An algorithm for finding weakly reversible deficiency zero realizations of polynomial dynamical systems

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Abstract

Systems of differential equations with polynomial right-hand sides are very common in applications. On the other hand, their mathematical analysis is very challenging in general, due to the possibility of complex dynamics: multiple basins of attraction, oscillations, and even chaotic dynamics. Even if we restrict our attention to mass-action systems, all of these complex dynamical behaviours are still possible. On the other hand, if a polynomial dynamical system has a weakly reversible deficiency zero ($WR_0$) realization, then its dynamics is known to be remarkably simple: oscillations and chaotic dynamics are ruled out and, up to linear conservation laws, there exists a single positive steady state, which is asymptotically stable. Here we describe an algorithm for finding $WR_0$ realizations of polynomial dynamical systems, whenever such realizations exist.

1 Introduction

By a polynomial dynamical system we mean a system of ODEs with polynomial right-hand side, of the form

$$\frac{dx_1}{dt} = p_1(x_1, \ldots, x_n),$$
$$\frac{dx_2}{dt} = p_2(x_1, \ldots, x_n),$$
$$\quad \vdots$$
$$\frac{dx_n}{dt} = p_n(x_1, \ldots, x_n),$$

where $p_i(x_1, \ldots, x_n) \in \mathbb{R}[x_1, \ldots, x_n]$. In general, such systems are very difficult to analyze due to nonlinearities and feedback that may give rise to bifurcations, multiple basins of attraction, oscillations, and even chaotic dynamics. The second part of Hilbert’s 16th problem (about the number of limit cycles of polynomial dynamical systems in the plane) is still essentially unsolved, even for quadratic polynomials [25]. Even the simplest object associated to (1), its steady state set, is central to real algebraic geometry.

In terms of applications, polynomial dynamical systems often show up in, for example, chemistry, biology, and population dynamics. In these models, the variable $x_i$ typically represents concentration, population, or another quantity that is strictly positive, so the domain of (1) is
restricted to the positive orthant. For example, in an infectious disease model, an infectious individual might covert a susceptible individual; this would contribute a “+ bxy” term to \( \frac{dx}{dt} \), where \( x \) is the population of susceptible individuals, \( y \) the infectious population, and \( b > 0 \) a parameter measuring the contact rate. Collecting all contributing terms results in an interaction network. An active area of research is to relate the structure of the interaction network to the dynamics generated by it [3, 4, 26–29, 32, 33, 37].

Conversely, one may start with (1) from experimental data, with little or no information on the generating interaction network. One may try to elucidate the underlying interaction network; however, without additional assumptions, a polynomial dynamical system is not uniquely generated by one interaction network, but infinitely many [14]. This lack of identifiability of the underlying network can actually be leveraged to analyze the dynamics: if a network with certain properties can be found to generate (1), then we may be able to immediately infer its dynamical behaviour.

A class of systems whose dynamics is very well understood is the family of complex-balanced systems [24], which are also called toric dynamical systems [9]. They can never exhibit oscillations or chaotic dynamics, and, up to linear conservation laws, there exists a single positive steady state, which is locally asymptotically stable [24]. Moreover, this steady state is conjectured to be a global attractor [23].

Not only are the dynamical properties of complex-balanced systems well understood, but also the network and parameter structures that characterize them [21]. While in general, there are algebraic conditions on the parameters necessary for complex-balancing, the exception to this rule is the case of weakly reversible and deficiency zero (WR\(_0\)) networks – these systems are complex-balanced for any choices of parameters, in a sense that will be made clear below. This fact is very important in applications, because the exact values of the coefficients in the polynomial right-hand sides of these dynamical systems are often very difficult to estimate accurately in practice.

In this paper we describe an efficient algorithm for determining whether a given polynomial dynamical system admits a WR\(_0\) realization, and for finding such a realization whenever it exists (see Algorithm 1). Our algorithm does not require solving the differential equation (1), nor does it require solving for its steady state set. Instead, the algorithm, making use of the geometric and log-linear structure of WR\(_0\) networks, requires as its inputs only the monomials and the matrix of coefficients. If a WR\(_0\) realization exists, in Theorem 3.12 we provide a bijection between the positive steady state set of (1) and the solution to a system of linear equations.

The paper is organized as follows. In Section 2 we introduce interaction networks as embedded in \( \mathbb{R}^n \) and formalize their relations to polynomial dynamical systems; we also introduce complex-balanced systems, WR\(_0\) networks, and other relevant notions and results. In Section 3.1 we describe our algorithm for finding a WR\(_0\) realization of a given polynomial dynamical system, whose steady state set is studied in Section 3.2. Our algorithm applies to the case of where the coefficients in the polynomials are unspecified; we consider such systems in Section 3.3.

## 2 Background

Throughout this work, we denote by \( \mathbb{R}^n_\geq \) and \( \mathbb{R}^n_\succ \) the sets of vectors with non-negative and positive entries respectively. Similarly, \( \mathbb{Z}^n_\geq \) is the set of vectors with non-negative integer components. Vectors are typically denoted \( \mathbf{x}, \mathbf{y}, \) or \( \mathbf{w} \). We denote by \( \dot{\mathbf{x}} \) the time-derivative \( \frac{d\mathbf{x}}{dt} \). For any \( \mathbf{x} \in \mathbb{R}^n_\succ \) and \( \mathbf{y} \in \mathbb{R}^n \), define the operation \( \mathbf{x}^\mathbf{y} = x_1^{y_1} x_2^{y_2} \cdots x_n^{y_n} \). If \( \mathbf{Y} = (y_1 \ y_2 \ \cdots \ y_n) \),
then $x^Y = (x^{y_1}, x^{y_2}, \ldots, x^{y_n})^\top$. The support of a vector $x \in \mathbb{R}^n$ is the set of indices $\text{supp}(x) = \{i: x_i \neq 0\}$.

2.1 Dynamical systems and Euclidean embedded graphs

In this section, we introduce the Euclidean embedded graph (E-graph), a directed graph in $\mathbb{R}^n$, and explain how a system of differential equations with polynomial right-hand side (a polynomial dynamical system) is defined by it.

Definition 2.1. A Euclidean embedded graph (E-graph) in $\mathbb{R}^n$ is a directed graph $(V, E)$, where $V$ is a finite subset of $\mathbb{R}^n_{\geq 0}$, and there are neither self-loops nor isolated vertices. Denote by $V_s$ the set of source vertices.

Let $V = \{y_1, y_2, \ldots, y_m\}$. An edge $(y_i, y_j)$, or $(i, j) \in E$, is also denoted $y_i \rightarrow y_j$. Since vertices are points in $\mathbb{R}^n$, an edge can be regarded as a bona fide vector between vertices. An edge vector $y_j - y_i$ is associated to the edge $y_i \rightarrow y_j$.

For the purpose of using E-graphs to study polynomial dynamical systems, we assume $V_s \subset \mathbb{Z}^n_{\geq 0}$, even though most results stated in this paper hold for $V \subset \mathbb{R}^n_{\geq 0}$.

The set of vertices $V$ of $(V, E)$ is partitioned by its connected components, which we identify by the subset of vertices that belong to that connected component. If every connected component is strongly connected, i.e., every edge is part of a cycle, then $(V, E)$ is said to be weakly reversible.

