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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 behaviors 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.

Key words. polynomial dynamical systems, mass action systems, weakly reversible, deficiency zero, stability

MSC codes. 37C75, 37N25, 92C42, 80A30, 92D25, 92C45

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1. Introduction.

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

$$
\begin{aligned}
\frac{dx_1}{dt} &= p_1(x_1, \ldots, x_n),\\
\frac{dx_2}{dt} &= p_2(x_1, \ldots, x_n),\\
&\vdots\\
\frac{dx_n}{dt} &= p_n(x_1, \ldots, x_n),
\end{aligned} \tag{1}
$$

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 feedbacks 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 [28]. Even the simplest object associated to (1), its steady state set, is central to real algebraic geometry.

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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 infect 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 model. An active area of research is to relate the structure of the interaction network to the dynamics generated by it [3, 4, 8, 21, 29, 31, 32, 35, 45].

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 [15]. 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 behavior.

A class of systems whose dynamics is very well understood is the family of *complex-balanced systems* [27], which are also called *toric dynamical systems* [10]. 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 [27]. Moreover, this steady state is conjectured to be a global attractor [26].

Not only are the dynamical properties of complex-balanced systems well understood but so are the network and parameter structures that characterize them [25]. While in general, there are algebraic restrictions 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, making use of the geometric and log-linear structure of WR_0 networks, the algorithm requires as its inputs 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 subsection 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 subsection 3.3. Our algorithm applies to the case where the coefficients in the polynomials are unspecified; we consider such systems in subsection 3.4.

2. Background.

2. Background. Throughout this work, we denote by $\mathbb{R}^n_{\geq}$ and $\mathbb{R}^n_{>}$ the sets of vectors with nonnegative and positive entries, respectively. Similarly, $\mathbb{Z}^n_{\geq}$ is the set of vectors with nonnegative integer components. Vectors are typically denoted $\boldsymbol{x}$, $\boldsymbol{y}$, or $\boldsymbol{w}$. We denote by $\dot{\boldsymbol{x}}$ the time-derivative $\frac{d\boldsymbol{x}}{dt}$. For any $\boldsymbol{x} \in \mathbb{R}^n_{>}$ and $\boldsymbol{y} \in \mathbb{R}^n$, define the operation $\boldsymbol{x}^{\boldsymbol{y}} = x_1^{y_1} x_2^{y_2} \cdots x_n^{y_n}$. If $\mathbf{Y} = \begin{pmatrix} \boldsymbol{y}_1 & \boldsymbol{y}_2 & \cdots & \boldsymbol{y}_n \end{pmatrix}$, then $\boldsymbol{x}^{\mathbf{Y}} = (\boldsymbol{x}^{\boldsymbol{y}_1}, \boldsymbol{x}^{\boldsymbol{y}_2}, \dots, \boldsymbol{x}^{\boldsymbol{y}_n})^\top$. The support of a vector $\boldsymbol{x} \in \mathbb{R}^n$ is the set of indices $\operatorname{supp}(\boldsymbol{x}) = \{i \colon x_i \neq 0\}$.

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. *An E-graph in $\mathbb{R}^n$ is a directed graph (V, E), where V is a finite subset of $\mathbb{R}^n_{\geq}$ and such that there are no self-loops and no isolated vertices.*

Let $V = \{\boldsymbol{y}_1, \boldsymbol{y}_2, \dots, \boldsymbol{y}_m\}$. An edge $(\boldsymbol{y}_i, \boldsymbol{y}_j)$, or $(i,j) \in E$, is also denoted $\boldsymbol{y}_i \to \boldsymbol{y}_j$, where $\boldsymbol{y}_i$ is said to be a source vertex. Let V_s denote the set of source vertices. Since vertices are points in $\mathbb{R}^n$, an edge can be regarded as a bona fide vector between vertices. An *edge vector* $\boldsymbol{y}_j - \boldsymbol{y}_i$ is associated to the edge $\boldsymbol{y}_i \to \boldsymbol{y}_j$.

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

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 $\{\boldsymbol{y}_0, \boldsymbol{y}_1, \dots, \boldsymbol{y}_r\} \subseteq V$ is the vertex set of a connected component, then the set of vectors $\{\boldsymbol{y}_j - \boldsymbol{y}_0 \colon j = 1, 2, \dots, r\}$ 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 $S(U) = \operatorname{span}\{\boldsymbol{y}_j - \boldsymbol{y}_i \colon \boldsymbol{y}_i, \boldsymbol{y}_j \in U\}$. The associated linear space of (V, E) is*

$$S = \operatorname{span}\{\boldsymbol{y}_j - \boldsymbol{y}_i \colon \boldsymbol{y}_i \to \boldsymbol{y}_j \in E\}.$$

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

Remark 2.4. Thus far, we have defined E-graphs, and we have introduced several objects and properties associated to them. Many of these objects are inspired by corresponding objects in *reaction network theory*, where E-graphs are known as reaction networks, edge vectors are known as reaction vectors, vertices are known as complexes, connected components are known as linkage classes, and associated linear spaces are known as stoichiometric subspaces. Below, we attach positive weights to edges; in reaction network theory these weights are called reaction rate constants.

We now turn our attention to how an E-graph is canonically associated to dynamics on $\mathbb{R}^n_{>}$ by assigning a positive weight to each edge.

DEFINITION 2.5. *Let (V, E) be an E-graph. For each $\boldsymbol{y}_i \to \boldsymbol{y}_j \in E$, let $\kappa_{ij} > 0$ be its weight, and let $\boldsymbol{\kappa} = (\kappa_{ij}) \in \mathbb{R}^E_{>}$. The associated dynamical system on $\mathbb{R}^n_{>}$ of the weighted E-graph $(V, E, \boldsymbol{\kappa})$ is*

$$\frac{d\boldsymbol{x}}{dt} = \sum_{(i,j)\in E} \kappa_{ij} \boldsymbol{x}^{\boldsymbol{y}_i}(\boldsymbol{y}_j - \boldsymbol{y}_i). \tag{2}$$

It is sometimes convenient to refer to κ_{ij} even though $\boldsymbol{y}_i \to \boldsymbol{y}_j$ may not be an edge in the network. In such cases, we set $\kappa_{ij} = 0$.

Remark 2.6. 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 $\mathbb{R}^n_>$ is indeed forward-invariant under (2) [40].

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 $\boldsymbol{x}_0 \in \mathbb{R}^n_>$ is confined to $(\boldsymbol{x}_0 + S) \cap \mathbb{R}^n_>$, which is called the *invariant polyhedron of* $\boldsymbol{x}_0$.

Example 2.7. We illustrate the notions and notations defined above. Figure 1 shows three examples of weighted E-graphs. The graphs in Figure 1(a) and 1(b) are weakly reversible, but the one 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 Figure 1(b) and 1(c) do not have affinely independent connected components.

The associated dynamical system of the weighted E-graphs in Figure 1(a) is

$$\begin{aligned}\frac{d}{dt}\begin{pmatrix}x_1\\x_2\end{pmatrix} &= 3\begin{pmatrix}2\\2\end{pmatrix} + 5x_1^2\begin{pmatrix}-2\\2\end{pmatrix} + 2x_1^2x_2^2\begin{pmatrix}-2\\-2\end{pmatrix} + 3x_2^2\begin{pmatrix}2\\-2\end{pmatrix}\\ &= \begin{pmatrix}6 - 10x_1^2 - 4x_1^2x_2^2 + 6x_2^2\\ 6 + 10x_1^2 - 4x_1^2x_2^2 - 6x_2^2\end{pmatrix}.\end{aligned} \tag{3}$$

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 Figure 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 2.10. This example demonstrates that while a weighted E-graph is associated to a unique dynamical system, the converse is not true; there are in general infinitely many realizations of a given polynomial dynamical system [15]. This work is concerned with finding a realization that guarantees 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.

