qualitative properties of the dynamics of the original and the transformed system (e.g. number and stability of equilibria, boundedness of solutions, existence of limit cycles, chaotic behavior etc.) are identical.

2.2.4. Conservation and the existence of a linear first integral

In classical chemical kinetics one assumes isotherm isobar conditions for a closed system where the chemical reactions take place. Therefore, the overall mass of the system should be conserved, that is expressed mathematically by the following conservation property.

Definition 2.3 (Conservation property)**.** The mass conservation property of a general (not necessarily linear) 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.

$$\underline{\mathbf{m}}M = \underline{\mathbf{0}} \tag{2.8}$$

with $\underline{\mathbf{0}} = [0, 0, ..., 0]$, that shows the rank deficiency of M in a MAL-CRN with mass conservation using the assumption that $n \leq m$.

Note that the elements of the positive row vector $\underline{\mathbf{m}}$ are the molecular weights of the species.

It is easy to see that *the mass conservation (2.8) implies the existence of a linear first integral* $\mathcal{M} = \sum m_i x_i(t) = \text{const}$, that is the overall mass of the system. By fixing $\mathcal{M}$ and specifying the initial condition of the ODE model accordingly, one can select an element from the stoichiometric compatibility class.

2.3. Quasi-polynomial (QP) and Lotka-Volterra (LV) systems

QP systems form a general descriptor class of dynamic systems with smooth nonlinearities in the sense that such systems can be embedded into QP form by adding new auxiliary variables to the system and thus extending the state-space [3].

2.3.1. Basic description of QP systems

Quasi-polynomial models are systems of autonomous ODEs defined in the positive orthant with quasi-polynomial RHS of the following form

$$\frac{dz_i}{dt} = z_i \left(\Lambda_i + \sum_{j=1}^{m} A_{ij} q_j \right), \quad i = 1, \ldots, n \tag{2.9}$$

where $q_j = \prod_{i=1}^{m} z_i^{B_{ji}}$ are the quasi-monomials, and $z \in \mathrm{int}(\mathbb{R}^n_+)$, $A \in \mathbb{R}^{n \times m}$, $B \in \mathbb{R}^{m \times n}$, $\Lambda_i \in \mathbb{R}$, $i = 1, \ldots, n$. Furthermore, $\Lambda = [\lambda_1 \ \ldots \ \lambda_n]^T$. The equilibrium point of interest of (2.9) as $z^* = [z_1^* \ z_2^* \ \ldots \ z_n^*]^T$ that gives rise to the equilibrium quasi-monomials q^*. Without the loss of generality it can be assumed that $rank(B) = n$ and $m \geq n$ [19]. The constant matrices and vectors (Λ, A, B) serve as an algebraic characterization for the class of quasi-polynomial systems.

2.3.2. Quasi-monomial transformation

The product $M = BA$ is a *descriptor*, that is invariant under a nonlinear coordinates transformation, the so called *quasi-monomial transformation* (shortly, QM transformation) that defines the transformed state variables as

$$x_j = \prod_{i=1}^{n} z_i^{\Gamma_{ji}}, \ j = 1, \ldots, n. \tag{2.10}$$

The parameter of the QM transformation is the real square invertible matrix $\Gamma \in \mathbb{R}^{n \times n}$.

It is easy to see, that the transformed system can be characterized algebraically by the following constants.

$$\tilde{B} = B\,\Gamma, \quad \tilde{A} = \Gamma^{-1} A, \quad \tilde{\Lambda} = \Gamma^{-1} \Lambda \tag{2.11}$$

It means, that (2.10) defines a partitioning that splits QP models into equivalence classes defined by the invariant matrix $M = B\,A = \tilde{B}\,\tilde{A}$.

2.3.3. Lotka-Volterra systems

From any QP-model with parameters (A, B, Λ) of an equivalence class, the corresponding LV model form that characterizes the class can be obtained *by QM-transformation and variable extension* such that $\hat{B} = I$ with $x = q$. Then the transformed matrix $\hat{A}$ becomes

$$\hat{A} = M = BA \tag{2.12}$$

The resulting transformed ODE in LV form

$$\frac{dx_l}{dt} = x_l \left(\Lambda_l + \sum_{j=1}^{m} M_{ij} x_j \right), \quad l = 1, ..., m \tag{2.13}$$

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 evolves in a lower n-dimensional manifold of the monomial space $\mathcal{Q}$.

Steady state points of LV systems The non-trivial nonnegative steady state points of the LV equation can be obtained (if they exist) by solving the linear equation

$$0 = \Lambda + M \cdot x^* \tag{2.14}$$

for x^*. From now on, we assume that *there exists at least one strictly positive equilibrium point* x^* *for the LV-system* (2.13).