Two geometric properties of the E-graph will become important to our analysis of polynomial dynamical systems. The first is a notion of affine independence within each connected component; the second is a notion of linear independence between connected components.

Definition 2.2. An E-graph $(V, E)$ has affinely independent connected components if the vertices in each connected component are affinely independent, i.e., if $\{y_0, y_1, \ldots, y_r\} \subseteq V$ is a connected component, then the set $\{y_j - y_0: j = 1, 2, \ldots, r\}$ is linearly independent.

Definition 2.3. Let $(V, E)$ be an E-graph. For any $U \subseteq V$, the associated linear subspace of $U$ is $S(U) = \text{span}\{y_j - y_i: y_i, y_j \in U\}$. The associated linear space\(^1\) of $(V, E)$ is

$$S = \text{span}\{y_j - y_i: y_i \rightarrow y_j \in E\}.$$ 

If $U$ defines a connected component of $(V, E)$, then $S(U) \subseteq S$. Indeed, if $V_1, V_2, \ldots, V_\ell$ are the connected components, then $S = S(V_1) + S(V_2) + \cdots + S(V_\ell)$.

Thus far, we have defined an E-graph, and introduced several objects and properties associated to it. We now turn our attention to how such a graph is canonically associated to dynamics, by assigning a positive weight to each edge.

Definition 2.4. Let $(V, E)$ be an E-graph. For each $y_i \rightarrow y_j \in E$, let $\kappa_{ij} > 0$ be its weight, and let $\kappa = (\kappa_{ij}) \in \mathbb{R}^E_{\geq 0}$. The associated dynamical system on $\mathbb{R}^n_{\geq 0}$ of the weighted E-graph $(V, E, \kappa)$ is

$$\frac{dx}{dt} = \sum_{(i,j) \in E} \kappa_{ij} x^{y_i}(y_j - y_i). \quad (2)$$

\(^1\)In reaction network theory literature, the associated linear space is called the stoichiometric subspace of the network.
It is sometimes convenient to refer to $\kappa_{ij}$ even though $y_i \rightarrow y_j$ may not be an edge in the network. In such cases, set $\kappa_{ij} = 0$.

**Remark 2.5.** We defined the domain of (2) to be $\mathbb{R}^n_>$. Systems of ODEs with polynomial right-hand side do not in general leave $\mathbb{R}^n_>$ forward-invariant, but if we assume $V \subset \mathbb{Z}^n_\geq$, the positive orthant $\mathbb{R}^n_\geq$ is indeed forward-invariant under (2) [35].

It is clear that the right-hand side of (2) lies in the associated linear space $S$, so any solution to (2) is confined to a translate of $S$. By the above remark, any solution to (2) where $V \subset \mathbb{Z}^n_\geq$ with initial condition $x_0 \in \mathbb{R}^n_>$ is confined to $(x_0 + S) \cap \mathbb{R}^n_\geq$, which is called the invariant polyhedron of $x_0$.

**Figure 1: Weighted E-graphs from Example 2.6.**

**Example 2.6.** We illustrate the notions and notations defined above. Figure 1 shows three examples of weighted E-graphs. The graphs in Figures 1(a) and 1(b) are weakly reversible, but that in Figure 1(c) is not. The graph in Figure 1(a) has two connected components, each of which is affinely independent; however, those in Figures 1(b) and 1(c) do not have affinely independent connected components.

The associated dynamical system of Figure 1(a) is

$$\frac{d}{dt} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 3 \begin{pmatrix} 2/2 \\ -2/2 \end{pmatrix} + 5x_1 \begin{pmatrix} -2 \\ -2 \end{pmatrix} + 2x_1^2 \begin{pmatrix} -2 \\ -2 \end{pmatrix} + 3x_2^2 \begin{pmatrix} 2 \\ -2 \end{pmatrix}$$

$$= \begin{pmatrix} 6 - 10x_1^2 - 4x_1^2x_2^2 + 6x_2^2 \\ 6 + 10x_1^2 - 4x_1^2x_2^2 - 6x_2^2 \end{pmatrix}. \quad (3)$$

The source vertices play the role of exponents in the monomials, thus the set of source vertices $V_s$ determines the monomials in the associated dynamical system.

It so happens that the weighted E-graphs in Figures 1(b) and 1(c) also have (3) as their associated dynamical systems. We say that the three weighted E-graphs in Figure 1 are dynamically equivalent, and the weighted graphs are realizations of the dynamical system (3); we define these terms precisely in Definition 2.9. This example demonstrates that while a weighted E-graph is associated to a unique dynamical system, the converse is not true; there is in general infinitely many realizations of a given polynomial dynamical system [14]. This work is concerned with finding a realization that guarantee certain algebraic and stability properties.

Another way to study the vector field generated by (2) is to use a linear combination of some fixed vectors, one for each monomial, with the coefficients given by the strength of the monomials at that point. We give a name to those fixed vectors.
Definition 2.7. Let \((V, E, \kappa)\) be a weighted E-graph, and \(y_i \in V_s\). The **net direction vector** from \(y_i\) is

\[
    w_i = \sum_{y_j \in V} \kappa_{ij}(y_j - y_i).
\]

The **matrix of net direction vectors** of \((V, E, \kappa)\) is

\[
    W = \begin{pmatrix} w_1 & w_2 & \cdots & w_m \end{pmatrix}.
\]

For convenience, we may refer to the net direction vector even if \(y_i \notin V_s\); in this case, let the net direction vector be zero. Such a net direction vector will not show up as a column of \(W\).

The matrix \(W\) from Definition 2.7 is also well defined when we start not with a weighted E-graph, but with a fixed polynomial dynamical system of the form

\[
    \frac{dx}{dt} = \sum_{i=1}^{m} x^i w_i. \tag{4}
\]

Note that any polynomial dynamical systems can be uniquely written as such, for some \(y_1, y_2, \ldots, y_m \in \mathbb{Z}_+^n\) distinct, and \(w_1, w_2, \ldots, w_m \in \mathbb{R}^n\) non-zero.

Definition 2.8. Consider the polynomial dynamical system (4). The **matrix of source vertices** \(Y_s\) and the **matrix of net direction vectors** \(W\) of (4) are

\[
    Y_s = \begin{pmatrix} y_1 & y_2 & \cdots & y_m \end{pmatrix} \quad \text{and} \quad W = \begin{pmatrix} w_1 & w_2 & \cdots & w_m \end{pmatrix}.
\]

Clearly, \(\dot{x} = W x Y_s\).

Thus far, we start with a weighted E-graph \((V, E, \kappa)\), and from it, define a dynamical system. The goal of the present work is the converse direction: start with a polynomial dynamical system, find some \((V, E, \kappa)\), ideally with certain properties, that gives rise to such dynamics. For example, (4) is generated by the graph \(y_i \xrightarrow{1} y_i + w_i\), for \(i = 1, 2, \ldots, m\). As Example 2.6 illustrates, there are in general many weighted E-graphs that can generate the same dynamics.

Definition 2.9. A **realization** of a polynomial dynamical system \(\dot{x} = f(x)\) is a weighted E-graph \((V, E, \kappa)\) whose associated dynamical system is precisely \(\dot{x} = f(x)\). Two realizations of \(\dot{x} = f(x)\) are said to be **dynamically equivalent**.

