Craciun´s E-MAK Method: A Dynamics-focused Approach to Poly-PL Kinetics

Daryl M. Magpantay[1,2*], Eduardo R. Mendoza[1,3,4,5] and Ederlina G. Nocon[1]

[1]Mathematics and Statistics Department, De La Salle University, Manila
[2]College of Arts and Sciences, Batangas State University, Batangas City
[3]Institute of Mathematical Sciences and Physics, University of the Philippines Los Baños, Laguna
[4]Max Planck Institute of Biochemistry, Martinsried, Munich, Germany
[5]LMU Faculty of Physics, Geschwister -Scholl- Platz 1, Munich 80539, Germany

*Corresponding author: magpantaydaryl@gmail.com

ABSTRACT

This paper studies chemical reaction networks with poly-PL kinetics, i.e. positive linear combinations of power law kinetics. The analysis of such systems is motivated by the study of Veloz et al., that proposed to analyze the dynamics of Evolutionary Game Theory models using Chemical Reaction Network Theory (CRNT) in the form of polynomial kinetics (POK). Our approach is based on the fact that poly-PL kinetics generate power law dynamical systems, which via a method recently introduced by G. Craciun can be mapped to EMAK systems. These are the analogue of mass action kinetics on Euclidean embedded graphs (E-graph). Our main structural results show the coincidence of the stoichiometric subspaces of the original network and its associated E-graph as well as the conservation of the positive dependency, which is a necessary condition for the existence of positive equilibria. However, our overall analysis shows Craciun´s method is only of limited use for studying PYK systems since only very special kinetics reflect the structural properties of the original chemical kinetic system.

Keywords: Chemical Reaction Networks, E-graph, Poly-PL Kinetics, power law kinetics

INTRODUCTION

Poly-PL kinetics (PYK) are kinetic systems consisting of non-negative linear combinations of power law functions. It contains the set PLK of power law kinetics as "mono-PL kinetics with coefficient 1." Like PLK, the definition domain of PYK is the positive orthant $\mathbb{R}^m_>$. However, as subsets, this may be extended to the whole non-negative orthant $\mathbb{R}^m_\geq$. PYK and PLK generate the same sets of species formation rate functions (SFRF), the power law dynamical systems (or GMA systems in BST terminology).

A poly-PL kinetics is rate constant-interaction decomposable, i.e. an element of rate constant-interaction map decomposable kinetics (RIDK). For each positive integer h, the set PYK_h consists of all poly-PL kinetics with h positive terms. The set $\{\mathrm{PYK}_h | h > 0\}$ forms a countable covering of PYK.

The set of polynomial kinetics (POK) was first introduced by Veloz et al. (2014) for the realization of replicator system-based evolutionary games with polynomial payoff func-

tions (mostly linear functions). Polynomial kinetics result in polynomial dynamical systems as ODEs, which is a classical area of research in mathematics. The domain of definition is usually extended to the whole non-negative orthant. The set of non-negative equilibria of polynomial dynamical system is a subset of an algebraic variety (and this may be a reason for algebraic geometry researchers to become interested in pursuing applicability of their theory). Veloz et al's proposal is the following:

> The replicator equation implies a reaction network: it can be written as
>
> $$\dot{x}_k = x_k(f_k(x) - \phi(x))$$
>
> where x_k is the proportion of players using strategy k, $f_k(x)$ is their fitness and $\phi(x) = \sum_{i=1}^{n} x_i f_i(x)$ the average fitness of the population (dilution flow in chemical reactions) represented by $x = (x_1, \dots, x_n)$. The reaction network consists of decay reactions of the form $x_k \rightarrow 0$ due to the dilution term $-x_k\phi(x)$. The production term $x_k f_k(x)$ implies catalytic reactions of the form
>
> $$x_k + i_1 + \cdots + i_m \rightarrow 2x_k + i_1 + \cdots + i_m,$$
>
> where $i_1, \dots, i_m$ are those species that are necessary for k to replicate, i.e., $f(x)$ is these species have positive concentrations in x.

As we want to see this case in the bigger set, our interest to study the concept of its superset PYK arises.

So far we have identified three (3) ways to study poly-PL kinetic systems. First is the direct way that deals with the proposed concept of Veloz et al. (2014). In this framework, evolutionary games with polynomial payoff functions lead to polynomial kinetic systems. The consideration of the superset of poly-PL kinetics, i.e. of real exponents instead of just non-negative integers, came from the observation that "sums of power law functions" occurred in power law approximations of some carbon cycle models (Fortun et al., 2018) which were analyzed with CRNT methods. Hence, we present a simple dynamically equivalent representation to which, in the case of poly-PL replicator systems, the Weakly Reversible Theorem for all complex factorizable poly-PL kinetics (PY-TIK) can be applied (Talabis et al., 2019).

Second is via dynamic equivalence to power kinetic systems using S-invariant Termwise Addition of Reactions (STAR) approach. STAR (S-invariant Termwise Addition of Reactions) is a network structure-oriented approach to poly-PL Kinetics based on the following basic observation: for the rate function $K_i(x)$ and for a reaction $r_i : y_i \rightarrow y_i'$ in a PYK system $(\mathcal{N}, K)$ with $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ we have $K_i(x) = k_i(a_{i1}M_{i1} + \dots + a_{ih}M_{ih})(y_i' - y_i) = k_i a_{i1} M_{i1}(y_i' - y_i) + \dots + k_i a_{ih} M_{ih}(y_i' - y_i)$ where M_{ij} are the h power law functions for the ith reaction. A STAR method introduces additional different reaction(s) for each of the h identical reaction vectors $y_i' - y_i$ in the sum. This enlarges the sets of reactions and complexes, so the new CRN $\mathcal{N}^* = (\mathcal{S}, \mathcal{C}^*, \mathcal{R}^*)$ and new kinetics $K^* : \mathbb{R}_>^{\mathcal{S}} \rightarrow \mathbb{R}^{\mathcal{R}^*}$ are constructed. One method focuses on the multiples of the reaction vectors and the other one uses the multiples of the maximal stoichiometric coefficients.

Lastly is via Craciun´s method which is the subject of this paper. Since poly-PL kinetics generates power law dynamical systems (called "polynomial dynamical systems by Craciun for various reasons), they can be represented as E-MAK systems. Polynomial dynamical system can be regarded as being generated by some "Euclidean Embed-

ded Graph" (also called E-graph). This paper aims to discuss the detailed description of the map PYK to EMAK, establish some network properties and produce results on positive equilibria of PYK systems based on EMAK representations.

The paper is organized as follows: In Section 2, necessary concepts and previous results in CRNT that are need to understand the latter sections are presented. In Section 3, the concept of Euclidean Embedded Graph will be explored. In Section 4, a detailed description of the map PYK (N) to E-Graph/EMAK will be discussed. In Section 5, some network structure relationships will be established and in Section 6, results on positive equilibria of PYK systems based on EMAK representations will be produced. This will be followed by sections exploring PYK systems with cycle terminal, t-minimal and PYK-SSK associated EMAK systems. Lastly, in Section 7, summary and conclusion of the results will be presented.

FUNDAMENTAL CONCEPTS OF CHEMICAL REACTION NETWORKS AND CHEMICAL KINETIC SYSTEMS

Chemical reaction networks and kinetic systems

In this section, we discuss fundamental concepts and results about chemical reaction networks (CRN) and chemical kinetic systems (CKS). We consider a CRN as a digraph with vertex labelling. On the other hand, our discussion on CKS focuses on power-law kinetic system.

Definition 1 A **chemical reaction network (CRN)** is a digraph $(\mathcal{C}, \mathcal{R})$ where each vertex has positive degree and stoichiometry, i.e., there is a finite set $\mathcal{S}$ (whose elements are called **species**) such that $\mathcal{C}$ is a subset of $\mathbb{Z}_{\geq}^{\mathcal{S}}$. Each vertex is called a **complex** and its coordinates in $\mathbb{R}_{\geq}^{\mathcal{S}}$ are called **stoichiometric coefficients**. The arcs are called **reactions**.