2.3.4. The homogeneous form of LV systems

In order to develop a compact vector-matrix form, the following notation is introduced

$$\mathrm{diag}(x) = \begin{bmatrix} x_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & x_m \end{bmatrix} \tag{2.15}$$

Then the dynamics (2.13) of a Lotka-Volterra system with a positive steady state point x^* can be written in the following form:

$$\frac{dx}{dt} = \mathrm{diag}(x) \cdot M \cdot (x - x^*) \tag{2.16}$$

In order to facilitate the joint analysis of MAL-CRNs and LV systems form a *homogeneous set of equations* is needed where the equilibrium point does not appear in the equations. Therefore, we augment the state vector x of the model (2.13) by a constant element to obtain the *compact homogeneous form* as follows

$$\frac{d\overline{x}}{dt} = \mathrm{diag}(\overline{x}) \left(\left[\begin{array}{c|c} M & \Lambda \\ \hline 0 & 0 \end{array} \right] \overline{x} \right) \tag{2.17}$$

where $\overline{m} = m + 1$, and $\overline{x} \in \mathbb{R}^{\overline{m}}$ is the new state vector.

2.3.5. Time-reparametrization transformation

There exists another nonlinear similarity transformation that preserve QP format, which is called *time-reparameterization* [30], time-rescaling or simply *new-time transformation* [19]. It introduces a nonlinear scaling of the time as follows.

$$dt = \prod_{k=1}^{n} z_k^{\Omega_k} dt' \tag{2.18}$$

Using (2.18) the original QP system (2.9) transforms to

$$\frac{dz_i}{dt'} = z_i \left(\sum_{j=1}^{m+1} \hat{A}_{i,j} \prod_{k=1}^{n} z_k^{\hat{B}_{j,k}} \right), \quad i = 1, \dots, n. \tag{2.19}$$

where the number of quasi-monomials formally increase by one, and thus $\hat{A} \in \mathbb{R}^{n \times (m+1)}$ and $\hat{B} \in \mathbb{R}^{(m+1) \times n}$ as follows

$$\hat{A}_{i,j} = A_{i,j}, \quad i = 1, \dots, n, \quad j = 1, \dots, m \tag{2.20}$$

$$\hat{A}_{i,m+1} = \lambda_i, \quad i = 1, \dots, n \tag{2.21}$$

$$\hat{B}_{i,j} = B_{i,j} + \Omega_j, \quad i = 1, \dots, m, \quad j = 1, \dots, n \tag{2.22}$$

$$\hat{B}_{m+1,j} = \Omega_j, \quad j = 1, \dots, n \tag{2.23}$$

It is important to note that the dynamic properties and the entire phase plot of the original and the transformed ODEs are the same including the steady state points and their stability properties, i.e. *the time-reparametrization transformation is indeed a similarity transformation.*

An essential difference between QM transformation (2.10) and time-reparametrization (2.18) is that while (2.10) is invariant in a QP class of invariance, this is not the case for (2.18). It is, however, possible to recast the transformed Lotka-Volterra system (which is in QP form) to the form (2.13).

The matrices characterizing the time-reparametrized Lotka-Volterra model are given as follows

$$\hat{A} = \left[\, M \middle| \Lambda \, \right], \quad \hat{B} = \left[\frac{I_{m \times m}}{0_{1 \times m}} \right] + 1_{(m+1) \times 1} \cdot \Omega \tag{2.24}$$

where $I_{m\times m}$ denotes the unit matrix of size m, and $a_{j\times k}$ stands for the constant matrix of size $j \times k$ with elements $a \in \{0, 1\}$, and $\Omega = [\Omega_1 \ ... \ \Omega_n]$ is the parameter vector of the transformation (2.18). The invariant matrix $\hat{M}$ of the QP model (2.24) is

$$\hat{M} = \hat{B}\hat{A} = \left[\begin{array}{c|c} M & \Lambda \\ \hline 0_{1\times m} & 0 \end{array}\right] + 1_{(m+1)\times 1} \cdot \Omega \cdot \hat{A}. \tag{2.25}$$

It is easy to see, that (2.25) depends linearly on the parameters Ω_i of (2.18).

2.3.6. Stability condition for QP systems

Thanks to the well characterized structure of QP systems with a positive equilibrium point expressed with the quasi-monomials q^*, an easy-to-check sufficient condition for their global (asymptotic) stability exists [10].

A QP system with a positive equilibrium point q^* is globally stable if the linear matrix inequality

$$M^T C + CM \leq 0 \tag{2.26}$$

is solvable for a positive diagonal matrix $C = \mathrm{diag}(c_1, .., c_m)$, with $M = BA$. In this case, the matrix M is called *diagonally stable*. (The stability is asymptotic, if the inequality (2.26) is strict.) Given the parameter matrix M of the system, the condition (2.26) can be checked effectively by solving a linear matrix inequality (LMI). Actually, it is shown it [9] that we can apply even milder conditions: if we assume (by appropriate ordering of the monomials) that the first n rows of B are linearly independent, then $c_i > 0$ for $i = 1, \ldots, n$ and $c_j \geq 0$ for $j = n + 1, \ldots, m$ still guarantee the global stability of q^*.

The above stability condition is derived using the following Lyapunov function candidate:

$$V_{QP}(q) = \sum_{i=1}^{m} c_i \left(q_i - q_i^* - q_i^* \ln \frac{q_i}{q_i^*} \right) \tag{2.27}$$

2.4. Dynamically similar linear ODEs

As we have seen before in the case of QM or LD transformations, invertible state transformations are equivalence transformations, and leave the properties of the system unchanged. Here we shall use a nonlinear phase space transformation that is not an equivalence transformation but leaves the phase portrait of a dynamic system unchanged in certain cases.

