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Node Balanced Steady States: Unifying and Generalizing Complex and Detailed Balanced Steady States

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Abstract

We introduce a unifying and generalizing framework for complex and detailed balanced steady states in chemical reaction network theory. To this end, we generalize the graph commonly used to represent a reaction network. Specifically, we introduce a graph, called a *reaction graph*, that has one edge for each reaction but potentially multiple nodes for each complex. A special class of steady states, called *node balanced steady states*, is naturally associated with such a reaction graph. We show that complex and detailed balanced steady states are special cases of node balanced steady states by choosing appropriate reaction graphs. Further, we show that node balanced steady states have properties analogous to complex balanced steady states, such as uniqueness and asymptotical stability in each stoichiometric compatibility class. Moreover, we associate an integer, called the *deficiency*, to a reaction graph that gives the number of independent relations in the reaction rate constants that need to be satisfied for a positive node balanced steady state to exist.

The set of reaction graphs (modulo isomorphism) is equipped with a partial order that has the complex balanced reaction graph as minimal element. We relate this order to the deficiency and to the set of reaction rate constants for which a positive node balanced steady state exists.

1 Introduction

Complex balanced steady states of a chemical reaction network are perhaps the most well-described class of steady states in chemical reaction network theory. Horn and Jackson built a theory for positive complex balanced steady states and showed that they are unique and asymptotically stable relatively to the linear invariant subspace they belong to [15]. Around the same time, Feinberg studied a structural network property, called the *deficiency*, and derived parameter-independent theorems concerning the existence of complex balanced steady states, based on the deficiency [5, 8].

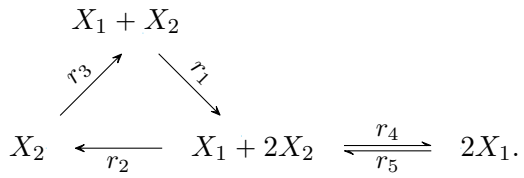
The graphical structure of a reaction network also plays an integral part of the present work. In fact we will not stick to a single graphical representation of a reaction network but to a collection of graphical representations, and build a theory that extends the classical theory of complex and detailed balanced steady states. In this theory detailed and complex balanced steady states arise as particular examples of the same phenomenon.

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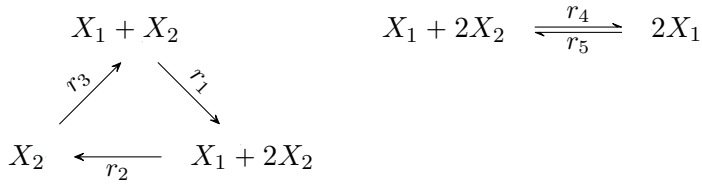
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The standard graphical representation of a reaction network is a digraph where the nodes are the complexes of the network and the directed edges are the reactions, as in the example below with two species. This representation appears so natural that a reaction network might be defined directly as a digraph with nodes labeled by linear combinations of the species [4] as follows:



(1)

In addition, we also consider digraphs where the same complex in different reactions might or might not be represented by the same node. These graphs, called *reaction graphs* (Definition 1), can be obtained from the standard graph by duplication of nodes. As an example, consider the digraph



(2)

where the node with label $X_1 + 2X_2$ is duplicated, such that the digraph (1) is split into two components. The digraph (1) is obtained by collapsing the two nodes for $X_1 + 2X_2$, that is, by reversing the duplication step.

We associate a *novel* type of steady states, called *node balanced steady states* with a given reaction graph (Definition 7). To set the idea, recall that a complex balanced steady state is an equilibrium point such that, for any complex y, the sum of the reaction flows out of y equals the sum of the reaction flows going into y. To illustrate this, consider the digraph (1) with mass-action kinetics. A complex balanced steady state $x = (x_1, x_2)$ fulfills

$$\kappa_1 x_1 x_2 = \kappa_3 x_2, \qquad \kappa_3 x_2 = \kappa_2 x_1 x_2^2, \qquad \kappa_2 x_1 x_2^2 + \kappa_4 x_1 x_2^2 = \kappa_1 x_1 x_2 + \kappa_5 x_1^2, \tag{3}$$

where κ_i is the reaction rate constant of the i-th reaction.

Analogously, we define a node balanced steady state with respect to a given reaction graph as a steady state fulfilling equations similar to (3), derived from the particular reaction graph. Thus, under mass-action kinetics, a node balanced steady state of the digraph (2) fulfills

$$\kappa_1 x_1 x_2 = \kappa_3 x_2, \qquad \kappa_3 x_2 = \kappa_2 x_1 x_2^2, \qquad \kappa_2 x_1 x_2^2 = \kappa_1 x_1 x_2, \qquad \kappa_4 x_1 x_2^2 = \kappa_5 x_1^2. \tag{4}$$

The equations in (3) can be obtained by adding the last two equations in (4). A node balanced steady state of the digraph (2) is therefore in particular complex balanced.

In this context complex balanced steady states are instances of node balanced steady states for a particular choice of reaction graph. As we will see, detailed balanced steady states are also node balanced steady states for a specific reaction graph. It is therefore not surprising that node balanced steady states satisfy properties analogous to complex (and detailed) balanced steady states. In fact, we show that many classical results carry over to node balanced steady states and might be defined in terms of properties of reaction graphs, rather than reaction networks. Particularly, if there is one positive node balanced steady state, then all steady states are node balanced, and if this is so, there is one positive node balanced steady state in each stoichiometric compatibility class. Furthermore, this steady state is asymptotically

stable relatively to the class (Theorem 1). Additionally, we give algebraic conditions on the reaction rate constants for which node balanced steady states exist with respect to a given reaction graph (Theorem 2). There are as many algebraic relations as the *deficiency* of the reaction graph. This also generalizes known results for complex balanced steady states [3].

We define a natural partial order on the set of reaction graphs. The standard graphical representation of a reaction network, as in (1), is the unique minimal element. Intuitively, a reaction graph G is smaller than, or included in, another reaction graph G', $G \preceq G'$, if G can be obtained from G' by collapsing some of the nodes of G'. We will show that if $G \preceq G'$, then the deficiency of G is smaller than or equal to that of G' (Proposition 4). As an example, the reaction graph in (1) is smaller than that of (2), but their deficiencies are the same.

Horn and Jackson showed that conditions for complex and detailed balanced steady states could be stated in terms of symmetry conditions on the reaction rates [15]. They also speculated that perhaps there were other classes of networks for which the steady states fulfilled similar symmetry conditions. We show that node balanced steady states might indeed be defined in terms of symmetry conditions, similar to those of Horn and Jackson.