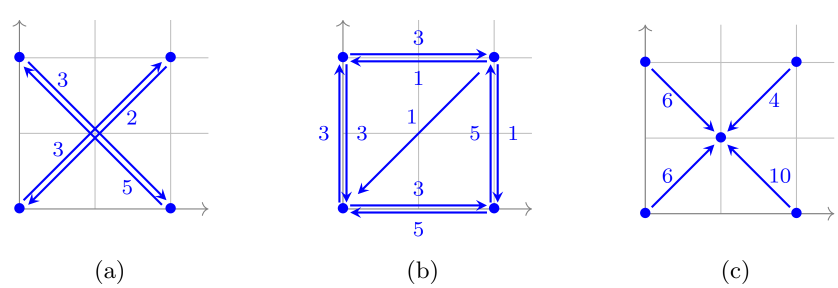

FIG. 1. *Weighted E-graphs from Example* 2.7.

Definition 2.8. *Let* $(V, E, \boldsymbol{\kappa})$ *be a weighted E-graph, and* $\boldsymbol{y}_i \in V_s$. *The net direction vector from* $\boldsymbol{y}_i$ *is*

$$\boldsymbol{w}_i = \sum_{\boldsymbol{y}_j \in V} \kappa_{ij}(\boldsymbol{y}_j - \boldsymbol{y}_i).$$

The matrix of net direction vectors of $(V, E, \boldsymbol{\kappa})$ *is*

$$\mathbf{W} = (\boldsymbol{w}_1 \quad \boldsymbol{w}_2 \quad \cdots \quad \boldsymbol{w}_m).$$

For convenience, we may refer to the net direction vector even if $\boldsymbol{y}_i \notin V_s$; in this case, let the net direction vector be zero. Such a net direction vector will *not* show up as a column of $\mathbf{W}$.

The matrix $\mathbf{W}$ from Definition 2.8 is also well defined when we start not with a weighted E-graph but with a fixed polynomial dynamical system of the form

$$\frac{d\boldsymbol{x}}{dt} = \sum_{i=1}^{m} \boldsymbol{x}^{\boldsymbol{y}_i} \boldsymbol{w}_i. \tag{4}$$

Note that any polynomial dynamical systems can be uniquely written as such, for some $\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_m \in \mathbb{Z}^n_{\geq}$ distinct, and $\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_m \in \mathbb{R}^n$ nonzero.

Definition 2.9. *Consider the polynomial dynamical system* (4). *The matrix of source vertices* $\mathbf{Y}_s$ *and the matrix of net direction vectors* $\mathbf{W}$ *of* (4) *are*

$$\mathbf{Y}_s = (\boldsymbol{y}_1 \quad \boldsymbol{y}_2 \quad \cdots \quad \boldsymbol{y}_m) \quad \text{and} \quad \mathbf{W} = (\boldsymbol{w}_1 \quad \boldsymbol{w}_2 \quad \cdots \quad \boldsymbol{w}_m).$$

Clearly, $\dot{\boldsymbol{x}} = \mathbf{W}\boldsymbol{x}^{\mathbf{Y}_s}$.

Thus far, we start with a weighted E-graph $(V, E, \boldsymbol{\kappa})$, and from it, we define a dynamical system. The goal of the present work is the converse direction: start with a polynomial dynamical system, find some $(V, E, \boldsymbol{\kappa})$, ideally with certain properties, that gives rise to such dynamics. For example, (4) is generated by the graph $\boldsymbol{y}_i \xrightarrow{1} \boldsymbol{y}_i + \boldsymbol{w}_i$, for $i = 1, 2, \ldots, m$. As Example 2.7 illustrates, there are in general many weighted E-graphs that can generate the same dynamics.

Definition 2.10. *A* ***realization*** *of a polynomial dynamical system* $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$ *is a weighted E-graph* $(V, E, \boldsymbol{\kappa})$ *whose associated dynamical system is precisely* $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$. *Two realizations of* $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$ *are said to be dynamically equivalent.*

Lemma 2.11 ([11]). *The weighted E-graphs* $(V, E, \boldsymbol{\kappa})$ *and* $(V', E', \boldsymbol{\kappa}')$ *are dynamically equivalent if and only if the net direction vector from* $\boldsymbol{y}_i$ *in* $(V, E, \boldsymbol{\kappa})$ *coincides with that in* $(V', E', \boldsymbol{\kappa}')$ *for all* $\boldsymbol{y}_i \in V_s \cup V'_s$.

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 behaviors, 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 2.12. *Let* $(V, E, \boldsymbol{\kappa})$ *be a weighted E-graph in* $\mathbb{R}^n$, *and let* $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$ *be its associated dynamical system. A state* $\boldsymbol{x}^* \in \mathbb{R}^n_>$ *is said to be a positive steady* *state if* $\boldsymbol{f}(\boldsymbol{x}^*) = \boldsymbol{0}$*. Let* $V_>(\boldsymbol{f})$ *be the set of positive steady states. A state* $\boldsymbol{x}^* > \boldsymbol{0}$ *is a complex-balanced steady state if, at every* $\boldsymbol{y}_i \in V$*, we have*

$$\sum_{(i,j)\in E} \kappa_{ij}(\boldsymbol{x}^*)^{\boldsymbol{y}_i} = \sum_{(j,i)\in E} \kappa_{ji}(\boldsymbol{x}^*)^{\boldsymbol{y}_j}.$$

The equation above can be interpreted as balancing the fluxes flowing across the vertex $\boldsymbol{y}_i$. If a weighted E-graph $(V, E, \boldsymbol{\kappa})$ admits one complex-balanced steady state, then every positive steady state is complex-balanced [27]; such a $(V, E, \boldsymbol{\kappa})$ is called a *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 [18, 24, 46].

THEOREM 2.13 ([27]). *Let* $(V, E, \boldsymbol{\kappa})$ *be a complex-balanced system, with steady state* $\boldsymbol{x}^* \in \mathbb{R}^n_>$ *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* $\boldsymbol{x}$ *satisfies* $\ln \boldsymbol{x} - \ln \boldsymbol{x}^* \in S^{\perp}$.
- (iii) *The function*

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

defined on $\mathbb{R}^n_>$*, is a strict Lyapunov function within each invariant polyhedron* $(\boldsymbol{x}_0 + S) \cap \mathbb{R}^n_>$*, 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 $V_>(\boldsymbol{f})$ admits a monomial parametrization [8, 10]. Each positive steady state $\boldsymbol{x}^*$ is in fact linearly stable with respect to its invariant polyhedron [7, 39]. Complex-balanced systems are also conjectured to be *persistent* and *permanent*[1] [14]. Moreover, the unique steady state is conjectured to be *globally* stable within its invariant polyhedron [26]. 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 $\mathbb{R}^2$ [14], or the E-graph is *strongly endotactic* [23], or the associated linear space S is of dimension two and all trajectories are bounded [37]. The *Global Attractor Conjecture* has also been proved if there is only one connected component [1, 6], or the E-graph is strongly endotactic [23], or the ambient state space is $\mathbb{R}^3$ [14], or when the associated linear space S is of dimension at most three [37].

Besides dynamical stability, complex-balanced systems are characterized graph-theoretically and algebraically. Horn proved in [25] that $(V, E, \boldsymbol{\kappa})$ is complex-balanced if and only if (V, E) is weakly reversible and $\boldsymbol{\kappa}$ satisfies some algebraic equations, the number of which is measured by a nonnegative integer called the *deficiency* of (V, E).

[1]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.

Definition 2.14. *Let (V,E) be an E-graph with ℓ 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 $V_1,\ V_2,\dots,V_\ell$ 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 $S(V_1),\ S(V_2),\dots,S(V_\ell)$ 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 $\boldsymbol{\kappa}$. This result is known as the Deficiency Zero Theorem [17, 25]. 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 WR_0 realizations for polynomial dynamical systems, which are automatically complex-balanced and therefore obey the properties listed in Theorem 2.13.