2.4.1. Nonlinear translated X-factorable transformation

Assume that the following set of ordinary differential equations

$$\frac{dX}{dt} = \mathbf{F}(X) \tag{2.28}$$

is defined on the positive orthant $\mathbb{R}^n_+$. The steady state solutions of Eq. (2.28) are defined by $\mathbf{F}(X) = 0$. Consider the following *nonlinear translated X-factorable phase (or state) space transformation* of Eq. (2.28)

$$\frac{dX}{dt} = \hat{\mathbf{F}}(X) = \mathrm{diag}(X_1, ..., X_n)\mathbf{F}(X - C), \tag{2.29}$$

where the elements of $C = [c_1, \ldots, c_n]^T$ are positive real numbers, and $X = [X_1, ..., X_n]^T$.

The original motivation of the application of the transformation (2.29) in [28] was to represent non-positive dynamical systems as kinetic systems. Clearly, the translation parameterized by C can be chosen such that the equilibrium points (or operating domain) of interest are moved to the strictly positive orthant, while the multiplication by $\mathrm{diag}(X)$ ensures the nonnegativity and the so-called geometrical separability of the transformed system. Moreover, it is easy to see that models of the form (2.29) are always kinetic, since they trivially fulfil the condition (2.2). It is shown in [28] that due to the transformation (2.29), a substantial compression of trajectories occurs close to the boundary of the positive orthant, however, this distortion is weak or negligible for trajectories far from the boundaries. Therefore, the dynamics of the solutions of Eqs. (2.28) and (2.29) will be called *dynamically similar*.

2.4.2. The underlying dynamically similar linear ODE model

Based on the above, the LV model in eq. (2.16) with a positive equilibrium point x^* can be considered as the X-factorable transformed version of the following *linear* system:

$$\frac{dx}{dt} = M \cdot (x - x^*) \tag{2.30}$$

2.5. Compartmental and Metzler matrices

To show the stability of weakly reversible linear CRN models, we use results from the theory of nonnegative and compartmental systems using mainly Chapter 2 of [21]. The review paper [23] is also devoted to the qualitative analysis of compartmental systems.

An $n \times n$ matrix F is called a compartmental matrix if it satisfies the following conditions

1. $F_{ij} \geq 0$, for $i, j = 1, \ldots, n$, $i \neq j$
2. $\sum_{i=1}^{n} F_{ij} \leq 0$, for $j = 1, \ldots, n$

Clearly, the Kirchhoff matrix A_k of CRN models is a compartmental matrix and thus a special type of Metzler matrix. We will use the following properties of compartmental matrices.

Consider a compartmental matrix F. Then, the following statements hold for the properties of the eigenvalues of F:

P1 The eigenvalues of F are either zero, or they have strictly negative real parts. (In other words, compartmental matrices cannot have unstable or purely imaginary eigenvalues.)

P2 If F is the Kirchhoff matrix of a weakly reversible CRN, then the number of zero eigenvalues of F is equal to the number of linkage classes (i.e. to the number of connected components of the reaction graph).

P3 If zero is an eigenvalue of F with algebraic multiplicity κ, then its geometric multiplicity is also κ (i.e. the eigenvectors corresponding to zero eigenvalues are always linearly independent).

3. Linear weakly reversible MAL-CRNs

Assume that every reaction in the MAL-CRN system is linear. This case forms the simplest class of MAL-CRNs, with interesting structural dynamic properties that are easy to investigate.

3.1. Basic structural properties

The basic structural elements of linear MAL-CRNs are in the following special form.

- The complexes are the species, i.e. $n = m$ and $C_i = X_i$. Therefore the complex composition matrix is the unit matrix, i.e. $Y = I$, and the state variable vector x is identical to the monomial variable vector $\varphi(x)$, i.e. $x = \varphi(x)$.
- The ODE model that describes the dynamics in the phase space $\mathcal{X}$ specializes to

$$\frac{dx}{dt} = A_k x \tag{3.1}$$

that is a linear ODE with constant coefficients that are collected in the Kirchhoff matrix A_k:

$$[A_k]_{ij} = \begin{cases} -\sum_{l=1, l\neq i}^{m} k_{il} & \text{if } i = j \\ k_{ji} & \text{if } i \neq j \end{cases} \tag{3.2}$$

where $k_{ji} \geq 0$.

Therefore, *A_k is a special compartmental matrix with zero column sums. This implies, that the eigenvalues of A_k are either zero or they have negative real parts, but there is at least one zero eigenvaule.*

It is very easy to see that the *realization $(Y = I, A_k)$ of a linear MAL-CRN is unique*, since $Y \cdot A_k = Y \cdot A'_k$ trivially implies $A_k = A'_k$ in this case. For the precise definition of CRN realizations, see e.g. [25].

3.2. Properties related to weak reversibility

It is known from the literature that in the weakly reversible linear CRN case $rank(A_k) = m - \ell$, where ℓ is the number of linkage classes [8].

Additionally, it is easy to see that *weakly reversible linear CRNs have always zero deficiency*: since the columns of Y are the standard basis vectors of $\mathbb{R}^m$, the rank of the reaction vectors in any strongly connected component of the reaction graph containing m complexes is exactly $m - 1$ (that is equal to the number of the edges in the spanning tree corresponding to the connected component). Therefore, the rank of the stoichiometric space with ℓ strongly connected components is $s = m - \ell$ resulting in zero deficiency.