The motivation for this work comes from the desire to build a general unifying framework for complex and detailed balanced steady states. However, as a consequence of our results, we are additionally able to state sufficient conditions on the reaction rate constants of a network such that a part of the network is at steady state whenever the whole system is at steady state. This is a relevant question in the context of biological modeling, since it is often the case that only subnetworks of a system are studied. It is therefore natural to wonder whether the small network is at steady state when the whole network is, and *vice versa*.

The structure of the paper is as follows. In the next section we introduce reaction networks and reaction graphs, together with basic properties of reaction graphs. In Section 3, we define node balanced steady states and discuss their properties. After that, in Section 4 and 5, we discuss the symmetry conditions of Horn and Jackson, and the relationship between a part and the whole of a reaction network. Finally, in Section 6, we provide proofs of the main theorems on node balanced steady states.

2 Reaction networks and reaction graphs

We let $\mathbb{R}^n_{\geqslant 0}$ and $\mathbb{R}^n_{>0}$ denote the nonnegative and positive orthants of $\mathbb{R}^n$, respectively. If $x \in \mathbb{R}^n_{>0}$ ($\mathbb{R}^n_{\geqslant 0}$), then we say that x is positive (nonnegative). Similarly, $\mathbb{Z}_{\geqslant 0}$ denotes the nonnegative integers. If $v_1, \ldots, v_k \in \mathbb{R}^n$ are vectors, then $\langle v_1, \ldots, v_k \rangle$ denotes the linear subspace generated by the vectors.

2.1 Reaction networks

This section introduces reaction networks and their associated ODE systems [7, 13]. A *reaction network* (or simply a network) is a triplet $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ where $\mathcal{S}$, $\mathcal{C} \subseteq \mathbb{Z}^{\mathcal{S}}_{\geqslant 0}$ and $\mathcal{R} \subseteq \mathcal{C} \times \mathcal{C}$ are finite sets, called respectively the *species, complex* and *reaction* set. We implicitly assume the sets are numbered and let

$$\mathcal{S} = \{X_1, \ldots, X_n\}, \quad \mathcal{C} = \{y_1, \ldots, y_m\}, \quad \text{and} \quad \mathcal{R} = \{r_1, \ldots, r_p\},$$

such that n, m, and p are their respective cardinalities. Hence $\mathbb{Z}^{\mathcal{S}}_{\geqslant 0} \cong \mathbb{Z}^n_{\geqslant 0}$, and a complex can be identified with a linear combination of species $y = (\lambda_1, \ldots, \lambda_n) = \sum_{i=1}^n \lambda_i X_i$. We further assume that $(y, y) \notin \mathcal{R}$, any $y \in \mathcal{C}$ is in at least one reaction and any $S \in \mathcal{S}$ is in at least one complex. In that case, $\mathcal{C}$ and $\mathcal{S}$ can be found from $\mathcal{R}$, and $\mathcal{N}$ is said to be *generated* from $\mathcal{R}$.

An element $r = (y, y')$ of $\mathcal{R}$ is written as $r\colon y \to y'$ or just $y \to y'$. A reaction $y \to y' \in \mathcal{R}$ is *reversible* if $y' \to y \in \mathcal{R}$ as well. If this is not the case, then the reaction is *irreversible*. A pair of reactions $y \to y'$ and $y' \to y$ is called a reversible reaction pair and denoted by $y \rightleftharpoons y'$. A reaction network is *reversible* if all reactions of the network are reversible.

The *stoichiometric matrix* $N \in \mathbb{R}^{n\times p}$ is the matrix with j-th column $N_j = y' - y$ where $r_j\colon y \to y'$. The columns of N generate the so-called *stoichiometric subspace* S of $\mathbb{R}^n$. We define $s = \operatorname{rank}(N) = \dim(S)$.

We let x_i denote the concentration of species X_i. A kinetics v for a reaction network is a $\mathcal{C}^1$-function from $\mathbb{R}^n_{\geqslant 0}$ to $\mathbb{R}^p_{\geqslant 0}$ such that $v(\mathbb{R}^n_{>0}) \subseteq \mathbb{R}^p_{>0}$. The j-th coordinate, v_j, is called the *rate function* of r_j. The main example of kinetics is *mass-action kinetics*, where

$$v_j(x) = \kappa_j x^y = \kappa_j \prod_{i=1}^{n} x_i^{\lambda_i}, \qquad \text{for} \quad r_j\colon y \to y', \quad \text{and} \quad y = (\lambda_1, \ldots, \lambda_n), \tag{5}$$

and $\kappa_j > 0$ denotes the *reaction rate constant* of r_j. By convention, $0^0 = 1$. Whenever the numbering of $\mathcal{R}$ is irrelevant, we write $v_{y\to y'}$ and $\kappa_{y\to y'}$, instead of v_j and κ_j, respectively.

Given a kinetics v, the evolution of the species concentrations over time is modeled by a system of ODEs,

$$\frac{dx}{dt} = Nv(x), \qquad x \in \mathbb{R}^n_{\geqslant 0}. \tag{6}$$

For reasonable kinetics, including mass-action kinetics, the solution of (6) is in the positive (nonnegative) orthant for all positive times in the interval of definition, if the initial condition is [20]. Furthermore, the solution is confined to one of the nonnegative polytopes known as the *stoichiometric compatibility classes*

$$\mathcal{P}_{x_0} = (x_0 + S) \cap \mathbb{R}^n_{\geqslant 0},$$

where $x_0 \in \mathbb{R}_{\geqslant 0}$ is the initial condition.