Deficiency also has a *geometric interpretation*; $\delta = 0$ if and only if (V,E) has affinely independent connected components $V_1,\ V_2,\dots,V_\ell$, and the subspaces $S(V_1)$, $S(V_2),\dots,S(V_\ell)$ are linearly independent [13, 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 $(V,E,\boldsymbol{\kappa})$ where $|V| = m$, its associated dynamical system (2) can be decomposed as $\dot{\boldsymbol{x}} = \mathbf{Y}\mathbf{A}_{\boldsymbol{\kappa}}\boldsymbol{x}^{\mathbf{Y}}$ [27], where

$$\mathbf{Y} = (\boldsymbol{y}_1 \quad \boldsymbol{y}_2 \quad \cdots \quad \boldsymbol{y}_m)$$

is a matrix whose columns are the vertices (including both sources and targets); $\boldsymbol{x}^{\mathbf{Y}}$ is the vector of monomials whose ith component is $\boldsymbol{x}^{\boldsymbol{y}_i}$, and the *Kirchhoff matrix*

$$[\mathbf{A}_{\boldsymbol{\kappa}}]_{ij} = \begin{cases} \kappa_{ji} & \text{if } \boldsymbol{y}_i \to \boldsymbol{y}_j \in E, \\ -\displaystyle\sum_r \kappa_{jr} & \text{for } i = j, \\ 0, & \text{otherwise,} \end{cases}$$

is the negative transpose of the graph Laplacian of $(V,E,\boldsymbol{\kappa})$. In general, the ith component of $\mathbf{A}_{\boldsymbol{\kappa}}\boldsymbol{x}^{\mathbf{Y}}$,

$$[\mathbf{A}_{\boldsymbol{\kappa}}\boldsymbol{x}^{\mathbf{Y}}]_i = \sum_{(j,i)\in E} \kappa_{ji}\boldsymbol{x}^{\boldsymbol{y}_j} - \boldsymbol{x}^{\boldsymbol{y}_i} \sum_{(i,j)\in E} \kappa_{ij},$$

measures the net flux passing through the ith vertex, so a complex-balanced steady state $\boldsymbol{x}^*$ is a solution to the equation $\mathbf{A}_{\boldsymbol{\kappa}}(\boldsymbol{x}^*)^{\mathbf{Y}} = \mathbf{0}$.

A subgraph $(V_0,E_0) \subseteq (V,E)$ is a *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 $\mathbf{A}_{\boldsymbol{\kappa}}$ is supported on the terminal strongly connected components.

THEOREM 2.15 ([20]). *Let $\mathbf{A}_{\boldsymbol{\kappa}}$ be the Kirchhoff matrix of $(V, E, \boldsymbol{\kappa})$ with terminal strongly connected components $V_1,\, V_2, \ldots, V_t$. There exists a basis $\{\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_t\}$ for* $\ker \mathbf{A}_{\boldsymbol{\kappa}}$ *with $\boldsymbol{c}_p \in \mathbb{R}^m_{\geq}$ and*

$$\begin{cases} [\boldsymbol{c}_p]_i > 0, & \text{if } \boldsymbol{y}_i \in V_p, \\ [\boldsymbol{c}_p]_i = 0, & \textit{otherwise.} \end{cases}$$

According to the Matrix-Tree Theorem [10, 25], there is an explicit formula for the entries of $\boldsymbol{c}_p$. Each nonzero $[\boldsymbol{c}_p]_i$ is a polynomial of κ_{ij} with positive coefficients, given by the maximal minors of $\mathbf{A}_{\boldsymbol{\kappa}}$ [10, 22, 36].

If (V, E) is weakly reversible, then $\delta = \dim(\ker \mathbf{Y} \cap \operatorname{im} \mathbf{A}_{\boldsymbol{\kappa}})$. More generally, $\dim(\ker \mathbf{Y} \cap \operatorname{im} \mathbf{A}_{\boldsymbol{\kappa}}) = |V| - \ell - t$, when $(V, E, \boldsymbol{\kappa})$ has t terminal strongly connected components [20]. Therefore if (V, E) is WR_0, then $\ker(\mathbf{Y}\mathbf{A}_{\boldsymbol{\kappa}}) = \ker \mathbf{A}_{\boldsymbol{\kappa}}$, and the matrix of net direction vectors $\mathbf{W}$ coincides with $\mathbf{Y}\mathbf{A}_{\boldsymbol{\kappa}}$ (see Lemma 3.1).

For the purpose of this work, we assume that we are given $\mathbf{W}$ and the matrix of source vertices $\mathbf{Y}_s$, but we do not know the decomposition of $\mathbf{W}$ into the product $\mathbf{Y}\mathbf{A}_{\boldsymbol{\kappa}}$, where the columns of $\mathbf{Y}_s$ are also columns of $\mathbf{Y}$. Because $\ker \mathbf{A}_{\boldsymbol{\kappa}}$ is well characterized [19, 20, 24], we make use of it in our search for WR_0 realizations.

Example 2.16. Consider the weighted E-graph $(V, E, \boldsymbol{\kappa})$ 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 labeled in the figure, the Kirchhoff matrix of $(V, E, \boldsymbol{\kappa})$ is

$$\mathbf{A}_{\boldsymbol{\kappa}} = \begin{pmatrix} -\kappa_{12} & \kappa_{21} & & & & & & \\ \kappa_{12} & -\kappa_{21} & & & & & & \\ & & -\kappa_{34} & \kappa_{43} & & & & \\ & & \kappa_{34} & -\kappa_{43} & & & & \kappa_{84} \\ & & & & -\kappa_{56} & 0 & \kappa_{75} & \\ & & & & \kappa_{56} & -\kappa_{67} & 0 & \\ & & & & 0 & \kappa_{67} & -\kappa_{75} & \kappa_{87} \\ & & & & & & & -\kappa_{84} - \kappa_{87} \end{pmatrix}.$$

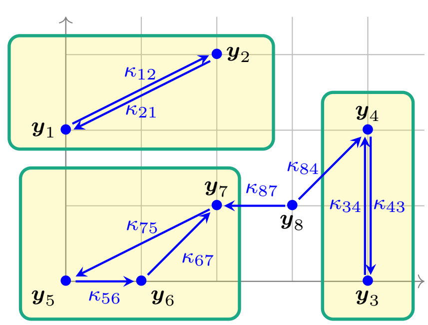

FIG. 2. *A weighted E-graph with two connected components but three terminal strongly connected components (boxed). Its Kirchhoff matrix* $\mathbf{A}_{\boldsymbol{\kappa}}$ *and a basis for* $\ker \mathbf{A}_{\boldsymbol{\kappa}}$ *are given in Example* 2.16.

A basis for its kernel is given by the vectors

$$\boldsymbol{c}_1 = \begin{pmatrix} \kappa_{21} \\ \kappa_{12} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad \boldsymbol{c}_2 = \begin{pmatrix} 0 \\ 0 \\ \kappa_{43} \\ \kappa_{34} \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad \boldsymbol{c}_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \kappa_{67}\kappa_{75} \\ \kappa_{56}\kappa_{75} \\ \kappa_{56}\kappa_{67} \\ 0 \end{pmatrix}.$$

The supports of the basis vectors $\boldsymbol{c}_p$ are precisely the terminal strongly connected components of (V, E). If the graph is weakly reversible, then the basis of $\ker \mathbf{A}_{\boldsymbol{\kappa}}$ given in Theorem 2.15 provides a way to partition the set of vertices.

2.3. Connection to reaction network theory. As hinted at in Remark 2.4, the present work comes at the heel of various results on realizations in reaction network theory. It was first recognized in the early 1970s that two mass-action systems with distinct rate constants and network structures (what we call E-graphs) can give rise to *the same* dynamics [27, 33]. The capacity of networks to be dynamically equivalent was studied in depth in [2, 15, 41]. An algorithm based on mixed-integer linear programming was proposed to compute realizations with additional properties [42], followed by various improvements in subsequent years; see [30, 34, 38, 43, 44]. The authors of these works note that the algorithms for complex-balanced realizations (of which WR_0 realizations are a subset) require as input the set of candidate complexes (i.e., candidate vertices). This issue was resolved when it was proved that, for complex-balanced realizations (as well as for weakly reversible, reversible, or detailed balanced realizations), *it suffices to use the set of monomial exponents as the set of vertices* [11].