3.3. Markov chains as linear weakly reversible CRNs

Consider continuous time Markov chains with positive equilibrium probabilities p_j^* [12]. The dynamics of the probability distribution $p_i, i = 1, ..., N$ satisfies the Master equation:

$$\frac{dp_i}{dt} = \sum_{j,j\neq i} q_{ij}p_j - q_{ji}p_i \tag{3.3}$$

where the coefficients $q_{ij}, (i \neq j)$ are non-negative, and

$$\sum_i p_i = 1 \quad , \quad 0 \leq p_i \leq 1 \tag{3.4}$$

Here we can establish the following correspondence with the CRN description

– p_i corresponds to the concentration x_i of the specie X_i (normalized)
– the term $q_{ij}p_j$ is the reaction rate of the reaction $X_j \to X_i$ with the reaction rate coefficient q_{ij}
– each reaction is reversible.

Note that (3.4) implies that the total mass of the system is constant (i.e. there is mass conservation). Let us form the matrix $\overline{Q}$ as

$$\overline{Q}_{ji} = \begin{cases} q_{ij} & \text{if} \quad j \neq i \\ \sum_j q_{ij} & \text{if} \quad j = i \end{cases}$$

Then $\overline{Q}$ is a Kirchhoff matrix and (3.3) can be written as

$$\frac{dp}{dt} = \overline{Q}p$$

For chains with a positive equilibrium distribution $p_j^*, j = 1, ..., N$ another equivalent form is convenient:

$$\frac{dp_i}{dt} = \sum_{j,j\neq i} q_{ij}p_j^* \left(\frac{p_j}{p_j^*} - \frac{p_i}{p_i^*}\right) \tag{3.5}$$

where p_i^* and q_{ij} are connected by the identity (coming form the steady state version of (3.3))

$$\sum_{j,j\neq i} q_{ij}p_j^* = \left(\sum_{j,j\neq i} q_{ji}\right) p_i^* \tag{3.6}$$

3.3.1. Level-set equivalent Lyapunov functions

A unified form of modern relative entropies defined for Markov chains is the Csiszár-Morimoto function over a discrete probability distribution p

$$H_h(p) = H_h(p||p^*) = \sum_i p_i^* h\left(\frac{p_i}{p_i^*}\right) \tag{3.7}$$

where $h(x)$ is an extended real-valued proper convex function defined on the open ($x > 0$) or closed ($x \geq 0$) semi-axis. The above required property of h is equivalent to the Jensen inequality

$$h(ax + (1-a)y) \leq ah(x) + (1-a)h(y) \quad \text{for all} \quad x, y \in U \ , \ a \in [0,1] \tag{3.8}$$

These relative entropies are the Lyapunov functions for all Markov chains with the positive equilibrium $p^* = [p_1^*, ..., p_N^*]$. [12]

Two special cases will be of interest in this paper.

- **Kullback-Leibler divergence** Here we use the function $h(x) = -x\ln(x)$ the results in the relative entropy

$$H_h(p) = H_h(p||p^*) = -\sum_i p_i \ln\left(\frac{p_i}{p_i^*}\right) = V_{CRN}(p) \tag{3.9}$$

  This is the same as the logarithmic Lyapunov function commonly used in the theory of CRNs (see Eq. (3.13)).
- **Relative Burg entropy** Here the convex function is chosen as $h(x) = -\ln(x)$, and then

$$H_h(p) = H_h(p||p^*) = -\sum_i p_i^* \ln\left(\frac{p_i}{p_i^*}\right) = V_{QP-sim}(p) \tag{3.10}$$

  This is similar to the logarithmic Lyapunov function candidate commonly used in the theory QP systems (see Eq. (2.27)).

Lemma 3.1 (Gorban [12])**.** *For Markov chain type dynamics and for the mathematically equivalent linear CRNs the normalized relative Burg entropy (that is the QP-style Lyapunov function candidate) is level set equivalent to the Kullback-Leibler divergence (that is the CRN-style Lyapunov function).*

3.4. Stability and Lyapunov functions of linear weakly reversible CRNs

The Deficiency Zero Theorem ensures the global asymptotic stability of the equilibrium point x^* within the stoichiometric compatibility class on the positive orthant.

3.4.1. The quadratic Lyapunov function

It follows from the theory of linear time-invariant systems that weakly reversible linear CRNs of the form (3.1) are globally stable with a quadratic Lyapunov function. Of course, the stability cannot be asymptotic, since weak reversibility guarantees that the intersection of the positive orthant and the kernel of A_k is non-empty (i.e. there exist infinitely many equilibrium points in the positive orthant). Therefore, we can use the following quadratic Lyapunov function:

$$V_2(x) = (x - x^*)^T P (x - x^*) \tag{3.11}$$

with an appropriate positive definite symmetric P. Taking the derivative of V_2 along the solution of (3.1), we obtain the classical non-strict Lyapunov inequality as the stability condition:

$$A_k^T P + P A_k \preceq 0, \tag{3.12}$$

where '$\preceq 0$' means negative semi-definiteness.