We denote the number of species with m, the number of complexes with n, and the number of reactions with r. Also, we denote this nonempty finite collection of reactions as $\mathcal{R} \subset (\mathcal{C} \times \mathcal{C})$. We implicitly assume the sets are numbered and let

$$\mathcal{S} = \{X_1, X_2, \dots, X_m\} \qquad \mathcal{C} = \{C_1, C_2, \dots, C_n\}$$
$$\text{and} \quad \mathcal{R} = \{R_1, R_2, \dots, R_r\}$$

where m, n and r are their respective cardinalities. Thus, $\mathbb{R}_{\geq}^{\mathcal{S}} \cong \mathbb{R}_{\geq}^{m}$. Consider the reaction

$$\alpha X_1 + \beta X_2 \to \gamma X_3,$$

X_1, X_2 and X_3 are the species. The complexes are $\alpha X_1 + \beta X_2$ and γX_3. In particular, $\alpha X_1 + \beta X_2$ is called the **reactant** (or **source**) **complex** and γX_3 the **product complex**. The number of reactant complexes is denoted by n_r.

The stoichiometric coefficients are the non-negative coefficients α, β and γ. Under mass action kinetics (MAK), the rate at which the reaction occurs is given by the monomial

$$K = kX_1^{\alpha} X_2^{\beta}$$

with rate constant $k > 0$. We can generalize this by considering power-law kinetics. The reaction rate can be

$$K = kX_1^{a} X_2^{b}$$

where a and b can be any real number. We call a and b as **kinetic orders**. Within a network involving additional species and reactions, the above reaction contributes to the dynamics of the species concentration as

$$\dot{X} = \begin{bmatrix} \dot{X}_1 \\ \dot{X}_2 \\ \dot{X}_3 \\ \vdots \end{bmatrix} = kX_1^{a} X_2^{b} \begin{pmatrix} -\alpha \\ -\beta \\ \gamma \\ \vdots \end{pmatrix} + \cdots$$

The **reactant map** $\rho : \mathcal{R} \to \mathcal{C}$ maps a reaction to its reactant complex while the **product map** $\pi : \mathcal{R} \to \mathcal{C}$ maps it to its product complex.

Definition 2 The **linkage classes** of a CRN are the subnetworks of a reaction graph where for any complexes C_i, C_j of the subnetwork, there is path between them. The number of linkage classes is denoted by ℓ.

A linkage class is said to be a **strong linkage class** if there is a directed path from C_i to C_j and vice versa for any complexes C_i, C_j of the subnetwork. The number of strong linkage classes is denoted by $s\ell$. Moreover, **terminal strong linkage classes**, the number of which is denoted as t, are the maximal strongly connected subnetworks where there are no edges (reactions) from a complex in the subgraph to a complex outside the subnetwork. The terminal strong linkage classes can be of two kinds: cycles (not necessarily simple) and singletons (which we call "terminal points").

Example 1 Given a chemical reaction network (CRN):

$R_1 : 2A \to B$
$R_2 : B \to 2A$
$R_1 : A + 3B \to 2A + B$
$R_1 : 2A + B \to A + 3B$

As observed, $m = 2$ (species), $n = 4$ (complexes), $n_r = 4$ (reactant complexes) and $r = 4$ (reactions). Also, we have

$\mathcal{S} = \{A, B\}$
$\mathcal{C} = \{C_1 = 2A, C_2 = B, C_3 = A + 3B, C_4 = 2A + B\}$

The number of linkage classes is two ($\ell = 2$), $\mathcal{L}_1 = \{R_1, R_2\}$ and $\mathcal{L}_2 = \{R_3, R_4\}$. Both subnetworks are strong linkage classes which implies that the number of strong linkage classes is two ($s\ell = 2$).

Definition 3 A CRN is called

1. **weakly reversible** if $s\ell = \ell$;
2. **t-minimal** if $t = \ell$;
3. **point-terminal** if $t = n - n_r$; and
4. **cycle terminal** if $n - n_r = 0$.

The above example is weakly reversible, t-minimal and cycle terminal.

The dynamical system of the CRN of our running example can be written as

$$\dot{X} = \begin{bmatrix} \dot{A} \\ \dot{B} \end{bmatrix} = \begin{array}{c} \begin{matrix} R_1 & R_2 & R_3 & R_4 \end{matrix} \\ \begin{bmatrix} -2 & 2 & 1 & -1 \\ 1 & -1 & -2 & 2 \end{bmatrix} \end{array} \cdot \begin{bmatrix} k_{12}A^{f_{11}} \\ k_{21}B^{f_{21}} \\ k_{34}A^{f_{31}}B^{f_{32}} \\ k_{43}A^{f_{41}}B^{f^{42}} \end{bmatrix} = NK(x).$$

N is called the stoichiometric matrix and $K(x)$ is called the **kinetic vector** (or **kinetics**). The pairing of $(\mathcal{N}, K)$ is called a **chemical kinetic system (CKS)**. The kinetics aboce belong to **power law kinetics** which have the form

$$K_i(x) = k_i \prod_{i=1}^{r} x^{F_{ij}} \quad where \quad 1 \leq i \leq r$$

with $k_i \in \mathbb{R}^m_>$ and $F_{ij} \in \mathbb{R}$. Power law kinetics is defined by an $r \times m$ matrix $F = [F_{ij}]$, called the **kinetic order matrix**, and vector $k \in \mathbb{R}^r$, called the **rate vector**. A particular example of power law kinetics is the well-known mass action kinetics where the kinetic order matrix consists of stoichiometric coefficients of the reactants. In the running example, we assume power law kinetics so that the kinetic order matrix is

$$F = \begin{array}{c} \begin{matrix} A & B \end{matrix} \\ \begin{bmatrix} f_{11} & 0 \\ 0 & f_{21} \\ f_{31} & f_{32} \\ f_{41} & f_{42} \end{bmatrix} \end{array} \begin{matrix} R_1 \\ R_2 \\ R_3 \\ R_4 \end{matrix},$$

where $f_{ij} \in \mathbb{R}$. However, in this paper, we are more interested in a kinetic system composed of non-negative linear combinations of power law functions.

We further decompose the stoichiometric matrix N. Writing the stoichiometric complexes as column vectors of the **(molecularity) matrix** Y, we have

$$Y = \begin{array}{c} \begin{matrix} C_1 & C_2 & C_3 & C_4 \end{matrix} \\ \left[\begin{array}{cccc} 1 & 0 & 1 & 2 \\ 0 & 1 & 3 & 1 \end{array}\right] \end{array} \begin{matrix} A \\ B \end{matrix},$$

Considering the digraph of our CRN, the **incidence matrix**

$$(I_a)_{(i,j)} = \begin{cases} -1 & if\ i\ is\ the\ reactant\ complex\ of\ reaction\ j \in \mathcal{R} \\ 1 & if\ i\ is\ the\ product\ complex\ of\ reaction\ j \in \mathcal{R} \\ 0 & otherwise \end{cases}$$

will be

$$I_a = \begin{array}{c} \begin{matrix} R_1 & R_2 & R_3 & R_4 \end{matrix} \\ \left[\begin{array}{cccc} -1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 \end{array}\right] \end{array} \begin{matrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{matrix},$$

Note that stoichiometric matrix $N = YI_a$. Hence, the stoichiometric map $N : \mathbb{R}^r \to \mathbb{R}^m$ is defined as the composition $Y \circ I_a$. The linear subspace of $\mathbb{R}^m$ defined by $Im\ N$ is called the **stoichiometric subspace**, denoted as S.

The linear transformation $A_k : \mathbb{R}^{\mathcal{C}} \to \mathbb{R}^{\mathcal{C}}$ called **Laplacian map** is the mapping defined by

$$A_h x := \sum_{(i,j)\in\mathcal{R}} k_{ij} x_i (\omega_j - \omega_i),$$

where x_i refers to the i^{th} component of $x \in \mathbb{R}^{\mathcal{C}}$ relative to the standard basis. Its matrix representation is the $n \times n$ matrix such that

$$(A_k)_{i,j} = \begin{cases} k_{ji} & if\ \ i \neq j, \\ k_{jj} - \sum_{i'=1}^{n} k_{ji'} & if\ \ i = j \end{cases}$$

where k_{ji} is the label (called the rate constant) associated to the reactions $(j,i) \in \mathcal{R}$.