Meanwhile, although there is in general no unique E-graph associated to a system of ODEs, it was conjectured that uniqueness does hold for WR_0 realizations. For networks with a single connected component, a proof was first presented in [16] using a linear algebraic method, and a proof based on the geometric interpretation of deficiency was given in [13]. The proof for the general case was provided in [12]. It was from [12] that we sought to use the geometry of the network to find WR_0 realizations, and the present work originates from that effort.

3. Main results. In this section, we present Algorithm 1 (see also Figure 3) that finds a WR_0 realization of a given system of polynomial differential equations,

$$\frac{d\boldsymbol{x}}{dt} = \sum_{i=1}^{m} \boldsymbol{x}^{\boldsymbol{y}_i} \boldsymbol{w}_i, \tag{5}$$

whenever one exists; here $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m \in \mathbb{Z}^n_{\geq}$ are distinct, and $\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_m \in \mathbb{R}^n \backslash \{\mathbf{0}\}$. Recall that whenever (5) admits a WR_0 realization it follows that the system is complex-balanced and enjoys all the properties listed in Theorem 2.13. In particular, 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. Moreover, if no WR_0 realization exists for (5), our algorithm would conclude as much. Finally, our algorithm is valid even if the $\boldsymbol{w}_i$'s are only known up to a positive scalar multiple; we prove this in Theorem 3.13.

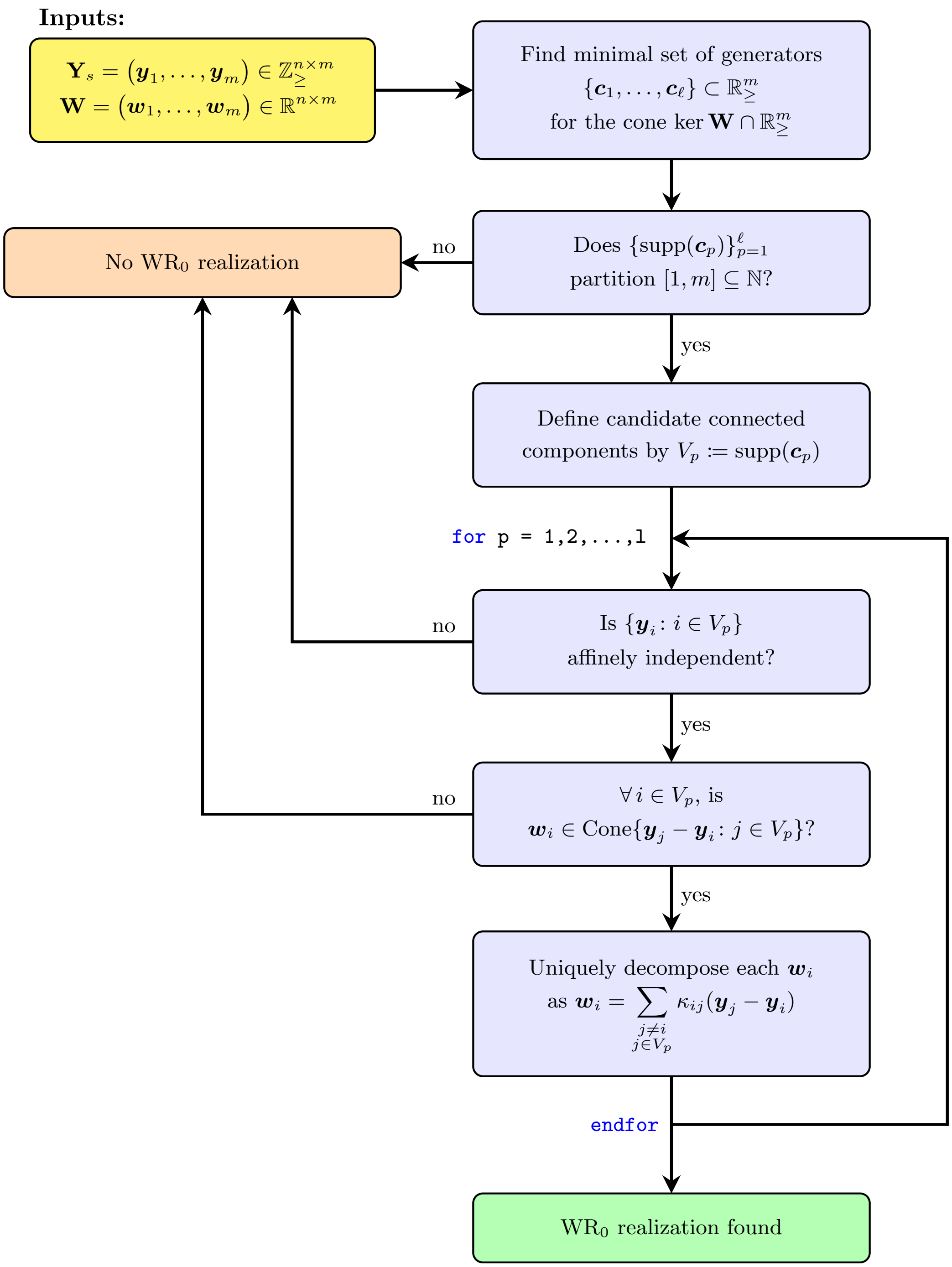

FIG. 3. *Algorithm 1 for finding WR_0 realization of a polynomial dynamical system* $\dot{\boldsymbol{x}} = \sum_{i=1}^{m} \boldsymbol{x}^{\boldsymbol{y}_i} \boldsymbol{w}_i$.

Algorithm 1 (WR_0 algorithm).

Input: Matrices $\mathbf{Y}_s = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m)$ and $\mathbf{W} = (\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m)$ that define $\dot{\boldsymbol{x}} = \sum_{i=1}^{m} \boldsymbol{x}^{\boldsymbol{y}_i} \boldsymbol{w}_i$.
Output: Either return the unique WR_0 realization or print that such a realization does not exist.

Find the minimal set of generators $\{\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_\ell\}$ of the pointed convex cone $\ker \mathbf{W} \cap \mathbb{R}^m_{\geq}$.
if the sets $\mathrm{supp}(\boldsymbol{c}_1), \mathrm{supp}(\boldsymbol{c}_2), \ldots, \mathrm{supp}(\boldsymbol{c}_\ell)$ do *not* form a partition of $\{1, 2, \ldots, m\}$, **then**
  Print: `WR0 realization does not exist.` **Exit.**
else
  Define the candidate connected components to be $V_p := \mathrm{supp}(\boldsymbol{c}_p)$ for $p = 1, 2, \ldots, \ell$.
  for $p = 1, 2, \ldots, \ell$ **do**
    if the vectors $\{\boldsymbol{y}_i : i \in V_p\}$ are *not* affinely independent, **then**
      Print: `WR0 realization does not exist.` **Exit.**
    else
      for each $i \in V_p$ **do**
        if $\boldsymbol{w}_i \notin \mathrm{Cone}\{\boldsymbol{y}_j - \boldsymbol{y}_i : j \in V_p\}$, **then**
          Print: `WR0 realization does not exist.` **Exit.**
        else
          Uniquely decompose $\boldsymbol{w}_i = \sum_{j \in V_p, j \neq i} \kappa_{ij} (\boldsymbol{y}_j - \boldsymbol{y}_i)$ with $\kappa_{ij} \geq 0$.
          Add $\{\boldsymbol{y}_i \to \boldsymbol{y}_j : \kappa_{ij} > 0\}$ to the edge set E.
        end if
      end for
    end if
  end for
end if
Print: `The WR0 realization does exist and has` ℓ `connected components.`
Print: `The connected components of this realization are given by` $\{V_p\}_{p=1}^{\ell}$.
Print: `The edges are listed in` E`, with weights` κ_{ij}.

3.1. Algorithm for finding $\mathbf{WR_0}$ realization. The inputs of Algorithm 1 are the source vertices and their net direction vectors via $\mathbf{Y}_s$ and $\mathbf{W}$, respectively. To find a WR_0 realization $(V, E, \boldsymbol{\kappa})$ is to find a matrix decomposition of $\mathbf{W} = \mathbf{Y}_s \mathbf{A}_{\boldsymbol{\kappa}}$, where $\mathbf{A}_{\boldsymbol{\kappa}}$ encodes the graph structure of (V, E). In the following lemma, we prove properties that can be expected should a WR_0 realization exist.