A nice property of stable Metzler matrices (and therefore of Kirchhoff matrices) is that they are diagonally stable, i.e. *there exists a positive definite diagonal* P *that satisfies* (3.12) [26].

3.4.2. The entropy-like logarithmic Lyapunov function

The zero deficiency property of weakly reversible linear CRNs implies that the logarithmic Lyapunov function

$$V_{CRN}(x) = -\sum_{i=1}^{n} x_i \ln\left(\frac{x_i}{x_i^*}\right) \tag{3.13}$$

proposed e.g. in [22] can also be used for proving the stability of such CRNs. It is important to remark that the stability of any equilibrium point x^* is asymptotic if we restrict the dynamics to the corresponding stoichiometric compatibility class.

3.5. LD transformation of linear CRNs

Assume we have a linear CRN with a coefficient matrix A_k and $Y = I$. If one applies an LD transformation (2.7) to (3.1), then

$$A'_k = TA_kT^{-1} \tag{3.14}$$

is obtained. Therefore, A_k and A'_k do not only encode the same reaction graph structure (only the edge weights are scaled), but the eigenvalues of the two realization matrices are also the same.

This means that the (non-weighted) reaction graph structure (including weak reversibility) and its dynamical consequences are *system properties* in the linear MAL case. Moreover, the sign pattern of the two matrices A_k and A'_k should be the same, and should follow the sign pattern of Kirchhoff matrices (3.2), i.e. they should be Metzler matrices. However, the zero column sum property is changed with the application of (3.14).

3.6. The conservation property of linear MAL-CRNs

It is important to note that (2.8) can be rewritten in the form

$$\left[\frac{m_1}{c_1}, ..., \frac{m_n}{c_n}\right] \mathrm{diag}(c_1, ..., c_n)M = \underline{\mathbf{0}} \tag{3.15}$$

that shows the invariance of the conservation with respect to the LD transformation (or variable rescaling), where the elements of the re-scaled row vector $\underline{\mathbf{m}}'$ are $\frac{m_i}{c_i}, i = 1, ..., n$. Furthermore, it is easy to see that a quadratic matrix M keeps its conservation property unchanged if it is multiplied by a positive diagonal matrix from the right, i.e. $M' = MC$ has also the conservation property, if $C = \mathrm{diag}(c),\ c_i > 0$.

It is important to note that the conservation and the Kirchhoff properties are identical in the linear MAL-CRN case. The zero column-sums within the Kirchhoff property of A_k can be expressed as

$$\underline{\mathbf{1}}A_k = \underline{\mathbf{0}} \tag{3.16}$$

where $\underline{\mathbf{1}} = [1, 1, ..., 1]$ [16], that shows the rank-deficient nature of A_k, i.e. $rank(A_k) \leq m - 1$. Here A_k has the conservation property with $\underline{\mathbf{m}} = \underline{\mathbf{1}}$.

4. Linear kinetic systems and their Lyapunov functions

This section is devoted to a special class of positive linear systems and their level set equivalent Lyapunov functions. The results will be generalized to the nonlinear case of Lotka-Volterra systems in section 5.

4.1. Non-degenerate linear kinetic systems and their properties

Now consider a linear ODE

$$\frac{dx}{dt} = \overline{M}x \tag{4.1}$$

with the constant square coefficient matrix $\overline{M}$ that obeys the kinetic condition (2.2). This implies that

$$m_{ij} \geq 0,\ i \neq j \quad , \quad m_{ii} \leq 0 \tag{4.2}$$

should hold. We shall say that a *matrix $\overline{M}$ is kinetic* if it has the sign pattern in (4.1). It is easy to check that a linear system (4.1) is kinetic if and only if $f = \overline{M}x$ is essentially nonnegative (i.e. if and only if $\overline{M}$ is a Metzler matrix).

Definition 4.1 (Non-degenerate linear kinetic system)**.** A linear ODE in the form of (4.1) models a non-degenerate linear kinetic system, if the right-hand side of each differential equation is different from zero, i.e. it contains at least one linear term, and each variable x_i appears in at least one right-hand side.

This implies that each row and also column of the coefficient matrix $\overline{M}$ contains at least one non-zero element that obey the sign pattern condition (4.2).

Let us associate a weighted directed graph to the linear ODE (4.1) that helps in analysing its structure.

Definition 4.2 (Variable-structure graph)**.** A directed graph $\boldsymbol{G}_{\overline{M}} = (V_{\overline{M}}, \boldsymbol{E}_{\overline{M}})$ is the variable-structure graph of $\overline{M}$ of (4.1), if $V_{\overline{M}} = \{x_1, ..., x_n\}$, and the directed edge $\boldsymbol{e}_{ij} = (x_i, x_j)$ is in $\boldsymbol{E}$ if $\overline{M}_{ji} > 0$.

Some important simple properties are as follows.

1. the row or column scaling of a matrix M leaves its variable-structure unchanged, i.e. $\boldsymbol{G}_M = \boldsymbol{G}_{TM} = \boldsymbol{G}_{MT}$ if $T = \mathrm{diag}(t_1, ..., t_n)$ is an element-wise positive diagonal matrix, i.e. $T \in \mathcal{D}_+$,
2. the transposition of a matrix M reverses the direction of the edges in $\boldsymbol{G}_M$, i.e. $\boldsymbol{G}_M = \overleftarrow{\boldsymbol{G}}_{M^T}$.