The *steady states* of (6) are the nonnegative solutions to the equation $Nv(x) = 0$. For mass-action kinetics, this equation becomes:

$$\sum_{r_j\colon y\to y'} \kappa_j x^y (y' - y) = 0, \qquad x \in \mathbb{R}^n_{\geqslant 0}. \tag{7}$$

Example 1 (part A). We use a variant of a reaction network in [15, equation (7.3)] and [9, Example 2.3] as a 'running' example throughout the paper. The set $\mathcal{R}$ of reactions consists of

$$\begin{array}{llllll} r_1\colon & 3X_1 \to X_1 + 2X_2 & r_2\colon & X_1 + 2X_2 \to 3X_2 & r_3\colon & 3X_2 \to 2X_1 + X_2 \\ r_4\colon & 2X_1 + X_2 \to 3X_1 & r_5\colon & 3X_1 \to 3X_2 & r_6\colon & 3X_2 \to 3X_1, \end{array}$$

with $\mathcal{C} = \{3X_1, X_1 + 2X_2, 3X_2, 2X_1 + X_2\}$ and $\mathcal{S} = \{X_1, X_2\}$. There is one reversible reaction pair, r_5 and r_6, and four irreversible reactions. The stoichiometric matrix is

$$N = \begin{pmatrix} -2 & -1 & 2 & -1 & -3 & 3 \\ 2 & 1 & -2 & 1 & 3 & -3 \end{pmatrix},$$

with rank $s = 1$. Thus, the stoichiometric compatibility classes $(x_0 + \langle(-1, 1)\rangle) \cap \mathbb{R}^2_{\geqslant 0}$ are one-dimensional. Mass-action kinetics implies $v(x) = (\kappa_1 x_1^3, \kappa_2 x_1 x_2^2, \kappa_3 x_2^3, \kappa_4 x_1^2 x_2, \kappa_5 x_1^3, \kappa_6 x_2^3)$.

2.2 Reaction graphs

In this subsection we introduce novel graphical representations of a reaction network, the main object of this work.

Definition 1. Let $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ be a reaction network. A *reaction graph* associated with $\mathcal{N}$ is a node labeled digraph $G = (V_G, E_G, Y)$ with no isolated nodes, where $V_G = \{1, \dots, m_G\}$ and

(i) Y is a surjective labeling of the node set with values in $\mathcal{C}$:

$$V_G \xrightarrow{Y} \mathcal{C}, \qquad \text{such that} \qquad i \mapsto Y_i,$$

(ii) Y induces a bijection R between E_G and $\mathcal{R}$ as follows:

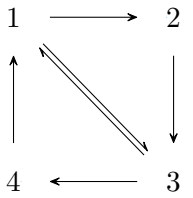
$$E_G \xrightarrow{R} \mathcal{R}, \qquad \text{such that} \qquad i \to j \quad \mapsto \quad R_{i\to j} = Y_i \to Y_j.$$

We say that a reaction graph is *weakly reversible* if all connected components of G are strongly connected, that is, there exists a directed path between two nodes, whenever there is a directed path between the nodes in opposite direction.

In what follows, we generically denote a complex of a network as y_i and a label of a node in a reaction graph as Y_i. For a reaction graph G', we denote objects related to it with $'$. Note that two nodes can have the same label in $\mathcal{C}$, but each reaction of $\mathcal{N}$ corresponds to exactly one edge of G. For two reaction graphs G, G' of $\mathcal{N}$, the bijections R, R' induce a correspondence $R^{-1} \circ R'$ between $E_{G'}$ and E_G: An edge $i' \to j'$ of G' *corresponds* to the edge $i \to j$ of G, if the two edges map to the same reaction of $\mathcal{N}$.

Any permutation of the node set V_G of a reaction graph gives an identical reaction graph, except for the numbering of the nodes. In the Introduction, 'reaction graph' was used in the sense of 'up to a numbering of the nodes' without mentioning it explicitly.

Example 1 (part B). The following digraph and labeling function



$$Y_1 = 3X_1, \qquad Y_2 = X_1 + 2X_2,$$
$$Y_3 = 3X_2, \qquad Y_4 = 2X_1 + X_2,$$

define a reaction graph for the reaction network in Example 1 (part A). This reaction graph is weakly reversible. In general we draw the node labels next to the nodes and add labels (r_j) to the edges, as in the digraph G_1 of Figure 1. The edge labels are redundant information, because the bijection R of a reaction graph (V_G, E_G, Y) is explicitly determined. However, it makes comparison between reaction graphs easier.

Figure 1 shows seven reaction graphs for the reaction network in Example 1 (part A) that will be used to illustrate results. The reaction graphs except for G_5, G_6 and G_7 are weakly reversible.

The following definition names some special reaction graphs. Recall that we assume that numberings of the reaction and complex sets are given.