Recall that a set X is a *polyhedral cone* if $X = \{\boldsymbol{x} : \mathbf{M}\boldsymbol{x} \leq \mathbf{0}\}$ for some matrix $\mathbf{M}$. 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 $\mathbb{R}^m_{\geq}$ is always pointed. A pointed polyhedral cone admits a unique minimal set of generators (up to scalar multiple) [9].

LEMMA 3.1. *Suppose a polynomial dynamical system $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$ admits a WR_0 realization $(V, E, \boldsymbol{\kappa})$ with ℓ connected components. Let $\mathbf{Y}_s$ be the matrix of source vertices, and let $\mathbf{W}$ be the matrix of net direction vectors of the polynomial dynamical system $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$. Let S be the associated linear space, and let $\mathbf{A}_{\boldsymbol{\kappa}}$ be the Kirchhoff matrix of the weighted E-graph $(V, E, \boldsymbol{\kappa})$. Then we have*

(i) $\mathbf{W} = \mathbf{Y}_s \mathbf{A}_{\boldsymbol{\kappa}}$ *and* $\ker \mathbf{W} = \ker \mathbf{A}_{\boldsymbol{\kappa}}$,
(ii) $S = \mathrm{im}\, \mathbf{W}$, *and the rank of* $\mathbf{W}$ *is* $|V| - \ell$,

(iii) $\ker \mathbf{W} \cap \mathbb{R}^m_{\geq}$ *is a pointed polyhedral cone, and*
(iv) *a minimal set of generators for* $\ker \mathbf{W} \cap \mathbb{R}^m_{\geq}$ *has* ℓ *elements, whose supports correspond to the connected components of* (V, E).

Proof. Consider the matrix $\mathbf{Y}_s = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_m)$, whose columns correspond to the monomials in $\boldsymbol{f}(\boldsymbol{x})$. Because the realization (V, E) is weakly reversible, all vertices in V are sources; in particular, $\{\boldsymbol{y}_i\}_{i=1}^m \subseteq V$. Moreover, because the deficiency of (V, E) is zero, by [12, Proposition 3.5], the net direction vector from any $\boldsymbol{y}_i$ is nonzero, so in fact $V = \{\boldsymbol{y}_i\}_{i=1}^m$.

(i) By Definition 2.9, $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}) = \mathbf{W}\boldsymbol{x}^{\mathbf{Y}_s}$, and because $(V, E, \boldsymbol{\kappa})$ is a realization, we have $\boldsymbol{f}(\boldsymbol{x}) = \mathbf{Y}_s \mathbf{A}_{\boldsymbol{\kappa}} \boldsymbol{x}^{\mathbf{Y}_s}$. Since the coefficients of polynomial functions are uniquely determined, $\mathbf{W} = \mathbf{Y}_s \mathbf{A}_{\boldsymbol{\kappa}}$. Because $\dim(\ker \mathbf{Y}_s \cap \operatorname{im} \mathbf{A}_{\boldsymbol{\kappa}}) = \delta = 0$, we have $\ker \mathbf{W} = \ker \mathbf{A}_{\boldsymbol{\kappa}}$.

(ii) Note that

$$\operatorname{rank} \mathbf{W} = \operatorname{rank} \mathbf{A}_{\boldsymbol{\kappa}} = |V| - \ell = \dim S,$$

where the first and last equalities follow from $0 = \delta = \dim(\ker \mathbf{Y}_s \cap \operatorname{im} \mathbf{A}_{\boldsymbol{\kappa}}) = |V| - \ell - \dim S$, and the second equality follows from weak reversibility and Theorem 2.15. Clearly $\operatorname{im} \mathbf{W} \subseteq S$, so $\operatorname{im} \mathbf{W} = S$.

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

(iv) Let $\mathcal{B} = \{\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_\ell\}$ be a basis of $\ker \mathbf{A}_{\boldsymbol{\kappa}}$ as in Theorem 2.15, where $\boldsymbol{c}_p \geq \mathbf{0}$, and each $V_p = \{\boldsymbol{y}_i : i \in \operatorname{supp}(\boldsymbol{c}_p)\}$ is a connected component of (V, E). Clearly $\mathcal{B} \subseteq \ker \mathbf{W} \cap \mathbb{R}^m_{\geq}$; we claim that $\mathcal{B}$ is a *minimal* set of *generators* for the pointed cone.

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

$$\boldsymbol{\nu} = \sum_{p=1}^{\ell} \lambda_p \boldsymbol{c}_p$$

for some $\lambda_p \in \mathbb{R}$. By Theorem 2.15, each $\boldsymbol{c}_p$ 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 $\nu_i = \lambda_{p(i)} [\boldsymbol{c}_{p(i)}]_i$. Since $\boldsymbol{\nu}$, $\boldsymbol{c}_{p(i)} \in \mathbb{R}^m_{\geq}$, it must be the case that $\lambda_{p(i)} \geq 0$. In other words, $\mathcal{B}$ generates the cone $\ker \mathbf{W} \cap \mathbb{R}^m_{\geq}$. Because the vectors in $\mathcal{B}$ have disjoint supports, $\mathcal{B}$ is minimal. ∎

LEMMA 3.2. *If Algorithm* 1 *exits at lines* 3*,* 8*, or* 12*, then* $\dot{\boldsymbol{x}} = \sum_{i=1}^m \boldsymbol{x}^{\boldsymbol{y}_i} \boldsymbol{w}_i$ *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 $\{\boldsymbol{c}_1, \ldots, \boldsymbol{c}_\ell\}$ be a minimal set of generators of $\ker \mathbf{W} \cap \mathbb{R}^n_{\geq}$, and partition the vertices by $V_p := \operatorname{supp}(\boldsymbol{c}_p)$. If instead the algorithm exits at line 8, then again no WR$_0$ realization exists because WR$_0$ realizations have affinely independent connected components [13, Theorem 9]. Finally, exiting at line 12 means that some net direction vector $\boldsymbol{w}_i$ cannot be decomposed as edges from $\boldsymbol{y}_i$ 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). ∎

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, because it fails the **if** statement in line 12, all net direction vectors $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_m$ can be decomposed as edges from $\boldsymbol{y}_i$ to other vertices in V_p; thus 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 $\boldsymbol{c} := \boldsymbol{c}_p$. Suppose for a contradiction that $V^* \subsetneq U$ is a connected component of (V, E). Because the **if** statement in line 7 is false, U is affinely independent, so the linear subspaces

$$S(V^*) = \{\boldsymbol{y}_i - \boldsymbol{y}_j : \boldsymbol{y}_i, \boldsymbol{y}_j \in V^*\} \quad \text{and} \quad S(U \setminus V^*) = \{\boldsymbol{y}_i - \boldsymbol{y}_j : \boldsymbol{y}_i, \boldsymbol{y}_j \in U \setminus V^*\}$$

are linearly independent. Because $\boldsymbol{c} \in \ker \mathbf{W} \cap \mathbb{R}^m_{\geq}$ and $\operatorname{supp}(\boldsymbol{c}) = U$, we have

$$\mathbf{0} = \sum_{i \in V^*} c_i \boldsymbol{w}_i + \sum_{i \in U \setminus V^*} c_i \boldsymbol{w}_i, \tag{6}$$

with $c_i > 0$. Furthermore, the **if** statement in line 11 returning false implies that each $\boldsymbol{w}_i$ in (6) can be further decomposed as edges between vertices in U. For any $\boldsymbol{y}_i$ in V^*, which is a connected component, the net direction vector $\boldsymbol{w}_i$ is a positive linear combination of edge vectors between $\boldsymbol{y}_i$ and other vertices in V^*, so $\boldsymbol{w}_i \in S(V^*)$. In particular, $\boldsymbol{c}^* := \sum_{i \in V^*} c_i \boldsymbol{w}_i \in S(V^*)$. 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 $\boldsymbol{c}^*$ and $\boldsymbol{c} - \boldsymbol{c}^*$ are linearly independent. Both $\boldsymbol{c}^*$ and $\boldsymbol{c} - \boldsymbol{c}^*$ lie in the cone $\ker \mathbf{W} \cap \mathbb{R}^m_{\geq}$, so $\{\boldsymbol{c}_1, \ldots, \boldsymbol{c}_\ell\}$ is not a set of generators, which is a contradiction. ∎

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 [13, Theorem 9].