4.2. Conservation in linear kinetic systems

Similarly to the case of linear MAL-CRNs, the coefficient matrix $\overline{M}$ of a non-degenerate linear kinetic system (4.1) has the conservation property, if (2.8) holds, i.e. $\underline{\mathbf{m}}\overline{M} = \underline{\mathbf{0}}$. Such matrices will be called *conservation matrices*.

Theorem 4.3. *The coefficient matrix $\overline{M}$ of a non-degenerate linear kinetic system* (4.1) *is a conservation matrix if and only if there exists a positive diagonal matrix $T = \mathrm{diag}(t_1, ..., t_n),\ t_i > 0$ such that $T\overline{M} = A_k$ where A_k is a Kirchhoff matrix.*

Proof. Assume that $\overline{M}$ has the conservation property, i.e.

$$\underline{\mathbf{m}}\overline{M} = \underline{\mathbf{0}} \tag{4.3}$$

Because $\overline{M}$ is kinetic, it has the necessary sign-pattern of a Kirchhoff matrix. If one multiplies it with a positive diagonal matrix T, the product will also have this sign property.

Let us form the positive diagonal matrix T from the elements of the row vector $\underline{\mathbf{m}}$, i.e. $T = \mathrm{diag}(\mathbf{m}_1, ..., \mathbf{m}_n)$, where $\mathbf{m}_i > 0$. Then Eq. (2.8) can be written in the form

$$\underline{\mathbf{m}}\overline{M} = \underline{\mathbf{1}} \cdot T\overline{M} = \underline{\mathbf{0}} \tag{4.4}$$

that is equivalent to the required column conservation property (3.16) of the matrix $T\overline{M}$. Together with the sign property above, we can say that the matrix $T\overline{M}$ is a Kirchhoff matrix.

The proof of the reverse direction, when we have a positive diagonal matrix $T = \mathrm{diag}(t_1, ..., t_n),\ t_i > 0$ such that $A_k = T\overline{M}$ holds for a Kirchhoff matrix A_K uses also the identity (4.4). From this it follows that $\underline{\mathbf{m}} = [t_1, ..., t_n]$. □

Corollary 4.4. *A non-degenerate kinetic matrix $\overline{M}$ with the conservation property is a stability matrix.*

Proof. Let us use a variable transformation $\overline{x} = Tx$ of the original ODE (4.1) using the positive diagonal transformation matrix $T = \mathrm{diag}(\mathbf{m}_1, ..., \mathbf{m}_n)$. Then the following transformed ODE is obtained

$$\frac{d\overline{x}}{dt} = T\overline{M}T^{-1}\overline{x}$$

where the transformed coefficient matrix $T\overline{M}T^{-1}$ has the same eigenvalues as $\overline{M}$, but it is also a Kirchhoff matrix $\overline{A_k} = A_kT^{-1}$ according to Theorem 4.3 and also keeping in mind that T^{-1} is a positive diagonal matrix, too, that does not change the Kirchhoff property of a matrix. □

4.3. Positive equilibrium points and conservation of linear kinetic systems

We recall from section 2.2.2 (Lemma 2.2) that a linear MAL-CRN is weakly reversible if and only if there exists at least one strictly positive vector c in the kernel of its Kirchhoff matrix A_k. This vector determines the *unique positive equilibrium point of the system within the appropriate stoichiometric compatibility class*.

Moreover, we notice that the variable structure graph of A_k ($\boldsymbol{G}_{A_k}$) is the non-weighted version of the usual reaction graph of the MAL-CRN. Therefore, the linear MAL-CRN corresponding to A_k is weakly reversible if and only if $\boldsymbol{G}_{A_k}$ is strongly connected.

Lemma 4.5. *If the coefficient matrix $\overline{M}$ of a non-degenerate linear kinetic system* (4.1) *is a conservation matrix and its variable-structure graph is strongly connected, then there exists a linear weakly reversible MAL-CRN that can be obtained from* (4.1) *by using a suitable LD transformation.*

Proof. Theorem 4.3 implies that there is a positive diagonal matrix $T = (t_1, ..., t_n), t_i > 0$ such that the matrix $\overline{A}_k = T\overline{M}$ is a Kirchhoff matrix.

Moreover, the variable structure graphs of $\overline{A}_k$ and $\overline{M}$ are the same, i.e. $\boldsymbol{G}_{\overline{M}} = \boldsymbol{G}_{\overline{A}_k}$, because the two matrices are related by a positive diagonal transformation. Therefore, the strongly connected property of $\boldsymbol{G}_{\overline{M}}$ holds also for $\boldsymbol{G}_{\overline{A}_k}$. This implies that $\overline{A}_k$ corresponds to a weakly reversible linear MAL-CRN. □

The weak reversibility of $\boldsymbol{G}_{\overline{M}}$ can be checked using a well-known algebraic property. If $\boldsymbol{G}_{\overline{M}}$ contains one graph component (linkage class), then it is weakly reversible if and only if $\overline{M}$ is *irreducible* which is equivalent to the property that $\overline{M}$ cannot be transformed into block upper-triangular form by simultaneous row/column permutations. Consequently, linear kinetic systems containing more than one linkage class are weakly reversible if and only if the diagonal blocks (possibly after renumbering the variables) corresponding to the linkage classes in $\overline{M}$.