Lemma 2.10 ([10, Definition 2.6]). The weighted E-graphs \((V, E, \kappa)\) and \((V', E', \kappa')\) are dynamically equivalent if and only if the net direction vector from \(y_i\) in \((V, E, \kappa)\) coincides with that in \((V', E', \kappa')\), for all \(y_i \in V_s \cup V'_s\).

Proof. This follows from the linear independence of monomials as functions on \(\mathbb{R}_+^n\).

2.2 Complex-balanced systems and WR\(_0\) systems

General polynomial dynamical systems can display a wide range of dynamical behaviours, ranging from stable or unstable steady states, limit cycles, and even chaos. In this work, we are interested in the family of **complex-balanced systems**, which enjoy various algebraic and stability properties.
Definition 2.11. Let \((V, E, \kappa)\) be a weighted E-graph in \(\mathbb{R}^n\), and let \(\dot{x} = f(x)\) be its associated dynamical system. A state \(x^* \in \mathbb{R}^n_+\) is said to be a \textit{positive steady state} if \(f(x^*) = 0\). Let \(V_>(f)\) be the set of positive steady states. A state \(x^* > 0\) is a \textit{complex-balanced steady state} if at every \(y_i \in V\), we have

\[
\sum_{(i,j) \in E} \kappa_{ij}(x^*)^y_i = \sum_{(j,i) \in E} \kappa_{ji}(x^*)^y_j.
\]

The equations above can be interpreted as balancing the fluxes flowing across the vertex \(y_i\). If a weighted E-graph \((V, E, \kappa)\) admits one complex-balanced steady state, then every positive steady state is complex-balanced [24]; such a \((V, E, \kappa)\) is called a \textit{complex-balanced system}.

These systems first arose from the study of chemical systems under mass-action kinetics, as a generalization of thermodynamic equilibrium. The following theorem lists some of the most important results about complex-balanced systems. For more details, see [16, 20, 38].

Theorem 2.12 ([24]). Let \((V, E, \kappa)\) be a complex-balanced system, with steady state \(x^* \in \mathbb{R}^n_+\), and associated linear space \(S\). Then the following are true:

(i) All positive steady states are complex-balanced, and there is exactly one steady state within each invariant polyhedron.

(ii) Any complex-balanced steady state \(x\) satisfies \(\ln x - \ln x^* \in S^\perp\).

(iii) The function

\[
L(x) = \sum_{i=1}^n x_i (\ln x_i - \ln x_i^* - 1),
\]

defined on \(\mathbb{R}^n_+\), is a strict Lyapunov function within each invariant polyhedron \((x_0 + S) \cap \mathbb{R}^n_+\), with a global minimum at the corresponding complex-balanced steady state.

(iv) Every complex-balanced steady state is asymptotically stable with respect to its invariant polyhedron.

Beside these properties, complex-balanced systems enjoy other remarkable algebraic and dynamical properties. For example, the set of positive steady states \(V_>(f)\) admits a monomial parametrization [9, 32]. Each positive steady state \(x^*\) is in fact linearly stable with respect to its invariant polyhedron [7, 34]. Complex-balanced systems are also conjectured to be persistent and permanent\(^2\) [13]. Moreover, the unique steady state is conjectured to be globally stable within its invariant polyhedron [23]. The Persistence and Permanence Conjectures have been proved in several cases, such as when there is only one connected component [1, 6], or the ambient state space is \(\mathbb{R}^2\) [13], or the E-graph is strongly endotactic [19], or the associated linear space \(S\) is of dimension two and all trajectories are bounded [31]. The Global Attractor Conjecture has also been proved if there is only one connected component [1, 6], or the E-graph is strongly endotactic [19], or the ambient state space is \(\mathbb{R}^3\) [13], or when the associated linear space \(S\) is of dimension at most three [31].

\(^2\)Roughly speaking, persistence is the property that starting in \(\mathbb{R}^n_+\), the solution is always bounded away from the boundary of \(\mathbb{R}^n_+\), and permanence occurs when solutions always converge to a compact subset of the invariant polyhedron.
Besides dynamical stability, complex-balanced systems are characterized graph-theoretically and algebraically. Horn proved in [22] that \((V, E, \kappa)\) is complex-balanced if and only if \((V, E)\) is weakly reversible and \(\kappa\) satisfies some algebraic equations, the number of which is measured by a non-negative integer called the deficiency of \((V, E)\).

**Definition 2.13.** Let \((V, E)\) be an E-graph with \(\ell\) connected components, and let \(S\) be its associated linear space. The **deficiency** of \((V, E)\) is the integer \(\delta = |V| - \ell - \dim S\).

The notion of deficiency can also be applied to the connected components. Suppose \(V_1, V_2, \ldots, V_\ell\) are the connected components of \((V, E)\). The **deficiency of a connected component** \(V_p\) is \(\delta_p = |V_p| - 1 - \dim S(V_p)\). It is easy to see that

\[
\delta \geq \sum_{p=1}^{\ell} \delta_p,
\]

with equality if and only if \(S(V_1), S(V_2), \ldots, S(V_\ell)\) are linearly independent. If \(\delta = 0\), then necessarily \(\delta_p = 0\) for all \(p\).

If \((V, E)\) is weakly reversible and \(\delta = 0\), then the associated dynamical system is always complex-balanced, regardless of the choice of \(\kappa\). This result is known as the Deficiency Zero Theorem [15,21]. The deficiency is a property of the E-graph, not of the associated dynamical system, yet in the case of deficiency zero, it has strong implications on the dynamics. The goal of this paper is to search for weakly reversible and deficiency zero (WR\(_0\)) realizations for polynomial dynamical systems, which are automatically complex-balanced, and therefore obey the properties listed in Theorem 2.12.

Deficiency also has a geometric interpretation; \(\delta = 0\) if and only if \((V, E)\) has affinely independent connected components \(S_1, S_2, \ldots, S_\ell\), and the subspaces \(S(V_1), S(V_2), \ldots, S(V_\ell)\) are linearly independent [12, Theorem 9]. Later we make use of this interpretation when searching for WR\(_0\) realizations.

The system (2) admits a matrix decomposition that aids in studying complex-balanced steady states. For a weighted E-graph \((V, E, \kappa)\) where \(|V| = m\), its associated dynamical system (2) can be decomposed be as \(\dot{x} = YA_\kappa x^Y\) [24], where

\[
Y = \begin{pmatrix} y_1 & y_2 & \cdots & y_m \end{pmatrix}
\]

is a matrix whose columns are the vertices (including both sources and targets); \(x^Y\) is the vector of monomials whose \(i\)th component is \(x^{y_i}\), and the **Kirchoff matrix**

\[
[A_\kappa]_{ij} = \begin{cases} 
\kappa_{ji} & \text{if } y_i \to y_j \in E \\
-\sum_r \kappa_{jr} & \text{for } i = j \\
0 & \text{otherwise}
\end{cases}
\]

is the negative transpose of the graph Laplacian of \((V, E, \kappa)\). In general, the \(i\)th component of \(A_\kappa x^Y\)

\[
[A_\kappa x^Y]_i = \sum_{(j,i) \in E} \kappa_{ji} x^{y_j} - x^{y_i} \sum_{(i,j) \in E} \kappa_{ij}
\]

measures the net flux passing through the \(i\)th vertex, so a complex-balanced steady state \(x^*\) is a solution to the equation \(A_\kappa(x^*)^Y = 0\).
A subgraph \((V_0, E_0) \subseteq (V, E)\) is a \textbf{terminal strongly connected component} if it is strongly connected, and there does not exist an edge in \(E\) from a vertex in \(V_0\) to a vertex in \(V \setminus V_0\). The kernel of \(A_\kappa\) is supported on the terminal strongly connected components:

**Theorem 2.14** ([18]). Let \(A_\kappa\) be the Kirchoff matrix of \((V, E, \kappa)\) with terminal strongly connected components \(V_1, V_2, \ldots, V_t\). There exists a basis \(\{c_1, c_2, \ldots, c_t\}\) for \(\ker A_\kappa\) with \(c_p \in \mathbb{R}^n_{\geq}\) and

\[
\begin{cases}
[c_p]_i > 0 & \text{if } y_i \in V_p, \\
[c_p]_i = 0 & \text{otherwise.}
\end{cases}
\]

According to the Matrix-Tree Theorem [9, 21], there is an explicit formula for the entries of \(c_p\). Each non-zero \([c_p]_i\) is a polynomial of \(\kappa_{ij}\) with positive coefficients, given by the maximal minors of \(A_\kappa\) [9, 30, 36].

If \((V, E)\) is weakly reversible, then \(\delta = \dim(\ker Y \cap \im A_\kappa)\). More generally, \(\dim(\ker Y \cap \im A_\kappa) = |V| - \ell - t\), when \((V, E, \kappa)\) has \(t\) terminal strongly connected components [18]. Therefore if \((V, E)\) is VR\(_0\), then \(\ker (YA_\kappa) = \ker A_\kappa\), and the matrix of net direction vectors \(W\) coincides with \(YA_\kappa\) (see Lemma 3.1).

For the purpose of this work, we assume that we are given \(W\) and the matrix of source vertices \(Y_s\), but we do not know the decomposition of \(W\) into the product \(YA_\kappa\), where the columns of \(Y_s\) are also columns of \(Y\). Because \(\ker A_\kappa\) is well characterized [17, 18, 20], we make use of it in our search for VR\(_0\) realizations.

**Example 2.15.** Consider the weighted E-graph \((V, E, \kappa)\) in Figure 2. While \((V, E)\) has two connected components, it has three terminal strongly connected components (boxed in Figure 2). With the ordering of vertices as labelled in the figure, the Kirchoff matrix of \((V, E, \kappa)\) is

\[
A_\kappa = \begin{pmatrix}
-\kappa_{12} & \kappa_{21} & 0 & 0 & 0 & 0 & 0 & 0 \\
\kappa_{12} & -\kappa_{21} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\kappa_{34} & \kappa_{43} & 0 & 0 & 0 & 0 \\
0 & 0 & \kappa_{34} & -\kappa_{43} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -\kappa_{56} & 0 & \kappa_{67} & 0 \\
0 & 0 & 0 & 0 & \kappa_{56} & -\kappa_{67} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \kappa_{67} & -\kappa_{75} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \kappa_{75} & -\kappa_{87}
\end{pmatrix}.
\]
A basis for its kernel is given by the vectors

\[
c_1 = \begin{pmatrix}
\kappa_{21} \\
\kappa_{12} \\
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}, \quad c_2 = \begin{pmatrix}
0 \\
0 \\
\kappa_{43} \\
\kappa_{34} \\
0 \\
0 \\
0 \\
0
\end{pmatrix}, \quad c_3 = \begin{pmatrix}
0 \\
0 \\
\kappa_{67} \kappa_{75} \\
\kappa_{56} \kappa_{75} \\
\kappa_{56} \kappa_{67} \\
0
\end{pmatrix}.
\]

The supports of the basis vectors \( c_p \) are precisely the terminal strongly connected components of \((V, E)\). If the graph is weakly reversible, then the basis of \( \ker A_{\kappa} \) given in Theorem 2.14 provides a way to partition the set of vertices.

### 3 Main results

In this section, we present Algorithm 1 (see also Figure 3) that searches for a weakly reversible and deficiency zero (WR\(_0\)) realization of a given system of polynomial differential equations

\[
\frac{dx}{dt} = \sum_{i=1}^{m} x^{y_i} w_i,
\]

where \( y_1, \ldots, y_m \in \mathbb{Z}_n^+ \) are distinct, and \( w_1, w_2, \ldots, w_m \in \mathbb{R}^n \setminus \{0\} \). Whenever (5) admits a WR\(_0\) realization, the system is complex-balanced and enjoys all the properties listed in Theorem 2.12. Moreover, if no WR\(_0\) realization exists for (5), our algorithm would conclude as much. Whenever a WR\(_0\) realization exists, the set of positive steady states has a log-linear structure that allows us to easily find the steady states of (5), as outlined in Theorem 3.12. Finally, our algorithm is valid even if the \( w_i \)'s are only known up to a positive scalar multiple; we prove this in Theorem 3.13.

#### 3.1 Algorithm for WR\(_0\) realization

The inputs of Algorithm 1 are the source vertices and their net direction vectors via \( Y_s \) and \( W \) respectively. To find a WR\(_0\) realization \((V, E, \kappa)\) is to find a matrix decomposition of \( W = Y_s A_{\kappa} \), where \( A_{\kappa} \) encodes the graph structure of \((V, E)\). In the following lemma, we prove properties that can be expected should a WR\(_0\) realization exists.

Recall that a set \( X \) is a polyhedral cone if \( X = \{x : Mx \leq 0\} \) for some matrix \( M \). Such a cone is convex. It is pointed, or strongly convex, if it does not contain a positive dimensional linear subspace. Note that a cone contained in the positive orthant \( \mathbb{R}^m_+ \) is always pointed. A pointed polyhedral cone admits a unique (up to scalar multiple) minimal set of generators [8].
\( Y_s = (y_1, \ldots, y_m) \in \mathbb{Z}_{\geq}^{n \times m} \)
\( W = (w_1, \ldots, w_m) \in \mathbb{R}^{n \times m} \)

Find minimal set of generators 
\( \{c_1, \ldots, c_\ell\} \subset \mathbb{R}^m \)
for the cone \( \ker W \cap \mathbb{R}_{\geq}^m \)

Does \( \{\text{supp}(c_p)\}_{p=1}^\ell \) partition \([1, m] \subset \mathbb{N}\)?

Define candidate connected components by \( V_p := \text{supp}(c_p) \)

for \( p = 1, 2, \ldots, \ell \)

Is \( \{y_i : i \in V_p\} \) affinely independent?

\( \forall i \in V_p, \) is \( w_i \in \text{Cone}\{y_j - y_i : j \in V_p\}? \)

Uniquely decompose each \( w_i \) as \( w_i = \sum_{\substack{j \neq i \\ j \in V_p}} \kappa_{ij} (y_j - y_i) \)

for \( p = 1, 2, \ldots, \ell \)

endfor

WR_0 realization found

Figure 3: Algorithm 1 for finding WR_0 realization of a polynomial dynamical system \( \dot{x} = \sum_{i=1}^m x y_i w_i.\)
Algorithm 1 (WR₀ algorithm)

**Input:** Matrices \( Y_s = (y_1, \ldots, y_m) \) and \( W = (w_1, \ldots, w_m) \) that define \( \dot{x} = \sum_{i=1}^{m} x y_i w_i \).