Let $s = \dim\ S$. The **deficiency** δ is defined as $\delta = n - \ell - s$. This non-negative integer is, as Shinar and Feinberg (2011) pointed out, essentially a measure of the linear dependency of the network's reactions. In the running example, the deficiency of the network is 0 since $n = 4,\ \ell = 2$ and $s = 2$. It is an important parameter in CRNT in establishing claims regarding the existence, multiplicity, finiteness and parametrization of the set of **positive steady states**, defined as $E_+(\mathcal{N}, K) = \{x \in \mathbb{R}^m_> | NK(x) = 0\}$.

Horn and Jackson (1972) introduced a subset of E_+ called the set of **complex balanced of equilibria** denoted as Z_+. A kinetic system is complex-balanced at a state (i.e. a species composition) if for each complex, formation and degradation are at equilibrium.

Definition 4 A positive vector c in $\mathbb{R}^m$ is called **complex balanced** (CB) if $K(c)$ is contained in $ker\ I_a$. A chemical kinetic system is called **complex balanced** if it has complex balanced equilibria.

With regards of being complex balanced of a chemical kinetic system, the following are two known propositions.

Proposition 1 If a chemical kinetic system has a complex balanced steady state, then the underlying CRN is weakly reversible (Horn, 1972).

Proposition 2 If a chemical kinetic system has deficiency 0, then its equilibria are all complex balanced (Feinberg, 1972).

Poly-PL Kinetics (PYK)

Poly-PL kinetics (PYK) are kinetic systems consisting of non-negative linear combinations of power law functions. Power law kinetics is a subset of PYK represented as "mono-PL kinetics with coefficient 1".

After setting the standard ordering of species $X_1, \dots, X_m$, we have the following definition:

Definition 5 A kinetics $K : \mathbb{R}^m_> \to \mathbb{R}^r$ is a **poly-PL kinetics** if

$$K_i(x) = k_i(a_{i,1}x^{F_{i,1}} + \dots + a_{i,j}x^{F_{i,j}} \qquad (1)$$

where $1 \leq i \leq$, written in lexicographic order with $k_i \in \mathbb{R}^m_>$, $F_{i,j}, a_{i,j} \in \mathbb{R}^m$ and $1 \leq j \leq h_i$ (where h_i is the number of terms in reaction i). Power-law kinetics is defined by $r \times m$ matrices $F_{i,k} = [F_{ij}]$, called the **kinetic order** matrices, vectors $k = [k_i], a_{i,j} \in \mathbb{R}^r_>$, called the **rate vector** and **poly-rate vectors**, respectively.

Another concept on kinetics is defined as follows:

Definition 6 A **rate constant-interaction map decomposable (RID) kinetics** is a kinetics, such that for each reaction r, the coordinate function $K_r : \Omega \to \mathbb{R}$ can be written in the form $K_r(x) = k_r I_{K\,r}(x)$, with a positive real number k_r (called a rate constant) and $\Omega \in \mathbb{R}^m$. We call the map $I_K : \Omega \to \mathbb{R}^{\mathcal{R}}$ defined by $I_{K\,r}$ as the interaction map and the set of kinetics RIDK.

In the following, we consider **complex factorizable PYK systems**, i.e. reactions branching from a reactant all have the same interaction map

$$\psi_i(x) = a_{i,1}x^{F_{i,1}} + \dots + a_{i,j}x^{F_{i,j}} \quad where\ 1 \leq i \leq n_r.$$

We say that a reactant complex y is a CF-node for K if and only it is a CF-node for K_j for each j and the coefficients $a_{i,j}$ coincide for all reactions in its reaction set and for each j. Moreover, we extend the definition of reactant determined power-law kinetics (PL-RDK) of (Talabis et al. , 2019) to poly-PL kinetics.

Definition 7 A poly-PL kinetic system has **reactant-determined kinetics** if for any two reactions a, b with identical reactant complexes, the corresponding columns of kinetic orders for each F_K are identical, i.e., $(F_K)_{ai} = (F_K)_{bi}$ for $i = 1, \dots, m$.

We also note that the PYK systems with reactant-determined kinetics are precisely the complex factorizable ones. For each kinetic order matrix F_K where $1 \leq K \leq h$, we define the $m \times n$ matrix $\tilde{Y}_K$ defined as:

$$(\tilde{Y}_K)_{ij} = \begin{cases} (F_K)_{ri}, & if\ j\ is\ a\ reactant\ complex\ of\ reaction\ r. \\ 0, & otherwise \end{cases}$$

A PL-RDK kinetics is factor span surjective if and only if all rows with different reactant complexes in the kinetic order matrix F are pairwise different.

EUCLIDEAN EMBEDDED GRAPH (E-GRAPH) and E-MAK SYSTEM

Craciun (2018) formally introduced Euclidean Embedded Graph as follows:

Definition 8 A **Euclidean embedded graph (or E-graph)** is a finite oriented graph $G = (V, E)$ whose vertices are labeled by distinct elements of $\mathbb{R}^n$ for some $n \geq 1$.

With an abuse of notation, we identify the set V with the set of vertex labels, i.e., we assume that $V \subset \mathbb{R}^n$. Moreover, we associate to each edge $e = (s, t) \in E$ its edge vector $v(e) = t - s$. Also, we define its source vertex to be $s(e) = s$, and its target vertex to be $t(e) = t$.

Thus, according to this formulation, an E-graph is almost the same as the concept of chemical reaction network that we introduced.

Craciun's definition is slightly more special because an oriented graph is a digraph with no 2-cycles. However, the formulation above seems just a bit of sloppiness since later in his paper, he speaks of reversible E-graphs. Brunner and Craciun (2018) define an E-graph as a directed graph, not just an oriented graph. So, an E-graph is really identical with a chemical reaction network as defined above.

Craciun introduced the concept of polynomial dynamical system. Any autonomous polynomial dynamical system (i.e., system of differential equations with polynomial right-hand side) on the strictly positive orthant $R^n_>$ can be represented as

$$\frac{dx}{dt} = \sum_{i=1}^{m} x^{s_i} v_i \tag{2}$$

where $x = (x_1, \dots, x_n) \in \mathbb{R}^n_>$, $s_1, \dots, s_m$ are some vectors in $\mathbb{Z}^n_{\geq 0}$ called **exponent vectors**, x^{s_i} denotes the monomial $x_1^{s_{i1}} x_2^{s_{i2}} \cdots x_n^{s_{in}}$ and $v_1, \dots, v_m$ are vectors in $\mathbb{R}^n$. A **solution** of (2) is a function $x : I \to \mathbb{R}^n_{>0}$ that satisfies (2), where I is an interval in $\mathbb{R}$.

However, he broadened the scope of the term to include the "power law dynamical system" case. Note that, since the coordinates $x_1, \dots, x_n$ are positive, the monomials x^{s_i} are well-defined even if the coordinates of the exponent vectors s_i are arbitrary real numbers (i.e., $s_1, \dots, s_m$ are not necessarily in $\mathbb{Z}^n_{\geq 0}$). In that case we say that Equation 2 is a **power-law dynamical system**. The approaches and results discussed in this paper apply not only to polynomial dynamical systems, but also to power-law dynamical systems. In this paper, whenever we say "polynomial dynamical system", we mean "polynomial or power law dynamical system".

A further extension is to replace the constant rate with a variable (but bounded) function. In other cases, the interaction network we need to model is part of a larger network that contains variables or "external factors" that influence our system, but are not contained in our system. In that case we cannot use an autonomous dynamical system as a model, but we may be able to use a non-autonomous dynamical system of the form

$$\frac{dx}{dt} = \sum_{i=1}^{m} k_i(t) x^{s_i} v_i \tag{3}$$

where the functions k_i are positive and uniformly bounded, i.e., there exists some $\epsilon > 0$ such that $\epsilon \leq k_i(t) \leq \frac{1}{\epsilon}$ for all t. We will refer to models of the form (3) as **variable-k polynomial dynamical systems**.

Now, given a Euclidean embedded graph $G = (V, E)$, the polynomial dynamical systems generated by G are the dynamical systems on $\mathbb{R}^n_>$ given by

$$\frac{dx}{dt} = \sum_{e \in E} k_e x^{s(e)} v(e) \tag{4}$$

for some positive constants k_e. Note that if $V \subset \mathbb{Z}^n_{\geq 0}$ then (4) is just mass-action kinetics for a chemical reaction network represented by G, i.e, one where there is a reaction of the form $s(e) \to t(e)$ for each edge $e \in E$.