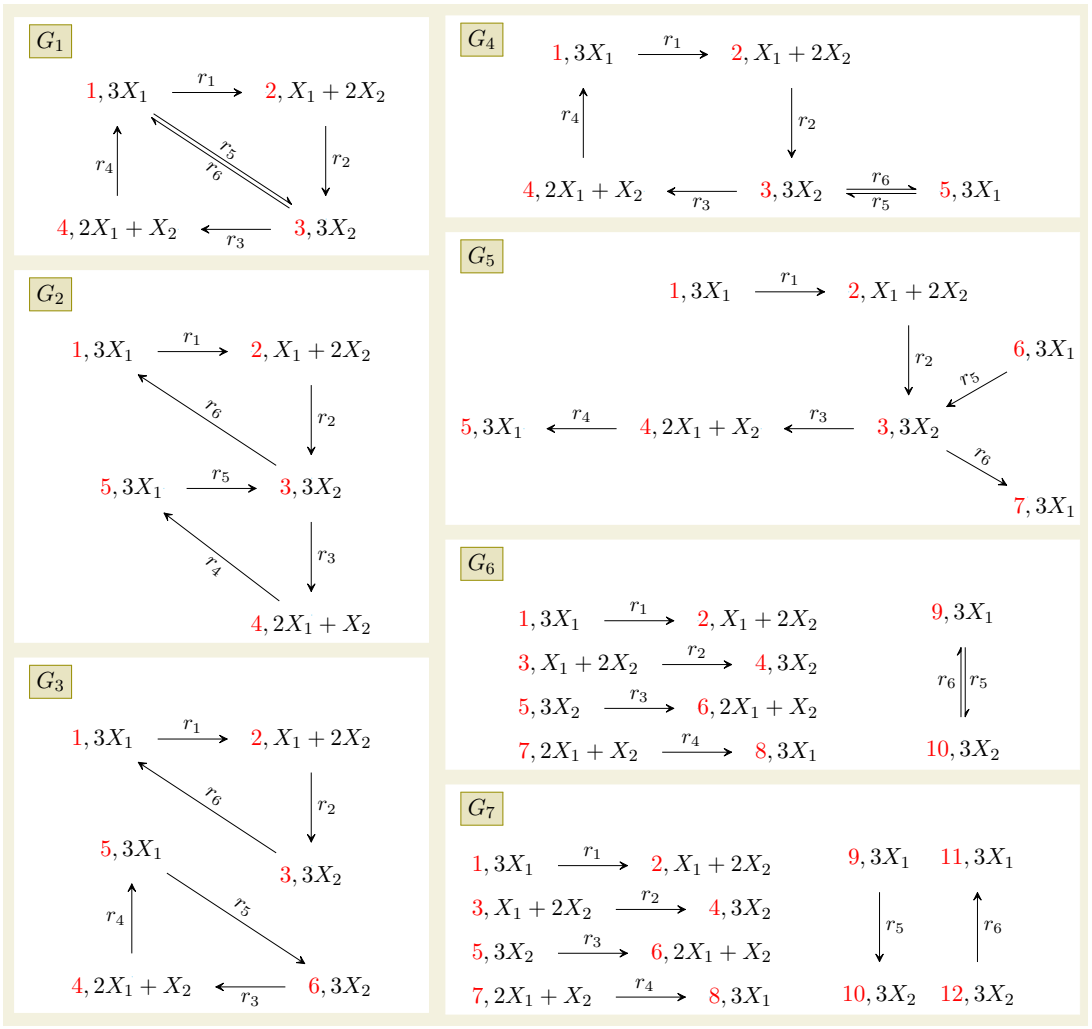


Figure 1: Reaction graphs for the network in Example 1 (part A). Reaction labels r_j are added for convenience.

Definition 2. Let $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ be a reaction network.

- A *complex reaction graph* G is a reaction graph with m nodes such that the labeling Y is a bijection between V_G and $\mathcal{C}$. The *canonical complex reaction graph* fulfills

$$Y_j = y_j, \qquad j = 1, \dots, m.$$

- A *detailed reaction graph* is a reaction graph with one connected component per reversible reaction pair and one per irreversible reaction.

- A *split reaction graph* is a reaction graph with $2p$ nodes and one connected component per reaction. The *canonical split reaction graph* fulfills

$$Y_{2j-1} = y, \qquad Y_{2j} = y', \qquad \text{if} \quad r_j \colon y \to y', \quad \text{for all } j = 1, \dots, p.$$

- We say that $\mathcal{N}$ *is weakly reversible* if any complex reaction graph is weakly reversible.

Example 1 (part C). Consider the reaction graphs in Figure 1. The reaction graph G_1 is a complex reaction graph, G_6 is a detailed reaction graph and G_7 is a split reaction graph (in fact, the canonical split reaction graph). The network is weakly reversible.

Intuitively, any reaction graph G is obtained by collapsing or joining nodes of a split reaction graph with the same labels. Oppositely, we can view a reaction graph as a graph where some nodes of a complex reaction graph are duplicated. Only nodes that are source or target nodes of multiple edges can be duplicated. For example, if node 1 of the reaction graph G_1 in Figure 1 is duplicated, then the reaction graphs G_4 and G_2 are obtained. Collapsing the node pairs $(9, 11)$, and $(10, 12)$ of the split reaction graph G_7 yields G_6. Node duplication does not determine the reaction graph uniquely. In contrast, by collapsing node pairs the reaction graph is uniquely determined. This is formalized in the next subsection.

2.3 Morphisms of reaction graphs and a partial order

In this subsection we consider the family of reaction graphs associated with a reaction network $\mathcal{N}$ and show that the set of equivalence classes of reaction graphs forms a lattice.

Definition 3. Let G, G' be two reaction graphs associated with a reaction network $\mathcal{N}$ and let Y, Y' be their labeling functions, respectively. A *morphism of reaction graphs* from G to G' is a map between the node sets

$$\varphi\colon V_G \to V_{G'},$$

such that

(i) $\varphi(i) \to \varphi(j)$ is an edge of G' if $i \to j$ is an edge of G.

(ii) $Y'_{\varphi(i)} = Y_i$ for all $i = 1, \ldots, m_G$ (equivalently, $Y = Y' \circ \varphi$).

An *isomorphism* of reaction graphs is a morphism that has an inverse morphism. It is simply a permutation of the nodes of the graph.

By definition, a morphism of reaction graphs is in particular a digraph morphism. Isomorphism of reaction graphs is an equivalence relation, which allows us to speak about the *equivalence class* $[G]$ of a reaction graph G. In this sense, two reaction graphs are *equivalent* if they are isomorphic. The complex reaction graphs form an equivalence class $\mathcal{G}_c$ and the split reaction graphs form another class $\mathcal{G}_{sp}$, with representatives given by the canonical reaction graphs. In the same way, the detailed reaction graphs also form an equivalence class. An equivalence class of reaction graphs can be depicted by omitting the numbering of the node set, as we did in (1) and (2) in the Introduction. We will use this representation in some examples to introduce an equivalence class without specifying a representative.

Lemma 1. *Any morphism of reaction graphs $\varphi\colon V_G \to V_{G'}$ is surjective.*

Proof. Definition 3 implies that $R_{i\to j} = Y_i \to Y_j = Y'_{\varphi(i)} \to Y'_{\varphi(j)} = R'_{\varphi(i)\to\varphi(j)}$. Therefore, $(R')^{-1} \circ R(i \to j) = \varphi(i) \to \varphi(j)$. Since $(R')^{-1} \circ R$ is a bijection between E_G and $E_{G'}$ and reaction graphs have no isolated nodes, all nodes of G' are in the image of φ, that is, φ is surjective. □

Let $G_{sp} = (V_{sp}, E_{sp}, Y_{sp})$ denote the canonical split reaction graph.

Definition 4. A partition $\mathcal{P}$ of $V_{G_{sp}} = \{1, \dots, 2p\}$ is called *admissible* if

$$Y_{sp,i} = Y_{sp,j} \quad \text{for all } i, j \text{ in the same subset } P \in \mathcal{P}.$$

Given an admissible partition $\mathcal{P} = \{P_1, \dots, P_q\}$, the associated reaction graph $G_{\mathcal{P}} = (V_{\mathcal{P}}, E_{\mathcal{P}}, Y_{\mathcal{P}})$ is defined as

$$\begin{aligned} V_{\mathcal{P}} &= \{1, \dots, q\}, \qquad (\text{so, } m_{G_{\mathcal{P}}} = q), \\ E_{\mathcal{P}} &= \{k \to k' \mid i \to j \in E_{G_{sp}},\, i \in P_k, j \in P_{k'}\}, \\ (Y_{\mathcal{P}})_k &= Y_{sp,i} \qquad \text{if} \qquad i \in P_k. \end{aligned}$$

Note that the associated reaction graph depends on the numbering of the sets in the partition, which we implicitly give when writing $\mathcal{P} = \{P_1, \dots, P_q\}$. The map $Y_{\mathcal{P}}$ is well defined because the partition is admissible. Moreover, $E_{\mathcal{P}}$ is in one-to-one correspondence with $\mathcal{R}$ because an edge $k \to k'$ arises from a unique choice of i, j. Otherwise, there would be two edges in G_{sp} corresponding to the same reaction, since the partition is admissible.