**Output:** Either return the unique WR₀ realization, or print that such a realization does not exist.

1: Find the minimal set of generators \( \{c_1, c_2, \ldots, c_\ell\} \) of the pointed convex cone \( \ker W \cap \mathbb{R}_m^0 \).
2: if the sets \( \text{supp}(c_1), \text{supp}(c_2), \ldots, \text{supp}(c_\ell) \) do not form a partition of \( \{1, 2, \ldots, m\} \) then
3: Print: WR₀ realization does not exist. Exit.
4: else
5: Define the candidate connected components to be \( V_p := \text{supp}(c_p) \), for \( p = 1, 2, \ldots, \ell \).
6: for \( p = 1, 2, \ldots, \ell \) do
7: if the vectors \( \{y_i; i \in V_p\} \) are not affinely independent then
8: Print: WR₀ realization does not exist. Exit.
9: else
10: for each \( i \in V_p \) do
11: if \( w_i / \in \text{Cone}\{y_j - y_i; j \in V_p\} \) then
12: Print: WR₀ realization does not exist. Exit.
13: else
14: Uniquely decompose \( w_i = \sum_j \kappa_{ij} (y_j - y_i) \) with \( \kappa_{ij} \geq 0 \).
15: Add \( \{y_i \to y_j; \kappa_{ij} > 0\} \) to edge set \( E \).
16: end if
17: end for
18: end if
19: end for
20: end if
21: Print: The WR₀ realization does exist, and has \( \ell \) connected components.
22: Print: The connected components of this realization are given by \( \{V_p\}_{p=1}^{\ell} \).
23: Print: The edges are given by \( E \), with weights \( \kappa_{ij} \).

Lemma 3.1. Suppose a polynomial dynamical system \( \dot{x} = f(x) \) admits a WR₀ realization \( (V, E, \kappa) \) with \( \ell \) connected components. Let \( Y_s \) be the matrix of source vertices, and \( W \) the matrix of net direction vectors of the polynomial dynamical system \( \dot{x} = f(x) \). Let \( S \) be the associated linear space, and \( A_\kappa \) the Kirchoff matrix of the weighted E-graph \( (V, E, \kappa) \). Then we have:

(i) \( W = Y_s A_\kappa \) and \( \ker W = \ker A_\kappa \),

(ii) \( S = \text{im} W \), and the rank of \( W \) is \( |V| - \ell \),

(iii) \( \ker W \cap \mathbb{R}_m^0 \) is a pointed polyhedral cone, and

(iv) a minimal set of generators for \( \ker W \cap \mathbb{R}_m^0 \) has \( \ell \) elements, whose supports correspond to the connected components of \( (V, E) \).

**Proof.** Because \( (V, E) \) is weakly reversible, all vertices in \( V \) are sources. Moreover, because the deficiency of \( (V, E) \) is zero, by [11, Proposition 3.5], the net direction vector from any \( y_i \) is non-zero, and the set of source vertices corresponds exactly to the columns of \( Y_s \).

(i) By definition, \( f(x) = W x Y_s \), and by dynamical equivalence, \( f(x) = Y_s A_\kappa x Y_s \). Since the coefficients of polynomial functions are uniquely determined, \( W = Y_s A_\kappa \). Because
Lemma 3.3. Suppose Algorithm 1 reaches line 23. Then the connected components of 

\[ \dim(\ker Y_s \cap \im A_\kappa) = \delta = 0, \] 

we have \( \ker W = \ker A_\kappa \).

(ii) Note that

\[ \text{rank } W = \text{rank } A_\kappa = |V| - \ell = \dim S, \]

where the first and last equalities follow from \( 0 = \delta = \dim(\ker Y_s \cap \im A_\kappa) = |V| - \ell - \dim S, \)

and the second equality follows from weak reversibility and Theorem 2.14. Clearly \( \im W \subseteq S, \)

so \( \im W = S. \)

(iii) The set \( \ker W \cap \mathbb{R}^m_\geq \) is the solution to \( W \nu \geq 0, -W \nu \geq 0, \) and \( \text{Id} \nu \geq 0; \) thus the set is a polyhedral cone. That \( \ker W \cap \mathbb{R}^m_\geq \) is pointed follows from it being a subset of \( \mathbb{R}^m_\geq. \)

(iv) Let \( B = \{c_1, c_2, \ldots, c_\ell\} \) be a basis of \( \ker A_\kappa \) as in Theorem 2.14, where \( c_p \geq 0, \) and each \( V_p = \{y_i : i \in \supp(c_p)\} \) is a connected component of \( (V, E). \) Clearly \( B \subseteq \ker W \cap \mathbb{R}^m_\geq; \) we claim that \( B \) is a minimal set of generators for the pointed cone.

Let \( \nu \in \ker W \cap \mathbb{R}^m_\geq \) be arbitrary. By (ii), \( B \) is a basis for \( \ker W, \) so decompose \( \nu \) accordingly:

\[ \nu = \sum_{p=1}^\ell \lambda_p c_p, \]

for some \( \lambda_p \in \mathbb{R}. \) By Theorem 2.14, each \( c_p \) is supported on the connected components of \( (V, E), \) which partition the set of vertices. In particular, for each \( i = 1, \ldots, m, \) there is exactly one \( p(i) \) such that \( \nu_i = \lambda_{p(i)}[c_{p(i)}]_i. \) Since \( \nu, c_{p(i)} \in \mathbb{R}^m_\geq, \) it must be the case that \( \lambda_{p(i)} \geq 0. \) In other words, \( B \) generates the cone \( \ker W \cap \mathbb{R}^m_\geq. \) Because the vectors in \( B \) have disjoint supports, \( B \) is minimal. \( \square \)

Lemma 3.2. If Algorithm 1 exits at lines 3, 8, or 12, then \( \hat{x} = \sum_{i=1}^m x^{y_i} w_i \) does not admit a WR_0 realization.

Proof. If the algorithm exits at line 3, then by the contrapositive of Lemma 3.1(iv) no WR_0 realization exists. Continuing with the algorithm, let \( \{c_1, \ldots, c_\ell\} \) be a minimal set of generators of \( \ker W \cap \mathbb{R}^m_\geq, \) and partition the vertices as \( V_p := \supp(c_p) \). If instead the algorithm exits at line 8, then again no WR_0 realization exists because WR_0 realizations have affinely independent connected components [12, Theorem 9]. Finally, exiting at line 12 means that some net direction vector \( w_i \) cannot be decomposed as edges from \( y_i \) to other vertices in \( V_p, \) which defines a connected component of a WR_0 realization if it exists according to Lemma 3.1(iv). \( \square \)

Lemma 3.3. Suppose Algorithm 1 reaches line 23. Then the connected components of \( (V, E) \) are given by \( V_1, V_2, \ldots, V_\ell. \)

Proof. If the algorithm reaches line 23, a realization has been found with edges among \( V_1, \ldots, V_\ell, \)

i.e., the connected components are subsets of \( V_p. \) We prove now that in fact, each \( V_p \) is connected in \( (V, E). \)