We claim that the minimal set of generators $\{\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_\ell\}$ forms a basis for $\ker \mathbf{W}$. Let $\boldsymbol{c} \in \ker \mathbf{W}$ be arbitrary. If $\boldsymbol{c}$ has nonnegative components, then it is a linear combination of $\boldsymbol{c}_p$'s. If $\boldsymbol{c} \notin \mathbb{R}^m_{\geq}$, then there exist sufficiently large constants $\mu_p > 0$ so that

$$\boldsymbol{c} + \sum_{p=1}^{\ell} \mu_p \boldsymbol{c}_p \in \mathbb{R}^m_{\geq}.$$

This vector is a nonnegative combination of $\boldsymbol{c}_1$, $\boldsymbol{c}_2, \ldots, \boldsymbol{c}_\ell$; thus, $\boldsymbol{c}$ is a linear combination of the generating vectors. Since $\mathbf{W} \in \mathbb{R}^{n \times |V|}$, we have $\operatorname{rank} \mathbf{W} = |V| - \ell$.

Let S be the associated linear space of (V, E), i.e., $S = \operatorname{span}\{\boldsymbol{y}_j - \boldsymbol{y}_i : \boldsymbol{y}_i \to \boldsymbol{y}_j \in E\}$. The falsity of the if statement in line 11 implies that $\operatorname{im} \mathbf{W} \subseteq S$, so $\dim S \geq |V| - \ell$. Hence, the deficiency of (V, E) is $\delta = |V| - \ell - \dim S \leq 0$. Because δ is always nonnegative, we conclude that $\delta = 0$. ∎

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

Proof. For weak reversibility, we need to show that each connected component is strongly connected. So without loss of generality, we assume (V, E) has one connected component. Because of deficiency zero, V is affinely independent and $\dim S = |V| - 1$, so $\delta = 0$. Moreover, $\dim(\ker \mathbf{Y} \cap \operatorname{im} \mathbf{A}_{\boldsymbol{\kappa}}) \leq \delta$ [24, Proposition 3.1],[2] so $\ker(\mathbf{Y}\mathbf{A}_{\boldsymbol{\kappa}}) = \ker \mathbf{A}_{\boldsymbol{\kappa}}$, and the generator $\boldsymbol{c}_1$ also spans $\ker \mathbf{A}_{\boldsymbol{\kappa}}$. By Theorem 2.15, $\boldsymbol{c}_1$ is supported on the terminal strongly connected component, which in this case is all of V. Therefore, (V, E) is in fact strongly connected. ∎

Remark 3.6. In the proof of Lemmas 3.3 and 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 $S(V_p)$:

$$\operatorname{span}\{\boldsymbol{y}_j - \boldsymbol{y}_i \colon \boldsymbol{y}_i, \boldsymbol{y}_j \in V_p\} = \operatorname{span}\{\boldsymbol{y}_j - \boldsymbol{y}_i \colon \boldsymbol{y}_i \to \boldsymbol{y}_j \in E_p\} = \operatorname{im} \mathbf{W}^{(p)},$$

where $\mathbf{W}^{(p)}$ has as its columns the net direction vectors of the vertices in V_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,*

$$\frac{d\boldsymbol{x}}{dt} = \sum_{i=1}^{m} \boldsymbol{x}^{\boldsymbol{y}_i} \boldsymbol{w}_i,$$

with distinct $\boldsymbol{y}_i \in \mathbb{Z}^n_{\geq}$, *and* $\boldsymbol{w}_i \in \mathbb{R}^n \setminus \{\mathbf{0}\}$, *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 the algorithm exits at lines 3, 8, or 12 by failing one of the **if** statements, or 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 WR_0 by Lemmas 3.4 and 3.5, respectively. The uniqueness of the realization follows from [12]. ∎

Remark 3.8. The uniqueness of the WR_0 realization is also a consequence of Algorithm 1. This is due to affine and linear independence, as well as the structure of $\ker \mathbf{W} = \ker \mathbf{A}_{\boldsymbol{\kappa}}$.

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 2.13 and 3.7.

THEOREM 3.9. *Suppose the system of differential equations*

$$\frac{d\boldsymbol{x}}{dt} = \sum_{i=1}^{m} \boldsymbol{x}^{\boldsymbol{y}_i} \boldsymbol{w}_i, \tag{7}$$

with distinct $\boldsymbol{y}_i \in \mathbb{Z}^n_{\geq}$ *and* $\boldsymbol{w}_i \in \mathbb{R}^n \setminus \{\mathbf{0}\}$, *passes Algorithm* 1. *Let* $\mathbf{W}$ *be the matrix of net direction vectors and* $S = \operatorname{im} \mathbf{W}$. *Then the following holds:*

[2] The author of [24] defines deficiency differently. He calls $\dim(\ker \mathbf{Y} \cap \operatorname{im} \mathbf{A}_{\boldsymbol{\kappa}})$ the deficiency, and Proposition 3.1 gives the inequality $\dim(\ker \mathbf{Y} \cap \operatorname{im} \mathbf{A}_{\boldsymbol{\kappa}}) \leq n - \ell - \dim S$, which is what we use here. In general, $\dim(\ker \mathbf{Y} \cap \operatorname{im} \mathbf{A}_{\boldsymbol{\kappa}}) = |V| - t - \dim S$, where t is the number of terminal strongly connected components [20].

(i) *A positive steady state* $\boldsymbol{x}^*$ *exists.*
(ii) *There is exactly one steady state within every invariant polyhedron* $(\boldsymbol{x}_0 + S) \cap \mathbb{R}^n_>$ *for any* $\boldsymbol{x}_0 \in \mathbb{R}^n_>$*, and it is complex-balanced.*
(iii) *Any positive steady state* $\boldsymbol{x}$ *satisfies* $\ln \boldsymbol{x} - \ln \boldsymbol{x}^* \in S^\perp$.
(iv) *The function*

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

defined on $\mathbb{R}^n_>$*, is a strict Lyapunov function of* (7) *within every invariant polyhedron* $(\boldsymbol{x}_0 + S) \cap \mathbb{R}^n_>$*, 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

$$\begin{aligned} \frac{dx_1}{dt} &= -12x_1 + x_3^2, \\ \frac{dx_2}{dt} &= 14x_1 - 4x_2^2 + 8x_3^2, \\ \frac{dx_3}{dt} &= 10x_1 + 4x_2^2 - 10x_3^2. \end{aligned} \tag{8}$$

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

$$\mathbf{Y}_s = \begin{pmatrix} \boldsymbol{y}_1 & \boldsymbol{y}_2 & \boldsymbol{y}_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix},$$
$$\mathbf{W} = \begin{pmatrix} \boldsymbol{w}_1 & \boldsymbol{w}_2 & \boldsymbol{w}_3 \end{pmatrix} = \begin{pmatrix} -12 & 0 & 1 \\ 14 & -4 & 8 \\ 10 & 4 & -10 \end{pmatrix},$$

respectively, which are inputs to Algorithm 1. Let $V = \{\boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_3\} \subset \mathbb{Z}^n_\geq$. A generator for the cone $\ker \mathbf{W} \cap \mathbb{R}^m_\geq$ is $\boldsymbol{c} = (48/1441, 120/131, 576/1441)^\top$. In the notation of Algorithm 1, $V_1 = [1, 3]$. Clearly V is affinely independent and the net direction vectors admit the following unique decompositions:

$$\begin{aligned} \boldsymbol{w}_1 &= 7(\boldsymbol{y}_2 - \boldsymbol{y}_1) + 5(\boldsymbol{y}_3 - \boldsymbol{y}_1), \\ \boldsymbol{w}_2 &= 2(\boldsymbol{y}_3 - \boldsymbol{y}_2), \\ \boldsymbol{w}_3 &= (\boldsymbol{y}_1 - \boldsymbol{y}_3) + 4(\boldsymbol{y}_2 - \boldsymbol{y}_3). \end{aligned}$$