Definition 4.6. A kinetic matrix $\overline{M}$ has the *p-property*, if its diagonal blocks (possibly after renumbering the variables) corresponding to the linkage classes are irreducible.

Lemma 4.5 implies that all of the vertices lie at least one of the circles in the variable structure graph $\boldsymbol{G}_{\overline{M}}$, there is no idle vertex and no sink or source vertices. This gives rise to the Corollary below.

Corollary 4.7. *The existence of positive equilibrium points of a linear kinetic system with a kinetic matrix $\overline{M}$ having the p-property follows through the following statements.*

A. The reaction graph of the transformed linear CRN with the Kirchhoff matrix $A_k = T\overline{M}$, where $T = \mathrm{diag}(\mathbf{m}_1, ..., \mathbf{m}_n)$, $\underline{\mathbf{m}}\overline{M} = 0$ is also strongly connected. Therefore, there is an element-wise positive vector c in the kernel of A_k, such that $A_kc = 0$.

B. This positive vector is also in the kernel of $\overline{M}$, because $\overline{M} = T^{-1}A_k$. Therefore, the element-wise positive vector c determines the positive equilibrium point of the original linear kinetic system, too (determined by the linear manifold given by the initial conditions).

The following theorem states the *equivalence of the existence of a positive equilibrium point and the conservation property for a class of kinetic matrices.*

Theorem 4.8. *The non-degenerate kinetic matrix $\overline{M}$ has the p-property, i.e. it has an element-wise positive vector p in its kernel ($\overline{M}p = 0$) if and only if $\overline{M}$ is a conservation matrix.*

Proof. Let us form the matrix $\overline{M}^T$. This is a conservation matrix with $\underline{\mathbf{m}} = p^T$, i.e. $\underline{\mathbf{m}}\overline{M}^T = 0$. It is also easy to see, that $\overline{M}^T$ is also a non-degenerate kinetic matrix with the p-property. This, together with its conservation property implies that its variable structure graph $\boldsymbol{G}_{\overline{M}^T}$ is strongly connected (see Lemma 4.5).

Furthermore, as Corollary 4.7.B states, there exists a positive vector c in the kernel of $\overline{M}^T$, such that $\overline{M}^T c = 0$. By transposing this equality we get $c^T\overline{M} = 0$ that shows, that $\overline{M}$ is indeed a conservation matrix with the conservation vector c^T. □

4.4. Stability and Lyapunov functions of linear kinetic systems

The above results on conservation and positive equilibrium points give rise to the following stability result.

Theorem 4.9. *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*

$$\overline{M}^T Q + Q\overline{M} \preceq 0 \tag{4.5}$$

Proof. First we use Theorem 4.8 that states that $\overline{M}$ is a stability matrix with an element-wise positive vector $\underline{\mathbf{m}}$. Let us form a Kirchhoff matrix from it by using the diagonal matrix $T = \mathrm{diag}(\mathbf{m}_1, ..., \mathbf{m}_n)$, i.e. $A_k = T\overline{M}$.

Because A_k is also a Metzler matrix, it is diagonally stable, i.e. there exists a positive diagonal matrix $Q \in \mathcal{D}_+$ such that $A_k^T Q + QA_k \preceq 0$. We can substitute the generating equation of A_k into it to obtain

$$\overline{M}^T(TP) + (PT)\overline{M} \preceq 0$$

As T and P are both positive diagonal matrices, their product is also a positive diagonal matrix, and $PT = TP$, therefore Eq. (4.5) holds with $Q = PT = TP$. □

4.4.1. Lyapunov functions for non-degenerate linear kinetic systems

Let us first define the set of coefficient matrices of non-degenerate kinetic systems with a strongly connected variable structure graph $\boldsymbol{G}_M$, and denote this set by $\mathcal{M}_{wrCRN}$.

Based on the results above we can now state the following theorem.

Theorem 4.10. *Assume that the coefficient matrix M of a non-degenerate kinetic system is in $\mathcal{M}_{wrCRN}$, i.e. the system has a strongly connected variable structure graph $\boldsymbol{G}_M$. Then this system allows to have* ***suitable scaled*** *Lyapunov functions V_2 (3.11), V_{CRN} (3.13) and V_{QP} (2.27) that are level set equivalent.*

Proof. First we show that by suitable variable re-scaling we can transform the ODE of the system to a model of a weakly reversible linear CRN. If $M \in \mathcal{M}_{wrCRN}$, then it is a conservation matrix and has a positive equilibrium point. Then there exists a positive diagonal matrix $T \in \mathcal{D}_+$ with $T = \mathrm{diag}(t_1, ..., t_n)$, such that $A_k = TM$ is a Kirchhoff matrix, and $A_k \in \mathcal{M}_{wrCRN}$, too. Applying state transformation $x_i' = t_i x_i$ to the ODE $\frac{dx}{dt} = Mx$ of the original system we obtain

$$\frac{dx'}{dt} = (TM)T^{-1}x' = A_k T^{-1}x' = A_k' x' \tag{4.6}$$

where A'_k s also a Kirchhoff matrix and $A'_k \in \mathcal{M}_{wrCRN}$, too. The state transformation implies $\frac{x_i}{x_i^*} = \frac{x'_i}{x'^*_i}$, therefore the CRN-type Lyapunov function of the transformed system (4.6) can be written in the original coordinates as

$$V_{CRN} = \sum_{i=1}^{n} t_i x_i \ln(\frac{x_i}{x_i^*}) \tag{4.7}$$

that is a *weighted or scaled version* (with the positive weights t_i) of the original CRN-type Lyapunov function (3.13).