For any \( p = 1, \ldots, \ell, \) let \( U := V_p \) be the support of \( c := c_p. \) Suppose for a contradiction that \( V^* \subsetneq U \) is a connected component. Because the if statement in line 7 is false, \( U \) is affinely independent, so the linear subspaces

\[ S(V^*) = \{y_i - y_j : y_i, y_j \in V^*\} \quad \text{and} \quad S(U \setminus V^*) = \{y_i - y_j : y_i, y_j \in U \setminus V^*\} \]
are linearly independent. Because \( c \in \ker W \cap \mathbb{R}_m^m \) and \( \text{supp}(c) = U \), we have

\[
0 = \sum_{i \in V^*} c_i w_i + \sum_{i \in U \setminus V^*} c_i w_i,
\]

with \( c_i > 0 \). Furthermore, the if statement in line 11 returning false implies that each \( w_i \) in (6) can be further decomposed as edges between vertices in \( U \). For any \( y_i \) in \( V^* \), which is a connected component, the net direction vector \( w_i \) is a positive linear combination of edge vectors between \( y_i \) and other vertices in \( V^* \), so \( w_i \in S(V^*) \). In particular, \( c^* := \sum_{i \in V^*} c_i w_i \in S(V^*) \). Similarly, any vertices in \( U \setminus V^* \) are only connected to other vertices in \( U \setminus V^* \). Linear independence of \( S(V^*) \) and \( S(U \setminus V^*) \) means that the vectors \( c^* \) and \( c - c^* \) are linearly independent. Both \( c^* \) and \( c - c^* \) lie in the cone \( \ker W \cap \mathbb{R}_m^m \), so \( \{c_1, \ldots, c_\ell\} \) is not a set of generators, which is a contradiction. \( \square \)

**Lemma 3.4.** Suppose Algorithm 1 reaches line 23. Then the deficiency of \((V, E)\) is zero.

**Proof.** The falsity of the if statement in line 7 and Lemma 3.3 imply that the connected components \( V_1, V_2, \ldots, V_\ell \) are affinely independent. To prove \( \delta = 0 \), it remains to show that \( S(V_1), S(V_2), \ldots, S(V_\ell) \) are linearly independent subspaces [12, Theorem 9].

We claim that the minimal set of generators \( \{c_1, c_2, \ldots, c_\ell\} \) forms a basis for \( \ker W \). Let \( c \in \ker W \) be arbitrary. If \( c \) has non-negative components, then it is a linear combination of \( c_p \)'s. If \( c \not\in \mathbb{R}_m^m \), then there exist sufficiently large constants \( \mu_p > 0 \) so that

\[
c + \sum_{p=1}^\ell \mu_p c_p \in \mathbb{R}_m^m.
\]

This vector is a non-negative combination of \( c_1, c_2, \ldots, c_\ell \); thus, \( c \) is a linear combination of the generating vectors. Since \( W \in \mathbb{R}^{n \times |V|} \), we have rank \( W = |V| - \ell \).

Let \( S \) be the associated linear space of \((V, E)\), i.e., \( S = \text{span}\{y_j - y_i : y_i \rightarrow y_j \in E\} \). The falsity of the if statement in line 11 implies that \( \text{im} W \subseteq S \), so \( \dim S \geq |V| - \ell \). Hence, the deficiency of \((V, E)\) is \( \delta = |V| - \ell - \dim S \leq 0 \). Because \( \delta \) is always non-negative, we conclude that \( \delta = 0 \). \( \square \)

**Lemma 3.5.** Suppose Algorithm 1 reaches line 23. Then \((V, E)\) is weakly reversible.

**Proof.** Without loss of generality, we reorder the vertices according to the connected components of the deficiency zero realization \((V, E, \kappa)\) found in line 23. Let \( y_1, y_2, \ldots, y_{m_1} \) form the first connected component; \( y_{m_1+1}, \ldots, y_{m_2} \) form the second connected component, and so on. Accordingly, reorder the columns of the matrix \( W \) of net direction vectors, the indices of the generators \( c_p \), and their supports \( V_p \). Under the new ordering of vertices, \( \text{supp}(c_p) = V_p = \{y_{m_p-1+1}, \ldots, y_{m_p}\} \) for \( p = 1, 2, \ldots, \ell \), where we take \( m_0 = 0 \).

With the new ordering of vertices, the Kirchoff matrix \( A_{\kappa} \) of \((V, E)\) is block-diagonal. Denote by \( A_{\kappa}^{(p)} \) the \( p \)th block, which encodes the connectivity of the connected component defined by \( V_p \). Indeed, \( A_{\kappa}^{(p)} \) is the Kirchoff matrix of the \( p \)th connected component when viewed as a weighted \( E \)-graph in the subgraph sense.

We now prove that the first component \((V_1, E_1)\) is strongly connected. Let \( Y^{(1)} \) be the first \( m_1 \) columns of \( Y \) and \( W^{(1)} \) be the first \( m_1 \) columns of \( W \), so that \( Y^{(1)} A_{\kappa}^{(1)} = W^{(1)} \). Let
\( c_1 = c'_1 + 0 \in \mathbb{R}^n_{>0} \), with \( c'_1 \in \mathbb{R}^{m_1} \) spanning the one-dimensional subspace \( \ker W^{(1)} \). Finally, let \( S_1 = \text{span}\{ y_j - y_i : y_i \in V_1 \} \).

Because \((V_1, E_1)\) is connected and \( V_1 \) is affinely independent, \( \dim S_1 = |V_1| - 1 \), so \( \delta_1 = 0 \). Moreover, if \( t \) denotes the number of terminal strongly connected components in \((V_1, E_1)\), then \( \dim(\ker Y^{(1)} \cap \text{im} A_\kappa^{(1)}) = |V_1| - t - \dim S_1 \leq \delta_1 \), we conclude that \( \ker (Y^{(1)} A_\kappa^{(1)}) = \ker A_\kappa^{(1)} \), and \( c'_1 \) also spans \( \ker A_\kappa^{(1)} \). By Theorem 2.14, \( c'_1 \) is supported on the terminal strongly connected component, which in this case is all of \( V_1 \). Therefore, \((V_1, E_1)\) is in fact strongly connected.

An analogous claim can be made about the other connected components. Consequently \((V, E)\) is weakly reversible.

**Remark 3.6.** In the proof of Lemma 3.3 and Lemma 3.4, we have proved that the associated linear subspace \( S(V_p) \) is in fact the span of the net direction vectors belonging to said connected component. Thus, there are multiple ways of generating \( S(V_p) \):

\[
\text{span}\{ y_j - y_i : y_i, y_j \in V_p \} = \text{span}\{ y_j - y_i : y_i \rightarrow y_j \in E_p \} = \text{im} W^{(p)}.
\]

The lemmas above provide the technical parts that we need to prove the main result of this paper.

**Theorem 3.7.** Given a system of differential equations

\[
\frac{dx}{dt} = \sum_{i=1}^{m} x^{y_i} w_i,
\]

with distinct \( y_i \in \mathbb{Z}_n^+ \) and \( w_i \in \mathbb{R}^n \setminus \{0\} \). Algorithm 1 returns the unique WR\(_0\) realization of the dynamical system if it exists, or concludes that no WR\(_0\) realization exists.

**Proof.** There are two possible scenarios: either (1) the algorithm exits at lines 3, 8, or 12 by failing one of the \textbf{if} statements, or (2) the algorithm successfully reaches line 23. In the first scenario, Lemma 3.2 implies that no WR\(_0\) realization exists. In the second scenario, the realization has connected components \( V_1, V_2, \ldots, V_\ell \) according to Lemma 3.3. The realization is weakly reversible and deficiency zero by Lemmas 3.4 and 3.5 respectively. The uniqueness of the realization follows from [11].