Lemma 2. *(i) For any reaction graph G there exists an admissible partition $\mathcal{P} = \{P_1, \dots, P_q\}$ with $q = m_G$ elements, such that $G = G_{\mathcal{P}}$.*

(ii) Two reaction graphs G, G' with respective admissible partitions $\mathcal{P} = \{P_1, \dots, P_q\}$, $\mathcal{P}' = \{P'_1, \dots, P'_{q'}\}$, as in (i), are equivalent if and only if $\mathcal{P} = \mathcal{P}'$.

Proof. (i) We construct the partition $\mathcal{P}$, such that there is one set P_k for each node $k \in V_G$. For each edge $i' \to j'$ of G_{sp}, let $i \to j$ be the edge of G corresponding to the same reaction. Then by definition $i' \in P_i$ and $j' \in P_j$. Each node of G_{sp} is the source or target of exactly one edge. Therefore, all nodes are assigned a unique set P_k, and each set P_k has at least one element. Thus $P_1, \dots, P_{m_G}$ is a numbered partition of $\{1, \dots, 2p\}$, which further is admissible. It is straightforward to check that $G = G_{\mathcal{P}}$.

(ii) Consider admissible partitions $\mathcal{P}, \mathcal{P}'$ and numberings of the subsets of the partitions such that $G = G_{\mathcal{P}}$ and $G' = G_{\mathcal{P}'}$. The isomorphism between G and G' translates into a permutation of the numbering of the subsets of the partitions, and thus $\mathcal{P} = \mathcal{P}'$. □

We conclude from Lemma 2 that an equivalence class of reaction graphs can be identified with an admissible partition $\mathcal{P}$ of the set $\{1, \dots, 2p\}$. This class is denoted by $\mathcal{G}_{\mathcal{P}}$. Using this, we can define a partial order on the set of equivalence classes.

Definition 5. Let $\mathcal{P}$ and $\mathcal{P}'$ be two admissible partitions. We say that $\mathcal{P}$ is a *refinement* of $\mathcal{P}'$, and write $\mathcal{P} \leqslant \mathcal{P}'$, if for each $P \in \mathcal{P}$ there exists $P' \in \mathcal{P}'$ such that $P \subseteq P'$.

Given two equivalence classes $\mathcal{G}_{\mathcal{P}}, \mathcal{G}_{\mathcal{P}'}$, we define $\mathcal{G}_{\mathcal{P}'} \preceq \mathcal{G}_{\mathcal{P}}$ if $\mathcal{P} \leqslant \mathcal{P}'$.

If $[G'] \preceq [G]$, then we write $G' \preceq G$ for convenience. We say that G' is included in G, or that G includes G'. Note that the objects are reversed in $[G'] \preceq [G]$ and $\mathcal{P} \leqslant \mathcal{P}'$.

The admissible partition for $\mathcal{G}_{sp}$ has $2p$ subset each with one element: $\{i\}$, for $i = 1, \dots, 2p$. The admissible partition $\mathcal{P}_c$ defining $\mathcal{G}_c$ has m elements, one for each complex:

$$P_{c,y} = \big\{j \in \{1, \dots, 2p\} \mid Y_{sp,j} = y\big\}, \qquad y \in \mathcal{C}.$$

Any admissible partition is a refinement of $\mathcal{P}_c$, and hence an admissible partition is a union of partitions, one for each subset of $\mathcal{P}_c$. Further, the partition for the split reaction graphs is a refinement of any other admissible partition. Hence, for any reaction graph G, it holds

$$\mathcal{G}_c \preceq [G] \preceq \mathcal{G}_{sp}. \tag{8}$$

The set of admissible partitions inherits a lattice structure from the lattice structure of the set of partitions in general. Recall that a lattice is a set with a partial order such that any pair of elements has an infimum and a supremum [12]. An admissible partition $\mathcal{P}$ defines an equivalence relation over $\{1,\dots,2p\}$ by letting $i \sim_{\mathcal{P}} j$ if $i,j \in P$ for some $P \in \mathcal{P}$. The *union* $\mathcal{P} \vee \mathcal{P}'$ is the partition such that $i \sim_{\mathcal{P}\vee\mathcal{P}} j$ if and only if there exists a sequence $i = i_0, i_1, \dots, i_{k-1}, i_k = j$ such that either $i_{\ell-1} \sim_{\mathcal{P}} i_\ell$ or $i_{\ell-1} \sim_{\mathcal{P}'} i_\ell$ for all $\ell = 1,\dots,k$. Similarly, the *intersection* $\mathcal{P} \wedge \mathcal{P}'$ is the partition such that $i \sim_{\mathcal{P}\wedge\mathcal{P}'} j$ if and only if $i \sim_{\mathcal{P}} j$ and $i \sim_{\mathcal{P}'} j$. It is straightforward to show that $\mathcal{P} \vee \mathcal{P}'$ and $\mathcal{P} \wedge \mathcal{P}'$ are both admissible.

Further, if $\mathcal{P} \leqslant \mathcal{P}'$, then there exists a (possibly non-unique) sequence of admissible partitions $\mathcal{P} = \mathcal{P}_0 \leqslant \mathcal{P}_1 \leqslant \cdots \leqslant \mathcal{P}_k = \mathcal{P}'$, such that at each step precisely two subsets of the partition are joined (cf. [12, Lemma 1 and Lemma 403]). This constitutes the proof of the following proposition.