We express this construction in terms of kinetics on a reaction network (or E-graph) instead of dynamical systems. Also, the same definition of a chemical kinetics on an E-graph as with a CRN.

Definition 9 A kinetics K on a reaction network (or E-graph) is called an **E-MAK** if for each reaction (or edge) $K_e(x) = k_e x^{s(e)}$, where $k_e > 0$ for all $x > 0$.

Any power law dynamical system can be realized as an E-MAK system. In particular, the kinetics is RDK (Reactant Determined Kinetics) and FSK (Factor Span Surjective).

Let us note that for any variable-k polynomial dynamical system (3) we can construct an E-graph G that generates it, and G is not unique. Assuming that the ordered pairs $(s_1, v_1), (s_2, v_2), \dots,$
(s_m, v_m) are distinct, the simplest way to construct such a G is to choose the set of vertices

$$V = \{s_i | i = 1, \dots, m\} \cup \{s_i + v_i | i = 1, \dots, m\},$$

and the set of edges

$$E = \{(s_i, s_i + v_i) | i = 1, \dots, m\}.$$

If we want to obtain a different E-graph that generates (2), we can, for example, write one of the vectors v_i as a positive linear combination of two different nonzero vectors, and use these new vectors to obtain a graph with $m + 1$ edges that also generates (2).

Note that if s_i and $s_i + v_i$ are non-negative for all i, then the E-graph is a CRN, and the E-MAK realization is a MAK-realization.

Example 2 Consider a dynamical system

$$\begin{aligned} \frac{dx_1}{dt} &= -3k_1(t)x_1 + 3k_2(t)x_2^2 \qquad (5) \\ \frac{dx_2}{dt} &= k_1(t)x_1 - k_2(t)x_2^2 \end{aligned}$$

for some functions $k_i(t)$ with $\epsilon < k_i(t) < \frac{1}{\epsilon}$ for all t.

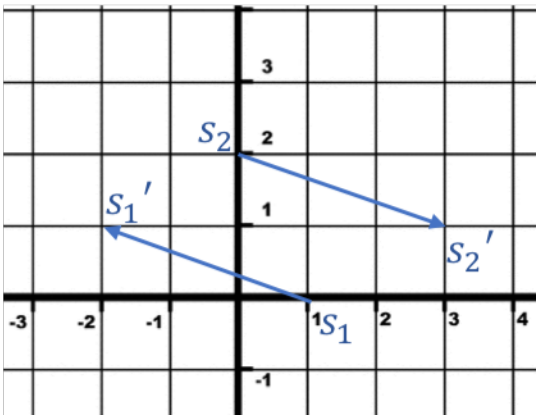
With this, we can write the vector form as follows:

$$\frac{dx}{dt} = k_1(t)x_1 \begin{pmatrix} -3 \\ 1 \end{pmatrix} + k_2(t)x_2^2 \begin{pmatrix} 3 \\ -1 \end{pmatrix} \qquad (6)$$

where $x = \binom{x_1}{x_2}$. Following (2), we can express the above as:

$$\frac{dx}{dt} = k_1(t)x^{s_1} \begin{pmatrix} -3 \\ 1 \end{pmatrix} + k_2(t)x^{s_2} \begin{pmatrix} 3 \\ -1 \end{pmatrix} \qquad (7)$$

where $s_1 = \binom{1}{0}$ and $s_2 = \binom{0}{2}$. Then, the simplest E-graph G that generates the dynamical system (5) has two edges, one edge from s_1 to $s_1' := s_1 + \binom{-3}{1} = \binom{1}{0} + \binom{-3}{1} = \binom{-2}{1}$, and other edge from s_2 to $s_2' := s_2 + \binom{3}{-1} = \binom{0}{2} + \binom{3}{-1} = \binom{3}{1}$ illustrated as follows:



DETAILED DESCRIPTION OF THE MAP PYK TO E-GRAPH/EMAK

We consider the Craciun map c_E from the set of power law dynamical systems on PLDS (also described as polynomial dynamical systems) to the set of Euclidean embedded graphs. It is defined to satisfy some conditions in order to avoid images that involve trivial graphs. This is to eliminate PLDS resulting to an E-graph with only one vertex. Note that, for $\frac{dx}{dt} = \sum x_i^{s_i} v_i$ to be satisfied, it must be the cases that the ordered pairs $(s_1, v_1), (s_2, v_2), \dots, (s_m, v_m)$ are distinct.

Denoting the PLDS subset satisfying the above condition as $PLDS_C$, we have $c_E : PLDS_C \to$ E-Graph. E-Graph consists of pairs $\mathcal{N}' = (\mathcal{S}, \mathcal{C}', \mathcal{R}')$ with $\mathcal{S} = \{x_i\}$ and $\mathcal{C}'$ can have arbitrary real coefficients. The essential property of c_E is that with the EMAK kinetics K', the chemical kinetic system is identical to the power law dynamical system. Craciun (2018) remarked that this map is not "unique" in the sense that there are many other E-Graph representations of the power law dynamical system.

Conversely, given an E-Graph, one can always construct a power law dynamical system coinciding with the right hand side of the ODE's of the associated EMAK system of the E-Graph. The second component is given the map from PYK to PLDS, where

$N = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ is a CRN and $\mathcal{S} = \{x_i\}$, which associates to poly-PL kinetics to its corresponding SFRF, i.e. the right hand side of $\frac{dx}{dt} = \sum_{r\in\mathcal{R}} K_r(x)(y'_r - y_r)$. Note that each K_r is a poly-PL vector function. Clearly, this second map is not surjective. The dynamic equivalence of $(\mathcal{N}, K)$ with the EMAK system is according to definition $\frac{dx}{dt} = \sum_{r\in\mathcal{R}} K_r(x)(y'_r - y_r) = \sum x_i^{s_i} v_i$. For an illustration we have:

Suppose the following are the PYK of a CRN with the corresponding reaction vectors

$$K_1(x) = k_1 x_1^4 x_2^{0.5}; (y'_1 - y_1) = \begin{pmatrix} 2 \\ 0 \end{pmatrix}$$

$$K_2(x) = k_2 x_1^7 x_2^{1.6}; (y'_2 - y_2) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

The corresponding SFRF is given by

$$\frac{dx}{dt} = k_1 x_1^4 x_2^{0.5} \begin{pmatrix} 2 \\ 0 \end{pmatrix} + k_2 x_1^7 x_2^{1.6} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

We can express this form to PLDS where $x = \binom{x_1}{x_2}$. That is

$$\frac{dx}{dt} = k_1 x^{s_1} v_1 + k_2 x^{s_2} v_2.$$

where $s_1 = \binom{4}{0.5}$, $s_2 = \binom{7}{1.6}$, $v_1 = \binom{2}{0}$ and $v_2 = \binom{1}{1}$.

This is an equality between two vector maps $\mathbb{R}^{\mathcal{S}} \to \mathbb{R}^{\mathcal{S}}$. One can, hence, set the coordinate functions equal so that conditions on the s_i and v_i. These conditions specify when an E-Graph (or its associated EMAK) is the image of a PYK system.

SOME NETWORK STRUCTURE RELATIONSHIPS

An E-graph is a more general concept than a CRN because the stoichiometric coefficients of an E-graph may be arbitrary real numbers, while those of a CRN are restricted to be non-negative integers.

Many concepts and results for CRNs also hold for E-graphs. In particular, all concepts and results involving only the digraph structure (and not the vertex labeling) are valid, such as those involving connectivity. For example, the concepts involving terminal classes such as cycle or point terminal, the numbers t, t_p and t_c, terminality, and their relationships all hold without any change.

From now on, to have a standard notation, if $\mathcal{N}$ is the underlying CRN of a PYK system, $\mathcal{N}_E$ denotes the associated E-graph. We write K for the poly-PL kinetics and K_E for the associated EMAK. We shall consistently use the subscript "E" for all objects associated with the E-graph, e.g. S_E is its stoichiometric subspace, δ_E its deficiency, etc.

The following proposition extends the geometric interpretation of deficiency to E-graphs (the proof is identical and extracted from the paper of Mendoza et. al (2018)).