**Remark 3.8.** The uniqueness of the WR\(_0\) realization is also a consequence of Algorithm 1. This is due to the affine and linear independences, as well as the structure of \( \ker W = \ker A_\kappa \).

If a WR\(_0\) realization exists, the polynomial dynamical system is complex-balanced. Therefore, if a system passes Algorithm 1, it automatically inherits all the algebraic and dynamical properties of complex-balanced system. Weak reversibility implies that a positive steady state exists [5]. The remaining statements in the theorem below are easy consequence of Theorems 2.12 and 3.7.

**Theorem 3.9.** Suppose the system of differential equations

\[
\frac{dx}{dt} = \sum_{i=1}^{m} x^{y_i} w_i,
\]

with distinct \( y_i \in \mathbb{Z}_n^+ \) and \( w_i \in \mathbb{R}^n \setminus \{0\} \), passes Algorithm 1. Let \( W \) be the matrix of net direction vectors and \( S = \text{im} \hat{W} \). Then the following holds.
(i) A positive steady state \( x^* \) exists.

(ii) There is exactly one steady state within every invariant polyhedron \((x_0 + S) \cap \mathbb{R}_n^+\) for any \( x_0 \in \mathbb{R}_n^+ \), and it is complex-balanced.

(iii) Any positive steady state \( x \) satisfies \( \ln x - \ln x^* \in S^\perp \).

(iv) The function
\[
L(x) = \sum_{i=1}^{n} x_i(\ln x_i - \ln x_i^* - 1),
\]
defined on \( \mathbb{R}_n^+ \), is a strict Lyapunov function of (7) within every invariant polyhedron \((x_0 + S) \cap \mathbb{R}_n^+\), with a global minimum at the corresponding complex-balanced steady state.

(v) Every positive steady state is locally asymptotically stable with respect to its invariant polyhedron.

**Example 3.10.** Consider the system of differential equations
\[
\begin{align*}
\frac{dx_1}{dt} &= -12x_1 + x^2_3, \\
\frac{dx_2}{dt} &= 14x_1 - 4x^2_2 + 8x^2_3, \\
\frac{dx_3}{dt} &= 10x_1 + 4x^2_2 - 10x^2_3;
\end{align*}
\]
(8)

We have \( n = 3 \) for the three state variables, and \( m = 3 \) for the three distinct monomials. The matrices of source vertices and net direction vectors are
\[
Y_s = (y_1 \ y_2 \ y_3) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix},
\]
\[
W = (w_1 \ w_2 \ w_3) = \begin{pmatrix} -12 & 0 & 1 \\ 14 & -4 & 8 \\ 10 & 4 & -10 \end{pmatrix},
\]
respectively, which are inputs to Algorithm 1. Let \( V = \{y_1, y_2, y_3\} \subset \mathbb{Z}_n^+ \). A generator for the cone \( \ker W \cap \mathbb{R}_n^+ \) is \( c = (48/1441, 120/131, 576/1441)^\top \). In the notation of Algorithm 1, \( V_1 = [1, 3] \). Clearly \( \tilde{V} \) is affinely independent and the net direction vectors admit the following unique decompositions:
\[
\begin{align*}
w_1 &= 7(y_2 - y_1) + 5(y_3 - y_1), \\
w_2 &= 2(y_3 - y_2), \\
w_3 &= (y_1 - y_3) + 4(y_2 - y_3).
\end{align*}
\]

Therefore (8) admits a WR\(_0\) realization, whose weighted E-graph is shown in Figure 4(b).

This implies that the system (8) has exactly one steady state within each invariant triangle given by \( 2x_1 + x_2 + x_3 = C \) for some \( C > 0 \), and this steady state is a global attractor within each such triangle. From Theorem 3.9, we know the steady state set admits a monomial parametrization of the form \((a_1s^2, a_2s, a_3s)\) for some constants \( a_i > 0 \). In fact, the set of steady states is given by
\[
(x^*_1, x^*_2, x^*_3) = \left(3s^2, \frac{\sqrt{330}}{2} s, 6s\right),
\]
and an explanation for the coefficients above will be provided in Theorem 3.12.

Example 3.11. Consider the system of differential equations

\[
\begin{align*}
\frac{dx_1}{dt} &= -\frac{1}{2}x_1 + x_3^2, \\
\frac{dx_2}{dt} &= -2x_1 - 4x_2^2 + 8x_3^2, \\
\frac{dx_3}{dt} &= 3x_1 + 4x_2^2 - 10x_3^2.
\end{align*}
\]

Again, we have \( n = 3 \) and \( m = 3 \). The monomials are the same as those in the previous example. The difference lies in the first column of the matrix of net direction vectors

\[
W = (w_1 \ w_2 \ w_3) = \begin{pmatrix}
-\frac{1}{2} & 0 & 1 \\
-2 & -4 & 8 \\
3 & 4 & -10
\end{pmatrix},
\]

whose kernel is spanned by \( c = (2, 1, 1)^\top \). As in the previous example, the vertices \( y_1, y_2, \) and \( y_3 \) are affinely independent. However, \( w_1 \not\in \text{Cone}\{y_j - y_1: j = 2, 3\} \), so no WR\(_0\) realization exists.

3.2 The set of positive steady states of a WR\(_0\) realization

Algorithm 1 determines whether a given polynomial dynamical system admits a WR\(_0\) realization. If it does, its steady state set is in fact log-linear. In this section, we write down a system of linear equations whose solution set is in bijection with the set of positive steady states; this provides an explicit parametrization of the set of positive steady states.

For any \( z \in \mathbb{R}^n \) and \( x \in \mathbb{R}_{>0}^n \), define the component-wise operations \( \exp z = (e^{z_1}, e^{z_2}, \ldots, e^{z_n})^\top \) and \( \log(x) = (\log x_1, \log x_2, \ldots, \log x_n)^\top \). We extend these operations to sets. If \( Z \subseteq \mathbb{R}^n \), then \( \exp(Z) = \{\exp z: z \in Z\} \), and if \( X \subseteq \mathbb{R}_{>0}^n \), then \( \log(X) = \{\log x: x \in X\} \).

Assume that the polynomial dynamical system

\[
\frac{dx}{dt} = \sum_{i=1}^{m} x^{y_i}w_i,
\]

Figure 4: (a) A weighted E-graph realizing (8) from Example 3.10, which admits (b) a WR\(_0\) realization. (c) A weighted E-graph realizing (9) from Example 3.11 that does not admit a WR\(_0\) realization.
with distinct $y_i \in \mathbb{Z}_+^n$ and $w_i \in \mathbb{R}^n \setminus \{0\}$, passes Algorithm 1, i.e., it admits a WR₀ realization $(V, E, \kappa)$. Without loss of generality, assume the vertices are ordered according to connected components in $(V, E)$, i.e., the first $m_1$ vertices belong to the connected component $(V_1, E_1)$, the next $m_2$ vertices belong to the connected component $(V_2, E_2)$, and so forth. Let $\{c_1, c_2, \ldots, c_\ell\}$ be a minimal set of generators of ker $W \cap \mathbb{R}_>^m$, ordered in an analogous way. From Algorithm 1, we know that the supports of the vectors $c_1, c_2, \ldots, c_\ell$ correspond to the connected components of $(V, E)$.