Proposition 1. *(i) The set of equivalence classes of reaction graphs with the partial order $\preceq$ is a finite lattice with maximal element $\mathcal{G}_{sp}$ and minimal element $\mathcal{G}_c$. Further, the infimum and supremum of two classes $\mathcal{G}_{\mathcal{P}}, \mathcal{G}_{\mathcal{P}'}$ are respectively*

$$\mathcal{G}_{\mathcal{P}} \wedge \mathcal{G}_{\mathcal{P}'} = \mathcal{G}_{\mathcal{P}\vee\mathcal{P}'}, \qquad \mathcal{G}_{\mathcal{P}} \vee \mathcal{G}_{\mathcal{P}'} = \mathcal{G}_{\mathcal{P}\wedge\mathcal{P}'}.$$

(ii) Let G, G' be reaction graphs associated with a reaction network. Assume $k = m_G - m_{G'} > 0$. Then $G' \preceq G$ if and only if there exists a sequence of $k-1$ reaction graphs $G' = G_0 \preceq G_1 \preceq \cdots \preceq G_{k-1} \preceq G_k = G$ such that

$$m_{G_i} = m_{G_{i-1}} + 1, \qquad i = 1,\dots,k.$$

Note that given two weakly reversible reaction graphs G, G', their infimum $G \wedge G'$ is also weakly reversible (cf. Proposition 2(iv)), but this is not necessarily the case for the supremum $G \vee G'$ as the next example will show.

Example 1 (part D). Table 1 shows the admissible partitions for the reaction graphs in Figure 1. Since $\mathcal{P}_5$ is a refinement of $\mathcal{P}_4$, we have $[G_4] \preceq [G_5]$. Further, $\mathcal{P}_2 \wedge \mathcal{P}_4 = \mathcal{P}_5$ and $\mathcal{P}_2 \vee \mathcal{P}_4 = \mathcal{P}_1$. It follows that $[G_2] \wedge [G_4] = \mathcal{G}_{\mathcal{P}_2\vee\mathcal{P}_4}$ is the equivalence class of the complex reaction graphs class with representative G_1, and similarly $[G_2] \vee [G_4] = \mathcal{G}_{\mathcal{P}_2\wedge\mathcal{P}_4} = [G_5]$. While G_2 and G_4 are weakly reversible, G_5 is not. Following Proposition 1(ii), the inclusion $G_1 \preceq G_3$ can be broken down into two sequences of inclusions $G_1 \preceq G_2 \preceq G_3$ and $G_1 \preceq G_2' \preceq G_3$, with $G_2' = G_{\mathcal{P}}$ and $\mathcal{P} = \big\{\{1,8,9,11\},\{2,3\},\{4,12\},\{6,7\},\{5,10\}\big\}$.

We conclude the section with an alternative description of the partial order.

Lemma 3. *$G' \preceq G$ if and only if there exists a morphism of reaction graphs $\varphi\colon V_G \to V_{G'}$.*

Proof. Let $\mathcal{P} = \{P_1,\dots,P_{m_G}\}$ and $\mathcal{P}' = \{P_1',\dots,P_{m_{G'}}'\}$ be the admissible partitions such that $G = G_{\mathcal{P}}$ and $G' = G_{\mathcal{P}'}$. Since $G' \preceq G$, we have $\mathcal{P} \leqslant \mathcal{P}'$. For each $i \in V_G$, let $\varphi(i) \in V_G'$ be the index such that $P_i \subseteq P_{\varphi(i)}$. Since the partitions are admissible, then

$$Y_i = (Y_{\mathcal{P}})_i = Y_{sp,k} = (Y_{\mathcal{P}'})_{\varphi(i)} = Y'_{\varphi(i)}, \quad \text{for all } k \in P_i \subseteq P'_{\varphi(i)}.$$

Further, if $i \to j \in E_G = E_{\mathcal{P}}$, then by definition there exist $i' \in P_i$ and $j' \in P_j$ such that $i' \to j'$ is an edge of G_{sp}. Since also $i' \in P'_{\varphi(i)}$ and $j' \in P'_{\varphi(j)}$, it follows that $\varphi(i) \to \varphi(j) \in E_{\mathcal{P}'} = E_{G'}$. By Definition 3, φ is a morphism of reaction graphs.

For the reverse implication, let $i \in V_G$ and $k \in P_i$. Since φ is a morphism and $G = G_{\mathcal{P}}$ it holds $(Y_{\mathcal{P}'})_{\varphi(i)} = (Y_{\mathcal{P}})_i = Y_{sp,k}$. Hence $k \in P'_{\varphi(i)}$. This shows $P_i \subseteq P'_{\varphi(i)}$ and thus $\mathcal{P} \leqslant \mathcal{P}'$ as desired. □

i	$\mathcal{P}_i$ such that $G_i = G_{\mathcal{P}_i}$	δ_{G_i}
1	$\{$ {1,8,9,11}, {2,3}, {4,5,10,12}, {6,7} $\}$	2
2	$\{$ {1,11}, {2,3}, {4,5,10,12}, {6,7},{8,9} $\}$	3
3	$\{$ {1,11}, {2,3}, {4,12}, {6,7},{8,9},{5,10} $\}$	3
4	$\{$ {1,8}, {2,3}, {4,5,10,12}, {6,7},{9,11} $\}$	3
5	$\{$ {1}, {2,3}, {4,5,10,12}, {6,7},{8},{9},{11} $\}$	5
6	$\{$ {1}, {2}, {3}, {4}, {5}, {6}, {7}, {8}, {9,11}, {10,12} $\}$	4
7	$\{$ {1}, {2}, {3}, {4}, {5}, {6}, {7}, {8}, {9}, {10}, {11}, {12} $\}$	5

Table 1: Partitions defining the reaction graphs in Figure 1 and their deficiencies.

The morphism φ associated with an inclusion $G' \preceq G$ identifies the nodes of G that are joined to form G', or, in terms of partitions, the subsets of the partition defining G that are joined to form the partition defining G'. By Lemma 3, two reaction graphs G and G' are isomorphic if and only if $G \preceq G'$ and $G' \preceq G$, which is consistent with Lemma 2.

Example 1 (part E). For the inclusion $G_4 \preceq G_5$ in Figure 1, the map $\varphi\colon V_{G_5} \to V_{G_4}$ is

$$\varphi(1) = \varphi(5) = 1, \quad \varphi(2) = 2, \quad \varphi(3) = 3, \quad \varphi(4) = 4, \quad \varphi(6) = \varphi(7) = 5.$$

2.4 Incidence matrix and weak reversibility

Given a reaction graph G with labeling Y, we consider the matrix $Y \in \mathbb{R}^{n \times m_G}$, called the *labeling matrix*, with j-th column being the vector Y_j (the same notation is used as for the labeling function, since both objects convey the same information).

We define a numbering on the edge set E_G by means of the bijection R and the numbering of $\mathcal{R}$. The *incidence matrix* C_G of the reaction graph G is the $m_G \times p$ matrix with nonzero entries defined by $(C_G)_{k_1 j} = -1$, $(C_G)_{k_2 j} = 1$, if the j-th edge is $k_1 \to k_2$. Each column of C_G has only two non-zero entries and the column sums are zero. The rank of the incidence matrix is $m_G - \ell_G$, where ℓ_G is the number of connected components of G [1, Prop. 4.3].