Proposition 3 The deficiency δ_E is equal to $dim\ (ker\ Y_E \cap Im\ I_{a\ E})$.

Proof.

Basic dimensional consideration implies

$$dim(ker(Y_E\ I_{a\ E})) = dim(ker(I_a)) + dim(ker(Y_E) \cap Im(I_{a\ E})).$$

From rank-nullity theorem,

$$dim(ker(Y_E\ I_{a\ E})) = r_E - dim(Im(Y_E I_a)) = r_E - s_E.$$

The rank of $I_{a\ E}$ corresponds to the number of complexes minus the number of linkage classes, so that

$$dim(Im(I_{a\ E})) = n_E - \ell_E.$$

It follows that

$$dim(ker(I_{a\ E})) = r_E - (n_E - \ell_E) = r_E + \ell_E - n_E.$$

And, hence,

$$dim(ker Y_E \cap Im\ I_A) = dim(ker(Y_E\ I_{a\ E})) - dim(ker(I_{a\ E}))$$

$= (r_E - s_E) - (r_E + \ell_E - n_E)$
$= n_E - \ell_E - s_E$
$= \delta_E$. □

We now extend the fundamental relationship between reactant deficiency, $\delta_{\rho\, E}$ and network deficiency, δ_E, to E-graphs. The following extracts are taken from the paper of Mendoza et. al (2018):

Proposition 4 Let G be an E-graph with deficiency δ_E and reactant deficiency $\delta_{\rho\, E}$. Then

$$\delta_E - \delta_{\rho\, E} = \tau(G)_E - t_{c\, E} - \Delta(G)_E.$$

In particular,

(i) if G is cycle terminal, then $0 \leq \delta_{\rho\, E} - \delta_E = \ell_E + \Delta(G)_E \leq \ell$;

(ii) if G is point terminal, then $\delta_E - \delta_{\rho\, E} = \tau(G)_E - \Delta(G)_E$;

(iii) if G is point terminal and cycle terminal, then $\delta_E - \delta_{\rho\, E} < \tau(G)_E - \Delta(G)_E$.

Proof.
$\delta_E - \delta_{\rho\, E} = n_E - \ell_E - s_E - n_{r\, E} + q_E = n_E - n_{r\, E} - \ell_E - s_E + q_E = \tau(G)_E - t_c - \Delta(G)_E$.

(i) If G is cycle terminal, $t_{p\, E} = n_E - n_{r\, E} = 0 \Leftrightarrow t_E = t_{c\, E} \Leftrightarrow \tau(G)_E - t_{c\, E} = -\ell_E$. Hence, $\delta_E - \delta_{\rho\, E} = -\ell_E - \Delta(G)_E$. Since $R_E = Im\ Y_E$, $q_E = c_E \geq s_E$ and $\Delta(G)_E$ is negative. Thus, $\delta_{\rho\, E} - \delta_E = \ell_E + \Delta(G)_E \leq \ell_E$. For the lower bound: $\delta_{\rho\, E} = n_{r\, E} - q_E = n_E - q_E \geq n_E - c_E = dim\ ker\ Y_E \geq dim(ker\ Y_E \cap Im\ I_{a\, E}) = \delta_E$.

(ii) If G is point terminal, $t_{c\, E} = 0$, hence the simpler formula.

(iii) If G is point terminal and cycle terminal, then $t_{c\, E} > 0$, which implies the inequality.

□

Since EMAK systems are similar to MAK systems, there are many results on MAK systems that are easily carried over to EMAK systems. Some examples can be found in the paper by Mendoza et al. (2018). A further example is the following early result from Feinberg (1972):

Proposition 5 If an E-Graph has zero deficiency, then any positive equilibrium is complex-balanced.

Proof.
Recall that $\delta_E = dim\ (Ker\ Y_E \cap Im\ I_{a\, E})$. Since $\delta_E = 0$, the only vector in the intersection is the zero vector. Hence, if $I_{a\, E}(K(x))$ is nonzero then it is not an equilibrium. Thus, the claim follows. □

If the power law dynamical system is generated by a poly-PL kinetics, then one can study the relationship of properties of the chemical kinetic system $(\mathcal{N}, K)$ and the EMAK system, whose reaction network we denote with $\mathcal{N}_E$.

We continue to analyze connections between network properties of PYK and EMAK systems. Note that through the use of the double-indexed sum notation, it became clear that the reaction vectors in the associated E-graph are not merely linear combinations of those in the PYK system, but were simply positive multiples.

Let h_i be the number of terms in the poly-PL kinetic function for the ith reaction of $\mathcal{N}$ where $i = 1, \dots, r$. Let $h := max_i\ h_i$. We order the terms in each kinetic function lexicographically and divide the last term into new terms to have h summands in each function. Thus the SFRF $f(x_1, \dots, x_m)$ can be written as a double sum $\sum_i \sum_j a_{ij} x^{F_{ij}} (y'_i - y_i)$, $i = 1, \dots, r$ and $j = 1, \dots, h$.

We show that the stoichiometric subspace of the given network is equal to the stoichiometric subspace of the associated E-graph.

Proposition 6 Let $(\mathcal{N}, K)$ be a PYK system and $\mathcal{N}_E$ the associated E-graph. Then $S_E = S$.

Proof. Recall that S_E is generated by v_{ij}'s. Since $v_{ij} = a_{ij}(y'_i - y_i)$ are the reaction vectors in $\mathcal{N}_E$, it clearly follows that $S_E = S$. □

Remark 1 Since the stoichiometric subspaces coincide, the Craciun map can be viewed as a transformation of a PYK system to an EMAK system.

We also use above notations to prove the following proposition on positive dependency.

Proposition 7 If $\mathcal{N}$ is positively dependent, the $\mathcal{N}_E$ is positively dependent.

Proof. Let $\sum_i \alpha_i(y'_i - y_i) = 0$ be the positive dependency relation in $\mathcal{N}$. Since $v_{ij} = a_{ij}(y'_i - y_i)$ are the reaction vectors in $\mathcal{N}_E$, we have $\sum_j(\sum_i(\frac{\alpha_i}{a_{ij}})v_{ij}) = \sum_j \sum_i \alpha_i(y'_i - y_i) = 0$. This means that $\mathcal{N}_E$ is positively dependent. □

Now, we explore the upper bounds for the deficiency of the E-graph. These considerations are important for the effective use of current CRNT results for the inference of properties of PYK systems. Most of the current CRNT results, which could be extended to EMAK systems, are about low deficiency systems.

In Proposition 3, we showed that for an E-graph, $\delta_E = dim(Ker\ Y_E \cap Im\ I_{a\ E})$.

The basis of our result is an upper bound for the number of complexes in the associated E-graph. Due to our "filling up" convention, the number of distinct kinetic order vectors (the F_{ij}'s) is at most hr. Since by assumption, each F_{ij} leads to a distinct reaction, $F_{ij} \to F_{ij} + v_{ij}$, it is also an upper bound for the number of reactions in $\mathcal{N}_E$. This infers the upper bound: $n_E \leq 2hr$. We have the following generic relationship:

Proposition 8 If $\mathcal{N}$ is the underlying CRN of a PYK system and $\mathcal{N}_E$ is the associated E-graph then $\delta_E \leq hr - s$.

Proof. We observe that the subspace $(Ker\ \ Y_E \cap Im\ \ I_{a\ E})$ is contained in $I_{a\ E}(Ker\ \ N_E)$, hence $\delta_E \leq dim\ \ I_{a\ E}(Ker\ \ N_E) \leq dim(Ker\ \ N_E) = r_E - s \leq hr - s$. □

Remark 2 An alternative proof is the following: from the above, $\delta_E := n_E - \ell_E - s$. We first consider the case $n_E = 2hr$, i.e. no vertices coincide, then $\ell_E = hr$ and $\delta_E = hr - s$. If two vertices coincide, both the number of vertices and the number of linkage classes are reduced by 1, hence the deficiency remains the same. With each further coincidence of vertices, the number of vertices is reduced by 1, but the number of linkage classes may be reduced by 1 or remain the same (if the vertices are in the same linkage class), hence the deficiency may be further reduced, but the upper bound remains valid.

Corollary 8.1 If $hr = s$, then $\delta_E = 0$ and $h = 1$.