The existence of a scaled quadratic Lyapunov function (3.11) follows immediately from Theorem 4.9.

Finally we can apply Lemma 3.1 to show that the system has a V_{QP}-type Lyapunov function, too. □

5. Kinetic Lotka-Volterra systems

Combining the notation (2.16) introduced for Lotka-Volterra systems with the result of Theorem 4.10 some further results can be derived as follows.

5.1. Kinetic Lotka-Volterra systems and their Lyapunov functions

Theorem 5.1. *Consider the special case of Lotka-Volterra systems*

$$\frac{dx}{dt} = \mathrm{diag}(x) \cdot M \cdot (x - x^*) \tag{5.1}$$

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

Proof. As a first step, 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.

Then the statement follows directly from Theorem 4.10. □

5.2. Kinetic Lotka-Volterra models via time-reparametrization

The key tool for forcing the sign pattern (4.2) for the Lotka-Volterra model having a positive equilibrium point (2.16) is time-reparametrization. As it was shown before, (2.18) is a similarity transformation that practically increases the chance of proving asymptotic stability.

If the Ω parameter vector of transformed Lotka-Volterra model (2.25) can be selected in such a way, that the resulting Lotka-Volterra model coefficient matrix $\hat{M}$ admits the sign pattern (4.2), then Theorem 5.1 can be applied.

The conditions (4.2) can be derived for (2.25) as the linear constraints (5.2).

$$\begin{aligned}
m_{ii} + \sum_{j=1}^{n} m_{ji}\Omega_j &< 0, && i = 1, \ldots, n \\
\sum_{j=1}^{n} \Lambda_j \Omega_j &< 0, && i = 1, \ldots, n \\
m_{ij} + \sum_{k=1}^{n} m_{kj}\Omega_k &< 0, && i = 1, \ldots, n, j = 1, \ldots, n, i \neq j \\
\Lambda_i + \sum_{j=1}^{n} \Lambda_j \Omega_j &> 0, && i = 1, \ldots, n \\
\sum_{j=1}^{n} m_{ji}\Omega_j &> 0, && i = 1, \ldots, n
\end{aligned} \tag{5.2}$$

Then a suitable time-reparametrization transformation Ω can be found by solving (5.2), if it exists.

5.2.1. Example

Consider the Lotka-Volterra system with following coefficient matrices

$$M = \begin{bmatrix} -0.1765 & -1.3320 \\ 0.7914 & -2.3299 \end{bmatrix}, \quad L = \begin{bmatrix} 1.5085 \\ 1.5385 \end{bmatrix} \tag{5.3}$$

The Lotka-Volterra model (5.3) has a positive eqilibrium point at $[1 \;\; 1]^T$.

Extending the constraints (5.2) with the linear objective function

$$\Phi(\Omega) = -\Omega_1 - \Omega_2$$

leads to a linear programming problem that can be solved by several software tools. A feasible solution of the problem in this case is

$$\Omega = \begin{bmatrix} -0.7193 & -0.1605 \end{bmatrix}.$$

With the above solution, it is possible to cast the original Lotka-Volterra system to the set of Kinetic Lotka-Volterra systems and use Theorem 5.1.

6. Conclusions

First an overview of the theory, methods and tools available for the two considered partially overlapping class of positive polynomial systems, chemical reaction networks with mass action law (MAL-CRNs) and quasi-polynomial systems (QP systems) were given. Both of them have an entropy-like Lyapunov function associated to them which are similar but not the same.

Then we have shown that linear kinetic systems with a linear first integral (that corresponds to conservation) and with the p-property can be transformed to linear weakly reversible MAL-CRNs using linear diagonal transformation, and the coefficient matrix of this system is diagonally stable. The equivalence of conservation and the existence of positive equilibrium points for linear kinetic systems with the p-property was also shown for this case.

The mathematical equivalence of Markov chains with positive equilibrium point and linear weakly reversible MAL-CRNs implies the existence of the weighted version of the various entropy level set equivalent Lyapunov functions described in the pioneering work of Gorban et al. [12] for linear kinetic systems with a linear first integral and with the p-property.

Using translated X-factorable phase space transformations and nonlinear variable transformations a dynamically similar linear ODE model has been associated to the QP system models that have a positive equilibrium point. The non-degenerate kinetic property together with the existence of the positive equilibrium point form a sufficient condition of the existence of the weighted version of the various entropy level set equivalent Lyapunov functions in this case. Further extension has been obtained by using the time re-parametrization transformation defined for QP models where the transformation parameters can be determined by solving a linear programming problem.

Future work includes the extension of the results to other types of weakly reversible MAL-CRNs, and the possible generalizations to the case of non-diagonal positive linear variable transformations.

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