Proposition 2. *Let G be a reaction graph associated with a reaction network $\mathcal{N}$. Then, the following holds:*

(i) $N = YC_G$.

(ii) The kernel of C_G contains a positive vector if and only if G is weakly reversible.

Assume G, G' are two reaction graphs associated with $\mathcal{N}$ such that $G' \preceq G$. Then, we have

(iii) There exists an $(m_{G'} \times m_G)$-matrix B such that $C_{G'} = BC_G$.

(iv) If G is weakly reversible, then so is G'.

Proof. (i) The j-th column of N is $y' - y$ if $r_j\colon y \to y'$. If $k_2 \to k_1$ is the j-th edge of G, then the j-th column of YC_G is the vector $Y_{k_2} - Y_{k_1}$. Since $r_j = R_{k_2 \to k_1}$, we have $Y_{k_2} = y$ and $Y_{k_1} = y'$, proving (i).

(ii) This is well known. For instance, use that the elementary cycles are the minimal generators of the polyhedral cone $\ker(C_G) \cap \mathbb{R}^p_{\geqslant 0}$ [11, Prop. 4] and that a digraph is weakly reversible if and only if each edge is part of an elementary cycle. See also [10, Remark 6.1.1] or [18, Lemma 3.3].

(iii) Let $V_G \xrightarrow{\varphi} V_{G'}$ be the surjective map from Lemma 1. Let $B \in \mathbb{R}^{m_{G'} \times m_G}$ such that the $(\varphi(i), i)$-th entry is 1, for $i = 1, \ldots, m_G$, and the rest of the entries are zero. If the j-th edge of G is $k_1 \to k_2$, then the nonzero entries of the j-th column of BC_G are -1 at row $\varphi(k_1)$ and 1 at row $\varphi(k_2)$. Thus $BC_G = C_{G'}$.

(iv) Follows from (ii) and (iii). □

2.5 Deficiency

The deficiency of a reaction network is an important characteristic in the study of steady states and their properties [2, 3, 5, 8, 19]. Here, we extend the classical definition of deficiency to an arbitrary reaction graph.

Definition 6. Let G be a reaction graph associated with a reaction network $\mathcal{N}$. The *deficiency* of G is the number

$$\delta_G = m_G - \ell_G - s,$$

where m_G is the number of nodes of G, ℓ_G is the number of connected components of G and s the rank of the stoichiometric subspace of $\mathcal{N}$.

The deficiency of a reaction graph depends only on the equivalence class of the reaction graph. Hence it makes sense to talk about the deficiency of an equivalence class $\mathcal{G}$, which we denote by $\delta_{\mathcal{G}}$. We have $\delta_{[G]} = \delta_G$. In particular, we refer to the *deficiency of* $\mathcal{N}$ as the the deficiency of the equivalence class $\mathcal{G}_c$ of the complex reaction graphs (in accordance with [5]).

The deficiencies of the reaction graphs in Figure 1 are given in Table 1, using that $s = 1$.

Example 2. A split reaction graph has $2p$ nodes and p connected components. Thus the deficiency of the split equivalence class $\mathcal{G}_{sp}$ is $\delta_{\mathcal{G}_{sp}} = 2p - p - s = p - s$.

Given a reversible network with $p = 2q$ reactions, then any detailed reaction graph has p nodes and q connected components. Thus the deficiency of the detailed equivalence class is $\delta = p - q - s = q - s$.

The deficiency of a reaction graph is a non-negative number, as we show below. For a given order $G_1, \ldots, G_{\ell_G}$ of the connected components of G, define the linear map Ψ_G by

$$\Psi_G \colon \mathbb{R}^{m_G} \to \mathbb{R}^{n+\ell_G} \qquad \text{with} \qquad \Psi_G(x) = \left(Yx, \sum_{i \in G_1} x_i, \ldots, \sum_{i \in G_{\ell_G}} x_i \right), \tag{9}$$

where Yx defines the first n coordinates of $\Psi_G(x)$. The following proposition is well known in the context of complex balanced steady states [3, 15]. We will use the result in Section 3.

Proposition 3. *For a reaction graph G with labeling function Y, the following equalities hold:*

$$\ker \Psi_G = \ker Y \cap \operatorname{im} C_G, \qquad \delta_G = \dim(\ker Y \cap \operatorname{im} C_G) = \dim \ker \Psi_G.$$

Proof. To prove the first equality, let e_i be the i-th unit vector of $\mathbb{R}^{m_G}$. For all $j \in \{1, \ldots, \ell_G\}$, we have $\omega_j := \sum_{i \in G_j} e_i \in (\operatorname{im} C_G)^\perp$. This gives ℓ_G linearly independent vectors in $(\operatorname{im} C_G)^\perp$.

Using that the rank of C_G is $m_G - \ell_G$, we conclude that $\omega_1, \dots, \omega_{\ell_G}$ form a basis of $(\operatorname{im} C_G)^\perp$. It follows that $x \in \operatorname{im} C_G$ if and only if $\omega_j \cdot x = 0$ for all $j \in \{1, \dots, \ell_G\}$. Further, $\omega_j \cdot x = \sum_{i \in G_j} x_i$.

Using this, we have $x \in \ker Y \cap \operatorname{im} C_G$ if and only if $Yx = 0$ and $\omega_j \cdot x = 0$, which is equivalent to $\Psi_G(x) = 0$. This concludes the proof of the first equality.

Consider now the linear map $\psi\colon \ker N \to \mathbb{R}^{m_G}$ defined by $w \mapsto C_G w$ on $\ker N \subseteq \mathbb{R}^p$. Since $\ker C_G \subseteq \ker N$ by Proposition 2(i), we have $\ker \psi = \ker C_G$. On the other hand,

$$\operatorname{im} \psi = \{C_G w \mid w \in \mathbb{R}^p, Nw = 0\} = \{C_G w \mid w \in \mathbb{R}^p, YC_G w = 0\} = \ker Y \cap \operatorname{im} C_G.$$

By the first isomorphism theorem, $\ker N / \ker C_G \cong \ker Y \cap \operatorname{im} C_G$. Using that $\ker C_G$ has dimension $p - m_G + \ell_G$, we have

$$\dim(\ker Y \cap \operatorname{im} C_G) = \dim \ker N - \dim \ker C_G = p - s - (p - m_G + \ell_G) = m_G - \ell_G - s = \delta_G$$

which concludes the proof of the second equality. □

The deficiency behaves surprisingly nice in connection with inclusion of reaction graphs. In particular, it is possible to iteratively compute the deficiency of any reaction graph from the split reaction graph. This will be further exploited in the coming section in relation to node balanced steady states.