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 $(a_1 s^2, a_2 s, a_3 s)$ for some constants $a_i > 0$. In fact, the set of steady states is given by

$$(x_1^*, x_2^*, x_3^*) = \left(3s^2, \frac{\sqrt{330}}{2}s, 6s\right),$$

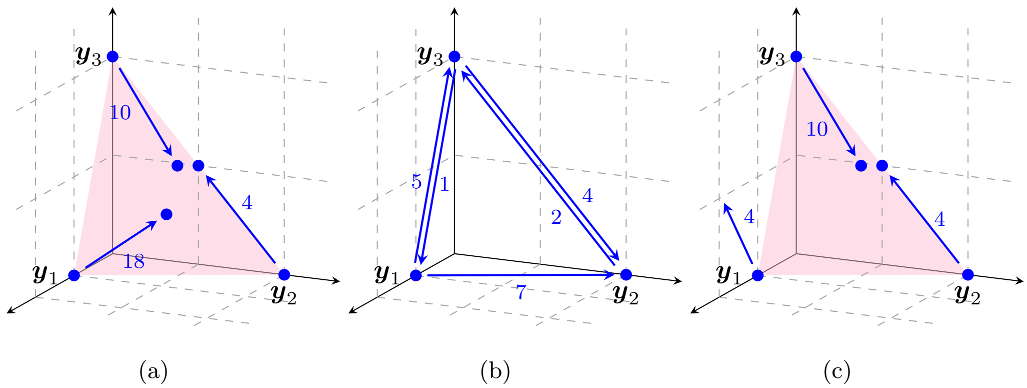

FIG. 4. (a) *A weighted E-graph realizing* (8) *from Example* 3.10*, which admits* (b) *a WR$_0$ realization.* (c) *A weighted E-graph realizing* (9) *from Example* 3.11 *that does not admit a WR$_0$ realization.*

and an explanation for the coefficients above will be provided in Theorem 3.12.

Example 3.11. Consider the system of differential equations

$$\begin{aligned} \frac{dx_1}{dt} &= -\frac{1}{2}x_1 + x_3^2, \\ \frac{dx_2}{dt} &= -2x_1 - 4x_2^2 + 8x_3^2, \\ \frac{dx_3}{dt} &= 3x_1 + 4x_2^2 - 10x_3^2. \end{aligned} \tag{9}$$

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

$$\mathbf{W} = \begin{pmatrix} \boldsymbol{w}_1 & \boldsymbol{w}_2 & \boldsymbol{w}_3 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & 0 & 1 \\ -2 & -4 & 8 \\ 3 & 4 & -10 \end{pmatrix},$$

whose kernel is spanned by $\boldsymbol{c} = (2, 1, 1)^\top$. As in the previous example, the vertices $\boldsymbol{y}_1$, $\boldsymbol{y}_2$, and $\boldsymbol{y}_3$ are affinely independent. However, $\boldsymbol{w}_1 \notin \text{Cone}\{\boldsymbol{y}_j - \boldsymbol{y}_1 \colon j = 2, 3\}$, so no WR$_0$ realization exists.

3.2. On the implementation and computational complexity of Algorithm 1.

Before proceeding, we briefly remark on Algorithm 1 and how it compares with an existing algorithm for WR$_0$ realizations in [34].

The algorithm we propose to find a WR$_0$ realization for $\dot{\boldsymbol{x}} = \mathbf{W}\boldsymbol{x}^{\mathbf{Y}_s}$ consists of three steps:

1. Check for the existence of a set of generators $\{\boldsymbol{c}_1, \ldots, \boldsymbol{c}_\ell\}$ with disjoint supports for the cone $\ker \mathbf{W} \cap \mathbb{R}^m_{\geq}$.
2. On the support V_p of each generator $\boldsymbol{c}_p$, check that $\{\boldsymbol{y}_i \colon i \in V_p\}$ is affinely independent.
3. For each $i \in V_p$, solve for (nonnegative) solutions κ_{ij} to $\boldsymbol{w}_i = \sum_{j \in V_p, j \neq i} \kappa_{ij}(\boldsymbol{y}_j - \boldsymbol{y}_i)$.

In reality, step 2 is no more than a rank condition, that the rank of $\{\boldsymbol{y}_i - \boldsymbol{y}_{i_0} \colon \boldsymbol{y}_i \in V_p\}$ is equal to $|V_p| - 1$, where $\boldsymbol{y}_{i_0}$ is a distinguished vertex in V_p. At first sight, it seems step 3 is a linear feasibility problem; however, it is in fact solving a linear *system.* By the time we reach step 3, we have already verified that, for a fixed i, the set $\{\boldsymbol{y}_j - \boldsymbol{y}_i \colon j \in V_p, j \neq i\}$ is linearly independent. Hence the system of linear equations $\boldsymbol{w}_i = \sum_{j\in V_p, j\neq i} \kappa_{ij}(\boldsymbol{y}_j - \boldsymbol{y}_i)$ either has no real solution, or there is a unique solution $(\kappa_{ij})_{ij}$, in which case we simply check whether $\kappa_{ij} \geq 0$ or not.

The "simplest" way to implement step 1 is to compute all the extreme rays of the cone $\ker \mathbf{W} \cap \mathbb{R}^m_{\geq}$. A much more efficient way to implement step 1 is via a series of linear programming problems. We find the first generator of the cone $\ker \mathbf{W} \cap \mathbb{R}^m_{\geq}$ by solving

$$\begin{aligned} \text{Minimize} \qquad & \boldsymbol{x}^\top \mathbf{1} \\ \text{subjected to} \qquad & \mathbf{W}\boldsymbol{x} = \mathbf{0}\,, \\ & x_1 = 1\,, \\ & \boldsymbol{x} \geq \mathbf{0}, \end{aligned}$$

because we are looking for vectors in $\ker \mathbf{W}$ that are nonnegative and nonzero and have minimal support. Denote the solution of the problem above by $\boldsymbol{c}_1$, and let $\Lambda = \operatorname{supp}(\boldsymbol{c}_1)$. We can then run another (analogous) linear programming problem, where we *remove* the columns whose indices are in Λ from the matrix $\mathbf{W}$. Let $\boldsymbol{c}_2$ be the solution to this second problem, augmented by zeros for indices in Λ. Replace the index set by $\Lambda = \bigcup_{p=1}^{2} \operatorname{supp}(\boldsymbol{c}_p)$, and repeat, until $\Lambda = \{1, 2, \dots, m\}$. Of course, if at any point the process fails, this means there is no such set of generators with disjoint support for the cone, and therefore no WR_0 realization exists. Hence, step 1 can be attained with the same computational cost as the solving of a number of linear programming problems (and this number is no larger than the number of connected components).

In the literature, there are also other approaches for computing WR_0 realizations. Technically speaking, these require the set of vertices as input; however, for WR_0 realizations, one can use the exponents of the monomials [11, Theorem 4.12]. The authors of [30] proposed a mixed-integer linear programming method to find a weakly reversible realization with minimal deficiency. The authors of [34] further reduced it to a linear programming method for the case of deficiency zero realizations. The methods in [30, 34] are algebraic in nature, while the algorithm proposed here relies on the geometric interpretation of deficiency.

3.3. The set of positive steady states of a $\mathbf{WR_0}$ 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 a WR_0 realization.

For any $\boldsymbol{z} \in \mathbb{R}^n$ and $\boldsymbol{x} \in \mathbb{R}^n_{>}$, define the componentwise operations $\exp \boldsymbol{z} = (e^{z_1}, e^{z_2}, \dots, e^{z_n})^\top$ and $\log(\boldsymbol{x}) = (\log x_1, \log x_2, \dots, \log x_n)^\top$. We extend these operations to sets. If $Z \subseteq \mathbb{R}^n$, then $\exp(Z) = \{\exp \boldsymbol{z} \colon \boldsymbol{z} \in Z\}$, and if $X \subseteq \mathbb{R}^n_{>}$, then $\log(X) = \{\log \boldsymbol{x} \colon \boldsymbol{x} \in X\}$.