Let $c_1 = (\alpha_1, \alpha_2, \ldots, \alpha_{m_1}, 0, \ldots, 0)^\top$. Define matrix $D_1 \in \mathbb{R}^{(m_1-1) \times n}$ whose rows are the affine vectors from $y_1$ to the remaining vertices of $V_1$, and define vector $J_1 \in \mathbb{R}^{m_1-1}$ using the log-differences of the components of $c_1$, i.e.,

$$D_1 = \begin{pmatrix} y_2 - y_1 \\ y_3 - y_1 \\ \vdots \\ y_{m_1} - y_1 \end{pmatrix} \quad \text{and} \quad J_1 = \begin{pmatrix} \log(\alpha_2/\alpha_1) \\ \log(\alpha_3/\alpha_1) \\ \vdots \\ \log(\alpha_{m_1}/\alpha_1) \end{pmatrix}.$$ 

For the connected component $(V_p, E_p)$, define $D_p$ and $J_p$ in a similar fashion. Define

$$D = \begin{pmatrix} D_1 \\ D_2 \\ \vdots \\ D_\ell \end{pmatrix} \in \mathbb{R}^{(m-\ell) \times n} \quad \text{and} \quad J = \begin{pmatrix} J_1 \\ J_2 \\ \vdots \\ J_\ell \end{pmatrix} \in \mathbb{R}^{m-\ell}. \quad (11)$$

**Theorem 3.12.** Suppose the system of differential equation (10) admits a WR₀ realization $(V, E, \kappa)$, and let $D \in \mathbb{R}^{(m-\ell) \times n}$ and $J \in \mathbb{R}_>^{m-\ell}$ be defined as in (11). Then the system $Dz = J$ is solvable. Let $z^* + \ker D$ be its solution set. Then the set of positive steady states of (10) is $\exp(z^* + \ker D)$.

**Proof.** First we prove that the linear system $Dz = J$ is solvable. Consider $D_1$. The vertices $y_1, y_2, \ldots, y_{m_1}$ in the first connected component are affinely independent, so the rows of $D_1$ are linearly independent. Moreover, as noted in Remark 3.6 the row-space of $D_1$ is the associated linear subspace $S(V_1)$. Therefore rank $D_1 = m_1 - 1$, and the matrix $D_1$ is surjective onto $\mathbb{R}^{m_1-1}$.

Similarly, for each $p = 2, \ldots, \ell$, the row-space of the matrix $D_p$ is $S(V_p)$, and the matrix $D_p$ is surjective. In addition, because the realization $(V, E, \kappa)$ has deficiency zero, $S(V_1), S(V_2), \ldots, S(V_\ell)$ are linearly independent; in other words, the $m - \ell$ rows of the matrix $D$ are linearly independent. Consequently, $D$ is surjective, and the system $Dz = J$ is solvable.

Let $z^* + \ker D$ be the set of solution to $Dz = J$. We next show that each solution can be related to a positive steady state of (10), which by definition satisfies

$$0 = \sum_{i=1}^m x^{y_i} w_i.$$

In other words, $(x^{y_1}, \ldots, x^{y_m})^\top$ lies in the steady state flux cone ker $W \cap \mathbb{R}_>^m$. Decomposing this vector with respect to the generators of the cone allows us to focus on one connected component at a time.
For simplicity of notation, consider the first connected component. At steady state, for some constant \( \lambda > 0 \), we have \( x^y_j = \lambda \alpha_j \) for \( j = 1, 2, \ldots, m_1 \). Thus
\[
x^y_j - y_1 = \frac{\alpha_j}{\alpha_1}
\]
for \( j = 2, 3, \ldots, m_1 \). Taking the logarithm of both sides, we obtain the system \( D_1 z = J_1 \) with \( z = \log x \).

Repeating this computation for each connected component, we conclude that \( x \) is a positive steady state for (10) if and only if \( x \) solves \( D z = J \) with \( z = \log x \). This leads us to the characterization of the set of positive steady states for (10) as \( \exp(z^* + \ker D) \), where \( z^* + \ker D \) is the set of solutions to \( D z = J \).

### 3.3 Extension to polynomial systems with unspecified coefficients

If instead of (10), we need to analyze
\[
\frac{dx}{dt} = \sum_{i=1}^{m} a_i x^y_i w_i
\]
for some unknown \( a_i > 0 \), it turns out that the answer as to whether a WR\(_0\) realization exists is the same:

**Theorem 3.13.** For any \( a_i > 0 \), the system (12) admits a WR\(_0\) realization \((V, E, \kappa)\) if and only if the system (10) admits a WR\(_0\) realization \((V, E, \kappa^*)\). Moreover, \( \kappa_{ij} = a_i \kappa^*_{ij} \).

**Proof.** The forward implication is trivial. We focus our attention on the other direction. For any \( i, j \), let \( \kappa_{ij} = a_i \kappa^*_{ij} \), so \( \kappa_{ij} > 0 \) if and only if \( \kappa^*_{ij} > 0 \). In other words, the weighted E-graph \((V, E, \kappa)\) shares the same set of edges as \((V, E, \kappa^*)\). Because the deficiency is characterized by affine and linear independence of the connected components, and the two graphs share the same structure, \((V, E, \kappa)\) is weakly reversible and deficiency zero if and only if \((V, E, \kappa^*)\) is.

Suppose \((V, E, \kappa^*)\) is a realization of (10). Then in \((V, E, \kappa)\), the net direction vector from \( y_i \) can be expanded using the realization \((V, E, \kappa^*)\), since
\[
a_i w_i = a_i \sum_{(i,j)\in E} \kappa^*_{ij}(y_j - y_i) = \sum_{(i,j)\in E} \kappa_{ij}(y_j - y_i).
\]
Therefore, \((V, E, \kappa)\) realizes (12).

### 3.4 Deficiency zero realizations that are not weakly reversible

If a polynomial dynamical system admits a deficiency zero realization that is not weakly reversible, then its dynamics is also greatly restricted: it can have no positive steady states, no oscillations, and no chaotic dynamics [15,17,21]. Actually, such realizations are special examples of mass-action system that are not consistent [2]. An E-graph \((V, E)\) is said to be consistent if there exist real numbers \( \alpha_{ij} > 0 \) such that
\[
\sum_{(i,j)\in E} \alpha_{ij}(y_j - y_i) = 0.
\]
It is easy to see that a polynomial dynamical system of the form (10) has a realization that is not consistent if and only if
\[ \ker \mathbf{W} \cap \mathbb{R}^m_+ = \emptyset. \] (13)

If a polynomial dynamical system has a realization that is not consistent, then it cannot have realization that is weakly reversible, because weakly reversible systems must have at least one positive steady state [5]. Therefore, if Algorithm 1 is accompanied by a preprocessing step that checks condition (13), then that step will decide whether our given system (10) has a realization that is not consistent; in particular, this step will also find all cases where our given system has a deficiency zero realization that is not weakly reversible.

Acknowledgements

The authors were supported in part by the National Science Foundation under grants DMS–1816238 and DMS–2051568. G.C. was also partially supported by the Simons Foundation.

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