RESULTS ON POSITIVE EQUILIBRIA OF PYK SYSTEMS BASED ON E-GRAPH/EMAK REPRESENTATIONS

This section includes different results that involve positive equilbria of PYK systems based on the associated E-graph. We will start with the case when the associated E-graph of a PYK system is weakly reversible.

Proposition 9 If $(\mathcal{N}, K)$ is a PYK system whose associated E-graph is weakly reversible, then there are rate constants such that $(\mathcal{N}, K)$ has a positive equilibrium.

Proof. If $(\mathcal{N}, K)$ is a PYK system whose associated E-graph is weakly reversible, then the reaction vectors (edge vectors) are positively dependent. With this, for each reaction (edge) (s, s'), there exists a positive number $\kappa_{(s,s')}$ such that

$$\sum_{(s,s')\in E} \kappa_{(s,s')}(s' - s) = 0. \tag{8}$$

Suppose for N, $\{\kappa_{(s,s')}\}_{s\to s'\in\mathcal{R}}$ is a set of positive numbers satisfying (8) and suppose $c \in R_{>}^{S}$ is any positive composition.

We assign to the network the set of the rate constants $\{k_{(s\to s')}\}_{s\to s'\in\mathcal{R}}$ that satisfy

$$k_{(s\to s')}(c^s) = \kappa_{(s,s')}, \forall s \to s' \in \mathcal{R} \tag{9}$$

This leads us to conclude that there are $k \in \mathbb{R}_{>}^{s}$ such that

$$\frac{dx}{dt} = \sum_{(s\to s')} k_{(s\to s')}(c^s)(s' - s) = 0$$

Hence, $(\mathcal{N}, K)$ has a positive equilibrium. □

Recall that a MAK system is weakly reversible and has zero deficiency if and only if it has positive equilibrium for each constant. The next proposition is an EMAK analogue of the said Deficiency Zero Theorem for MAK systems. This involves factor span surjective power law kinetics (PL-FSK).

Proposition 10 If $(\mathcal{N}, K)$ is a PYK system whose associated E-graph is the set of kinetic complexes of a weakly reversible (PL-FSK) system and has zero deficiency, then $(\mathcal{N}, K)$ has a positive equilibrium for each rate constant.

Proof. Let $(\mathcal{N}, K)$ be a PYK system, $(\mathcal{N}_E, K_E)$ be the associated EMAK system, $(\mathcal{N}', K')$ be a PL-FSK system and $\tilde{\mathcal{N}}'$ be the set of kinetic complexes of $(\mathcal{N}', K')$, also an E-graph.

Suppose $\mathcal{N}_E$ be a weakly reversible and $\delta_E(\mathcal{N}_E) = 0$.

By our assumption, $\mathcal{N}_E = \tilde{\mathcal{N}}'$ and weakly reversible. It follows that $\mathcal{N}'$ is also weakly reversible.

Using Müller-Regensburger Criterion (Muller S. and Regensburger G., 2014),

$$0 = \delta_E(\mathcal{N}_E) = \delta(\tilde{\mathcal{N}}') = \tilde{\delta}(\mathcal{N}')$$

implies that there exists a positive equilibrium for $(\mathcal{N}_E, K_E)$ and hence by dynamic equivalence for $(\mathcal{N}, K)$. □

It is then clear that weakly reversibility is an essential property to have a positive equilibrium. Now, it is important to find sufficient conditions for PYK to have a weakly reversible E-graph. The next proposition gives a condition of a PLDS to generate a weakly reversible E-graph. The proof is similar to the proof of Lemma 9.2 of the expository work of Gubberman (2003) on mass action systems and the deficiency zero theorem.

Proposition 11 If a polynomial dynamical system (PLDS) is complex balanced then the E-graph $G = (V, E)$ that generates the system is weakly reversible.

Proof. Suppose $PLDS$ is complex (vertex) balanced. Then there exists an E-graph, $G(V, E)$ that generates the system and there exists a point $\bar{x} \in R_{>0}^{n}$ such that for any vertex $s \in V$ we have

$$\sum_{e=(s,s')\in E} k_e \bar{x}^{s'} = \sum_{e=(s',s)\in E} k_e \bar{x}^{s}. \tag{10}$$

Consider a subset $\mathcal{N}$ of complex (vertex) indices such that, if $s' \in \mathcal{N}, s' \to s$ implies that $s \in \mathcal{N}$. Summing over elements of $\mathcal{N}$ in equation (10) gives

$$\sum_{s\in\mathcal{N}}\sum_{e=(s,s')\in E} k_e\bar{x}^{s'} = \sum_{s\in\mathcal{N}}\sum_{e=(s',s)\in E} k_e\bar{x}^{s}. \tag{11}$$

Clearly,

$$\sum_{s\in\mathcal{N}}\sum_{s'\in\mathcal{N}} k_{(s,s')}\bar{x}^{s'} = \sum_{s\in\mathcal{N}}\sum_{s'\in\mathcal{N}} k_{(s',s)}\bar{x}^{s} \tag{12}$$

is true, since the left-and-right-hand sums are the same. Combining these two equations gives

$$\sum_{s\in\mathcal{N}}\sum_{s'\in\mathcal{N}'} k_{(s,s')}\bar{x}^{s'} = \sum_{s\in\mathcal{N}}\sum_{s'\in\mathcal{N}'} k_{(s',s)}\bar{x}^{s}, \tag{13}$$

where $\mathcal{N}'$ is the set of all complex indices not in $\mathcal{N}$. However, by the definition of $\mathcal{N}$, the right-hand side of equation (13) is zero, since no complexes (vertices) in $\mathcal{N}$ react with complexes (vertices) outside $\mathcal{N}$. That means that the left hand side of the equation is also zero, so the conditions on $\mathcal{N}$ imply that, if $s' \in \mathcal{N}$ and $s \to s'$, then $s \in \mathcal{N}$ as well.

Now, for a complex (vertex) s, define the set s_+ as

$$s_+ = \{v| \text{ there is a directed path from } s \text{ to } v \ (s \Rightarrow v)\}.$$

This set satisfies the properties of $\mathcal{N}$ above, so if $s' \to s$, then $s' \in s_+$. Conversely, assume $s' \Rightarrow s$; then, the transitivity of the operation $\Rightarrow$ implies that $s \Rightarrow s'$; since this is true for all s', the system is weakly reversible. □

Corollary 11.1 If $(\mathcal{N}, K)$ is a PYK system which is mapped to a complex balanced PLDS, then the associated E-Graph is weakly reversible.

The following are extensions of two known theorems from MAK to EMAK systems.

Proposition 12 If an EMAK system has a complex balanced equilibrium, then its underlying network is weakly reversible (Horn, 1972).

Proof. Recall that a digraph is weakly reversible if and only if $ker\ I_a$ contains a positive vector. This is true also for E-graph. The image of the assumed complex balanced equilibrium is such a vector, hence the network is weakly reversible. □

Proposition 13 If an EMAK system has zero deficiency, then any positive equilibrium is complex balanced (Feinberg, 1972).

Proof. Zero deficiency means that $Ker\ Y_E \cap Im\ I_{a\ E}$ is the nullspace, hence the image of any positive equilibrium must be in $Ker\ I_{a\ E}$. □

PYK SYSTEM WITH CYCLE TERMINAL AND t-MINIMAL ASSOCIATED EMAK SYSTEMS

In this section, we study the poly-PL kinetics whose associated EMAK system is the set of kinetic complexes of a weakly reversible PL-FSK system and has zero deficiency. It follows from the results of Müller and Regensburger (2014) that the EMAK system has a complex balanced equilibrium for any set of rate constants.

Characteristics of Cycle Terminal Associated EMAK Systems

Recall that a digraph is cycle terminal if and only if each vertex is a source vertex, i.e. $n_r = n$. Since $n - n_r = t_p$, the number of terminal strong connected components that are single vertices, equivalently, it is a digraph where $t = t_c$, i.e. all terminal strong

connected components are cycles.

For the associated E-graph, this means that all the complexes are of the form s_{ij}, which leads to the following straightforward Proposition:

Proposition 14 An associated E-graph $\mathcal{N}_E$ is cycle terminal if and only if for each s_{ij}, there is another s_{kl} with $s_{ij}-s_{kl} \in r_i(y'_i-y_i)$, $r_i \in \mathbb{R}^m_>$.