Assume that the polynomial dynamical system

$$\frac{d\boldsymbol{x}}{dt} = \sum_{i=1}^{m} \boldsymbol{x}^{\boldsymbol{y}_i} \boldsymbol{w}_i, \tag{10}$$

with distinct $\boldsymbol{y}_i \in \mathbb{Z}^n_{\geq}$ and $\boldsymbol{w}_i \in \mathbb{R}^n \setminus \{\mathbf{0}\}$, passes Algorithm 1; i.e., it admits a WR_0 realization $(V, E, \boldsymbol{\kappa})$. Without loss of generality, assume the vertices are ordered according to the 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 $\{\boldsymbol{c}_1,\boldsymbol{c}_2,\ldots,\boldsymbol{c}_\ell\}$ be a minimal set of generators of $\ker \mathbf{W}\cap\mathbb{R}^m_{\geq}$, ordered in an analogous way. From Algorithm 1, we know that the supports of the vectors $\boldsymbol{c}_1$, $\boldsymbol{c}_2,\ldots,\boldsymbol{c}_\ell$ correspond to the connected components of (V,E).

Let $\boldsymbol{c}_1=(\alpha_1,\alpha_2,\ldots,\alpha_{m_1},0,\ldots,0)^\top$. Define matrix $\mathbf{D}_1\in\mathbb{R}^{(m_1-1)\times n}$ whose rows are the affine vectors from $\boldsymbol{y}_1$ to the remaining vertices of V_1, and define vector $\boldsymbol{J}_1\in\mathbb{R}^{m_1-1}$ using the log-differences of the components of $\boldsymbol{c}_1$, i.e.,

$$\mathbf{D}_1=\begin{pmatrix}\boldsymbol{y}_2-\boldsymbol{y}_1\\ \boldsymbol{y}_3-\boldsymbol{y}_1\\ \vdots\\ \boldsymbol{y}_{m_1}-\boldsymbol{y}_1\end{pmatrix}\quad\text{and}\quad \boldsymbol{J}_1=\begin{pmatrix}\log(\alpha_2/\alpha_1)\\ \log(\alpha_3/\alpha_1)\\ \vdots\\ \log(\alpha_{m_1}/\alpha_1)\end{pmatrix}.$$

For the connected component (V_p,E_p), define $\mathbf{D}_p$ and $\boldsymbol{J}_p$ in a similar fashion. Then define

$$\mathbf{D}=\begin{pmatrix}\mathbf{D}_1\\ \hline \mathbf{D}_2\\ \hline \vdots\\ \hline \mathbf{D}_\ell\end{pmatrix}\in\mathbb{R}^{(m-\ell)\times n}\quad\text{and}\quad \boldsymbol{J}=\begin{pmatrix}\boldsymbol{J}_1\\ \hline \boldsymbol{J}_2\\ \hline \vdots\\ \hline \boldsymbol{J}_\ell\end{pmatrix}\in\mathbb{R}^{m-\ell}. \tag{11}$$

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

Proof. First we prove that the linear system $\mathbf{D}\boldsymbol{z}=\boldsymbol{J}$ is solvable. Consider $\mathbf{D}_1$. The vertices $\boldsymbol{y}_1$, $\boldsymbol{y}_2,\ldots,\boldsymbol{y}_{m_1}$ in the first connected component are affinely independent, so the rows of $\mathbf{D}_1$ are linearly independent. Moreover, as noted in Remark 3.6, the row-space of $\mathbf{D}_1$ is the associated linear subspace $S(V_1)$. Therefore $\operatorname{rank}\mathbf{D}_1=m_1-1$, and the matrix $\mathbf{D}_1$ is surjective onto $\mathbb{R}^{m_1-1}$.

Similarly, for each $p=2,\ldots,\ell$, the row-space of the matrix $\mathbf{D}_p$ is $S(V_p)$, and the matrix $\mathbf{D}_p$ is surjective. In addition, because the realization $(V,E,\boldsymbol{\kappa})$ 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 $\mathbf{D}$ are linearly independent. Consequently, $\mathbf{D}$ is surjective, and the system $\mathbf{D}\boldsymbol{z}=\boldsymbol{J}$ is solvable.

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

$$\mathbf{0}=\sum_{i=1}^{m}\boldsymbol{x}^{\boldsymbol{y}_i}\boldsymbol{w}_i.$$

In other words, $(\boldsymbol{x}^{\boldsymbol{y}_1},\ldots,\boldsymbol{x}^{\boldsymbol{y}_m})^\top$ lies in the steady state flux cone $\ker\mathbf{W}\cap\mathbb{R}^m_{>}$. 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 $\boldsymbol{x}^{\boldsymbol{y}_j}=\lambda\alpha_j$ for $j=1,\,2,\ldots,m_1$, where α_j are components of the generator $\boldsymbol{c}_1$. Thus

$$\boldsymbol{x}^{\boldsymbol{y}_j-\boldsymbol{y}_1}=\frac{\alpha_j}{\alpha_1}$$

for $j=2,3,\ldots,m_1$. Taking the logarithm of both sides, we obtain the system $\mathbf{D}_1\boldsymbol{z}=\boldsymbol{J}_1$ with $\boldsymbol{z}=\log\boldsymbol{x}$.

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

3.4. Extension to polynomial systems with unspecified coefficients. If, instead of (10), we need to analyze

$$\frac{d\boldsymbol{x}}{dt}=\sum_{i=1}^{m}a_i\boldsymbol{x}^{\boldsymbol{y}_i}\boldsymbol{w}_i \tag{12}$$

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 $(V,E,\boldsymbol{\kappa})$ if and only if the system* (10) *admits a WR_0 realization $(V,E,\boldsymbol{\kappa}^*)$. 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 $(V,E,\boldsymbol{\kappa})$ shares the same set of edges as $(V,E,\boldsymbol{\kappa}^*)$. Because the deficiency is characterized by affine and linear independence of the connected components, and the two graphs share the same structure, $(V,E,\boldsymbol{\kappa})$ is WR_0 if and only if $(V,E,\boldsymbol{\kappa}^*)$ is.

Suppose $(V,E,\boldsymbol{\kappa}^*)$ is a realization of (10). Then in $(V,E,\boldsymbol{\kappa})$, the net direction vector from $\boldsymbol{y}_i$ can be expanded using the realization $(V,E,\boldsymbol{\kappa}^*)$, since

$$a_i\boldsymbol{w}_i=a_i\sum_{(i,j)\in E}\kappa_{ij}^*(\boldsymbol{y}_j-\boldsymbol{y}_i)=\sum_{(i,j)\in E}\kappa_{ij}(\boldsymbol{y}_j-\boldsymbol{y}_i).$$

Therefore, $(V,E,\boldsymbol{\kappa})$ realizes (12). ∎

3.5. 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; actually, such as system will admit a *linear* strict Lyapunov function, and therefore all its solutions have to converge to the boundary of the positive orthant, or to infinity [17, 19, 25]. Actually, such realizations are special examples of mass-action systems generated by E-graphs 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

$$\sum_{(i,j)\in E}\alpha_{ij}(\boldsymbol{y}_j-\boldsymbol{y}_i)=\mathbf{0}. \tag{13}$$

It is not hard to show that a polynomial dynamical system of the form (10) has a realization $(V,E,\boldsymbol{\kappa})$, where (V,E) is *not* consistent if and only if

$$\ker\mathbf{W}\cap\mathbb{R}^m_>=\emptyset. \tag{14}$$

If a given polynomial dynamical system admits a realization that is not consistent, then it cannot admit any positive steady state; hence, it cannot admit any 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 (14), then that step will decide whether our given system (10) has a realization that is not consistent, and, in particular, that step will also find all cases where our given system might a deficiency zero realization that is *not* weakly reversible.

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