For a cycle terminal digraph, S is contained in R and $0 \leq \delta_\rho - \delta \leq \ell$. In the next proposition, we present an upper bound of the deficiency of a cycle terminal E-graph.

Proposition 15 For a cycle terminal E-graph, $\delta_E \leq hr - 1 - s$.

Proof. Note that that hr is an upper bound for the number of s_{ij}'s . With this, $n_E \leq hr$.

The fact that $\ell_E \geq 1$ implies

$$\delta_E = n_E - \ell_E - s_E \leq hr - 1 - s.$$

□

Properties of t-minimal Associated EMAK Systems

For t-minimal E-graphs, we have the following extension of the Subspace Coincidence Theorem of Feinberg and Horn (1977):

Theorem 16 If an E-graph is t-minimal, then $K_E = S_E$.

Proof. Since an E-graph is t-minimal, that is $t_E - \ell_E = 0$, then $Im\ Y_E A_{kE} = S_E$ for all k. Now, we have to show that $K_E = Im\ Y_E A_{kE}$.

Observe that,

$$\begin{aligned} K_E &= span(Im\ f_E) \\ &= span(Y_E A_{kE} \psi_E(R^{\mathcal{S}})) \\ &= Y_E \cdot A_{kE}(\psi(R^{\mathcal{S}})) \\ &= Y_E I_{aE} I_{kE}(R^{\rho(\mathcal{R})}) \\ &= Y_E I_{aE}\ diag(k) \rho'_E(R^{\rho(\mathcal{R})}) \\ &= Y_E I_{aE}\ diag(k) \rho'_E(R^{\mathcal{C}}) \\ &= Y_E I_{aE} I_{kE}(R^{\mathcal{C}}) \\ &= Y_E \cdot A_{kE}(R^{\mathcal{C}}) \\ &= Y_E(Im\ A_{kE}) = Im\ Y_E A_{kE}. \end{aligned}$$

□

The proof is adapted from Theorem 2 of the paper of Arceo et. al (2015).

In a nonbranching network, $n_r = r$. If a network is nonbranching then it is t-minimal. Now, combining these properties to a cycle terminal E-graph, we have the following result.

Proposition 17 If the E-graph is cycle terminal and nonbranching, then $n_E = hr$.

Proof. If an E-graph is cycle terminal, then $n_E = n_{r\,E}$. Suppose it is also nonbranching. This implies that $n_{r\,E} = r_E = hr$. Hence, $n_E = hr$. □

Since a weakly reversible network is cycle terminal, Proposition 17 is true for weakly reversible nonbranching E-graph.

THE ASSOCIATED E-MAK SYSTEMS OF A CLASS OF PYK-SSK SYSTEMS

Recall that for a mono-PL kinetics, complex factorizability is equivalent to equality of the kinetic complexes (also called "kinetic order vectors" or "interactions" for PLK systems) and coefficients if two reactions have the same reactant complex. Factor span surjectivity in addition is equivalent to the converse implication. For any complex factorizable kinetics, the network is span surjective if

and only if it is nonbranching and K is factor span surjective.

First, we introduce a new term as follows:

Definition 10 A poly-PL system is **integral** if all its coefficients a_{ij} are positive integers. For a mono-PL system, we write a_i for a_{i1}.

We simplify the double indices "$i1$" to "i", i.e. $F_i = F_{i1}$, etc. where $i = 1, \dots, r$.

In the next proposition, we compare systems involving integral mono-PL kinetics.

Proposition 18 Let $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ be a cycle terminal CRN, and $\rho, \pi : \mathcal{R} \to C$ the reactant and product maps, respectively. Furthermore, let K be an integral mono-PL kinetics with the following properties:

i. K is span surjective.

ii. For each i, $F_i = F_j + a_j(y'_j - y_j)$ for $j \neq i$ if and only if $\pi(r_j) = \rho(r_i)$.

Then the associated E-MAK system $\mathcal{N}_E$ is the set of kinetic complexes of the system $\mathcal{N}' = (\mathcal{S}, \mathcal{C}', \mathcal{R}')$ where $\mathcal{R}'$ consists of the reactions $r'_i : a_i y_i \to a_i y'_i$ for each $r_i : y_i \to y'_i$ in $\mathcal{R}$ and $K'_{ri'}(x) = \frac{1}{a_i} K_{ri}(x)$. The nonbranching $\mathcal{N}$, $\mathcal{N}'$ and $\mathcal{N}_E$ are isomorphic as digraphs, and $N' = N\ diag(a)$ and $K' = diag(\frac{1}{a})K$, where $a = (a_1, \dots, a_r)$, so that all network and kinetic properties coincide.

Proof. Condition (i) infers that $\mathcal{N}$ is necessarily nonbranching. The first part is to show that $\mathcal{N} \cong \mathcal{N}' \cong \mathcal{N}_E$ as digraphs.

(a) Note that the vertices in $\mathcal{N}_E$ are F_i's and the arcs the reactions $F_i \to F_i + V_i$ where V_i's are the reaction vectors $a_i(y'_i - y_i)$ for each reaction in $\mathcal{N}'$, $r'_i : a_i y_i \to a_i y'_i$ of R'.

Define $\gamma : \mathcal{N} \to \mathcal{N}_E$ where $\gamma(\pi(r_j)) = F_i$. Now, considering condition (ii), it will lead to $\gamma(V) = V_E$ and $\gamma(A) = A_E$ ($\gamma(\mathcal{R}) = \mathcal{R}_E$). Thus, $\mathcal{N} \cong \mathcal{N}_E$.

(b) Also, we define $\omega : \mathcal{N} \to \mathcal{N}'$ where $\omega(y_i) = a_i y_i$. This implies that $\omega(V) = V'$ and $\omega(A) = A'$ ($\omega(\mathcal{R}) = \mathcal{R}'$) where A is the sets of arcs. Hence, $\mathcal{N} \cong \mathcal{N}'$.

By (a) and (b), $\mathcal{N} \cong \mathcal{N}_E \cong \mathcal{N}'$.

As a result, since $r'_i : a_i y_i \to a_i y'_i$ for each $r_i : y_i \to y'_i$ in R and $K'_{r'_i}(x) = \frac{1}{a_i} K_{r_i}(x)$ then $N' = N\ diag(a)$ and $K' = diag(1/a)K$, where $a = (a_1, \dots, a_r)$. □

Remark 3 We call the set of power law kinetics fulfilling (i) and (ii), **PL-ESK (ESK = EMAK Similar Kinetics)**. For these kinetics, $\mathcal{N}' = \mathcal{N}$. MAK systems always satisfies (ii) In fact, for these, the Craciun map is the identity, i.e. $(\mathcal{N}, K) = (\mathcal{N}_E, K_E)$. However, only span surjective MAK systems belong to MAK-ESK.

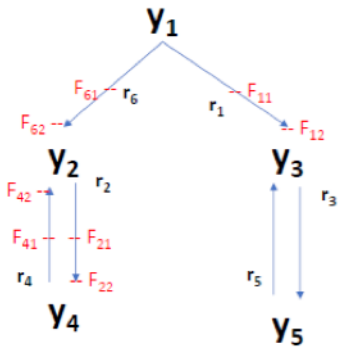
Corollary 18.1 For mono-PL systems satisfying assumptions (i) and (ii) of Proposition 18 , $\delta' = \delta = \delta_E$.

Proof. Since $\mathcal{N}' = \mathcal{N}\ diag(a)$, $S' = Im\ N' = Im\ N = S = S_E$. Since the digraphs are isomorphic, $n' - \ell' = n - \ell = n_E - \ell_E$, which proves the claim. □

We can clearly extend the kinetic deficiency concept of Müller and Regensburger from PLK to mono-PL systems, and conclude from the above that also $\delta = \tilde{\delta} = \tilde{\delta}'$. In particular, if N is weakly reversible and has zero deficiency, then it has complex balanced equilibria for each set of rate constants. Due to the dynamic equivalence and equal deficiency with N', the latter also has complex balanced equilibria for each set of rate constants. If N has positive deficiency, then the criterion for the existence of complex balanced equilibria of M*ü*ller-Regensburger for positive kinetic deficiency can be applied.

At this point, we extend our scope to CF integral poly-PL systems ($h > 1$). We first

consider an example of a bi-PL system to appreciate the challenge of extending the result to higher term numbers ($h > 1$). To relate network properties to its EMAK, we need to be able to map a reaction to a construct in the latter. One way to do this is to take the pair (F_{i1}, F_{i2}) of reaction r_i which we call the kinetic complex vector of the reaction and require that F_{i2} is the product of the reaction with reactant F_{i1}, or equivalently, $F_{i2} = F_{i1} + v_{i1} = F_{i1} + a_{i1}(y_i' - y_i)$.



However, we immediately see a potential difficulty: if two kinetic complexes are equal, then the topology of the E-graph will differ (maybe substantially) from that of the CRN. For example, branching reactions r_1 and r_6 will be identified or if $F_{41} = F_{21}$, two reversible reactions result from one. A simple way (it may not be the only one) to prevent such complications is to require that the kinetics be maximally span surjective, i.e. the kinetic complexes are pairwise distinct. This hypothesis has two immediate consequences: $\mathcal{N}$ and $\mathcal{N}_E$ are necessarily non-branching. Clearly, as in the mono-PL case, we need Property (ii) for all reactions, e.g. $F_{41} = F_{62} + v_{62}$. Hence, an extension of the previous result to PYK systems with $h > 1$ is the following:

Proposition 19 Let $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ be a cycle terminal CRN, and $\rho, \pi : \mathcal{R} \to \mathcal{C}$ the reactant and product maps respectively. Furthermore, let K be an integral poly-PL kinetics with the following properties:

i. K is maximally span surjective;

ii. for each i, $F_{i1} = F_{jh} + a_{jh}(y_j' - y_j)$ for $j \neq i$ iff $\pi(r_j) = \rho(r_i)$;

iii. for each i, $F_{i(j+1)} = F_{ij} + a_{ij}(y_i' - y_i)$ for $j = 1, \ldots, h-1$.

Then the associated E-MAK system $\mathcal{N}_E$ is the set of kinetic complexes of an integral mono-PL system $\mathcal{N}' = (\mathcal{S}, \mathcal{C}', \mathcal{R}')$ where $\mathcal{R}'$ consists of the reactions $r_{ij}' : a_{ij}y_i \to a_{ij}y_i'$ for each $r_i : y_i \to y_i'$ in $\mathcal{R}$ and $K'_{r_{ij}'}(x) = \frac{1}{a_{ij}} K_r(x)$. Hence, $\ell = \ell_E$, $\mathcal{N}'$ and $\mathcal{N}_E$ are isomorphic as digraphs, and $\mathcal{N}'$ is the $m \ x \ hr$ matrix $(N_1, N_2, \ldots, N_n)$, where $N_j = N \ diag(a_j)$, $a_j = (a_{ij}, \ldots, a_{rj}$ and $K_j' = diag(\frac{1}{a_j})K$.

Proof. Condition (i) implies that the kinetic complexes are pairwise distinct. With this, $\mathcal{N}$ and $\mathcal{N}_E$ are necessarily non-branching. Hence, $\ell = \ell_E$.

Define $\omega : \mathcal{N}_E \to$ where $\omega(F_{ij}) = a_{ij}y_i$. Using conditions (ii) and (iii), we have $\omega(V_E) = V'$ and $\omega(A_E) = A'$ ($\omega(\mathcal{R}_E) = \mathcal{R}'$). Hence, $\mathcal{N}_E \cong \mathcal{N}'$. We need condition (ii) as in the mono-PL case in Proposition 19.

Since $\mathcal{N}'$ is an integral mono-PL system, every j^{th}term in an integral poly-PL kinetics of each reaction corresponds to $N_j = N \ diag(a_j)$ where $a_j = (a_{ij}, \ldots, a_{rj})$. Hence, N' is $n \times hr$ matrix of the form $(N_1 \ N_2 \cdots N_h)$. □

Corollary 19.1 For PYK systems with $h > 1$, $\delta' = \delta_E = (h-1)n + \delta$.

Proof. Observe that

$$\delta' = \delta_E = n_E - \ell_E - s_E = hn - \ell - s = (h-1)n + \delta.$$

□

Remark 4 Note that Proposition 19 is an extension of Proposition 18 for nonbranching $\mathcal{N}$ since K maximally span surjective implies that it is span surjective which for CF systems is equivalent to $\mathcal{N}$ nonbranching and K factor span surjective. Note also that for $h = 1$, $\delta_E = (1-1)n + \delta = \delta$.

SUMMARY AND CONCLUSION

The topics covered in this paper are motivated by the fact that poly-PL kinetics generate power law dynamical systems, which via a method introduced by G. Craciun can be mapped to EMAK systems using E-graph. A map from PYK to EMAK or Craciun's E-graph is shown to establish some network relationships. From this, we identify results on positive equilibria of PYK systems based on their E-graph/EMAK representations. Our main structural results show the coincidence of the stoichiometric subspaces of the network and its associated E-graph as well as the conservation of the positive dependency, which is a necessary condition for the existence of positive equilibria. Analysis were also done on cases where the associated E-grpah is t-minimal and cycle terminal.

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Appendix

List of Acronyms

CF	complex factorizable
CKS	chemical kinetic system
CRN	chemical reaction network
CRNT	chemical reaction network theory
DZT	deficiency zero theorem
EMAK	embedded mass action kinetics
FSK	factor span surjective
MAK	mass action kinetics
ODE	ordinary differential equations
POK	polynomial kinetic system
PLDK	polynomial dynamical systems
PLK	power law kinetics
PL-ESK	power-law EMAK similar kinetics
PL-NDK	power-law non-reactant determined kinetics
PL-RDK	power-law reactant determined kinetics
PSK	power law kinetics system
PYK	poly-PL Kinetics
RID	rate constant-interaction map-decomposable
RDK	reactant determined kinetics
SFRF	species formation rate function

List of Symbols

(N, K)	Chemical Kinetic System
A_k	Laplacian map
$A_{k\ E}$	Laplacian map (E-graph)
$A(D)$	set of arcs
D	Digraph
$E_+(N, K)$	Set of positive equilibria
F	Kinetic Order Matrix
I_a	Incidence map
$I_{a\ E}$	Incidence map (E-graph)
K	Kinetics of a CRN
K_E	Kinetics of a CRN (E-graph)
K_{ij}	rate function
N	Stoichiometric map
R	Reactant Subspace

S	Stoichiometric Subspace
S_E	Stoichiometric Subspace (E-graph)
$V(D)$	set of vertices
Y	Map/matrix of complexes
Y_E	Map/matrix of complexes
$Z_+(N,K)$	Set of positive balanced steady states
δ	Deficiency of a CRN
δ_ρ	Reactant Deficiency
$\delta_{\rho\ E}$	Reactant Deficiency (E-graph)
ℓ	Number of lingkage classes
$\mathcal{C}$	Set of complexes
$\mathcal{K}$	Type of RID Kinetics
$\mathcal{R}$	Set of reactions
$\mathcal{S}$	Set of species
$N = \mathcal{S}, \mathcal{C}, \mathcal{R})$	Chemical Reaction Network
π	Product map
ρ	Reactant map
$\tau(N) = t - \ell$	terminality of the network
$\tau(G)_E = t - \ell$	terminality of the network (E-graph)
$\Delta(N)$	rank difference
$\Delta(G)_E$	rank difference (E-graph)
$i \to j$ or (i,j)	i reacts to j
e	Edge in E-graph
k	Rate vector
m	Number of species
n	Number of complexes
n_E	Number of complexes (E-graph)
n_r	Number of reactants
p_K	parameter map
q	Reactant Rank
r	Number of reactions
r_E	Number of reactions (E-graph)
s	Rank of a CRN
s_E	Rank of a CRN (E-graph)
$s\ell$	Number of strong linkage classes
$s\ell$	Number of strong linkage classes (E-graph)
$s(e)$	Source Vertex in E-graph
$t(e)$	Target Vertex in E-graph
t	Number of terminal strong linkage classes
t_c	number of cycle-terminal classes
t_p	number of point-terminal classes
$v(e)$	Edge Vector in E-graph