Proposition 4. *Assume $G' \preceq G$ for two reaction graphs associated with a reaction network $\mathcal{N}$ and let $\varphi\colon V_G \to V_{G'}$ be the morphism defining the inclusion, cf. Lemma 3.*

(i) Assume that $m_G = m_{G'} + 1$ and let i_1, i_2 be the only two nodes of G such that $\varphi(i_1) = \varphi(i_2)$. If i_1, i_2 belong to the same connected component of G, then $\delta_{G'} = \delta_G - 1$ and there is an undirected cycle through $\varphi(i_1) = \varphi(i_2)$ in G', which is not in G. Otherwise, $\delta_{G'} = \delta_G$.

(ii) $\delta_{G'} \leqslant \delta_G$.

(iii) If $\Delta = \delta_G - \delta_{G'} > 0$, then there exists a sequence of $\Delta + 1$ reaction graphs $G' = G_0 \preceq G_1 \preceq \cdots \preceq G_{\Delta - 1} \preceq G_\Delta = G$ such that

$$\delta_{G_i} = \delta_{G_{i-1}} + 1, \qquad i = 1, \dots, \Delta.$$

Proof. (i) Using that $m_G = m_{G'} + 1$, we have that

$$\delta_G - \delta_{G'} = m_{G'} + 1 - \ell_G - s - (m_{G'} - \ell_{G'} - s) = \ell_{G'} - \ell_G + 1.$$

Let G_1, G_2 be the connected components of G containing i_1, i_2 respectively. Outside G_1 and G_2, the morphism φ is a permutation of the nodes, while G_1 and G_2 are mapped to the connected component of G' containing $\varphi(i_1) = \varphi(i_2)$. Thus, if $G_1 = G_2$, $\ell_G = \ell_{G'}$, while if $G_1 \neq G_2$, then $\ell_{G'} = \ell_G - 1$. This gives the stated relation between δ_G and $\delta_{G'}$.

Furthermore, consider an undirected path without repeated nodes between i_1 and i_2 in G. The image by φ of this path is a path of G', with end points $\varphi(i_1) = \varphi(i_2)$. Thus there is an undirected cycle in G'. There are no repeated nodes since φ is one-to-one on $V_G \backslash \{i_1, i_2\}$.

(ii) and (iii) follow from (i) and Proposition 1. □

The above results have some interesting consequences. Assume $G' \preceq G$. If G, G' have exactly the same cycles (given the correspondence of edges between the two graphs), then their deficiency is the same by Proposition 4(i). Further, the deficiency of G' can be computed iteratively from that of G by joining pairs of nodes, one at a time, and checking whether two connected components merge or not.

Example 1 (part F). Consider the inclusion $G_1 \preceq G_2 \preceq G_3$ and the deficiencies given in Table 1. The inclusion $G_2 \preceq G_3$ is obtained by joining the nodes $3, 6$, which changes the number of connected components. Thus, $\delta_{G_2} = \delta_{G_3} = 3$. For the inclusion $G_1 \preceq G_2$ one joins the nodes $1, 5$, which does not alter the number of connected components and a new cycle is created in G_1, namely $1 \rightleftharpoons 3$. The deficiency is reduced by one, hence $\delta_{G_1} = \delta_{G_2} - 1 = 2$.

3 Node balanced steady states

In this section we introduce *node balanced steady states* for a given reaction graph, and show that complex and detailed balanced steady states, two well-studied classes of steady states, are examples of node balanced steady states. We use the partial order on the equivalence classes of reaction graphs to deduce further properties of node balanced steady states.

3.1 Definition and first properties

Definition 7. Let $\mathcal{N}$ be a reaction network, $G = (V_G, E_G, Y)$ an associated reaction graph and v a kinetics. A *node balanced steady state* of $\mathcal{N}$ with respect to G is a solution to the equation

$$C_G\, v(x) = 0, \qquad x \in \mathbb{R}^n_{\geqslant 0}.$$

Equivalently, $x^* \in \mathbb{R}^n_{\geqslant 0}$ is a node balanced steady state if for all nodes i of C_G it holds

$$\sum_{j \in V_G \mid i \to j \in E_G} v_{Y_i \to Y_j}(x^*) = \sum_{j \in V_G \mid j \to i \in E_G} v_{Y_j \to Y_i}(x^*), \tag{10}$$

where $v_{Y_i \to Y_j}$ is the rate function of the reaction $Y_i \to Y_j$.

By Proposition 2(i), any node balanced steady state is also a steady state of the network. Further, a direct consequence of Proposition 2 is the following result.

Proposition 5. *Let $\mathcal{N}$ be a reaction network with a kinetics v and let $G' \preceq G$ be two associated reaction graphs.*

(i) If there exists a positive node balanced steady state with respect to G, then G is weakly reversible.

(ii) Any node balanced steady state of $\mathcal{N}$ with respect to G is also a node balanced steady state with respect to G'.

By Proposition 5(ii), a node balanced steady state with respect to G is a node balanced steady state with respect to any reaction graph equivalent to G. Thus, we may equivalently refer to a node balance steady state with respect to an equivalence class of reaction graphs or to a particular reaction graph in that class. Further, a *complex balanced steady state* is a node balanced steady state with respect to the equivalence class of complex reaction graphs, and similarly, a *detailed balanced steady state* is a node balanced steady state with respect to the equivalence class of detailed reaction graphs.

By Proposition 5(ii) and equation (8), any node balanced steady state of $\mathcal{N}$ is also a complex balanced steady state and we recover the well-known fact that detailed balanced steady states are complex balanced steady states. In fact, more is true. We will show in Corollary 1 that if $G' \preceq G$ and $\delta_{G'} = \delta_G$, then the reverse implication of Proposition 5(ii) holds for mass-action kinetics. That is, both reaction graphs give rise to the same set of node

balanced steady states, and there exist node balanced steady states for the same set of reaction rate constants.

Since a split reaction graph is never weakly reversible, there cannot be positive node balanced steady states with respect to this graph. Similarly, if a reaction network contains irreversible reactions, then there are no positive detailed balanced steady states with respect to the detailed reaction graph.

Example 1 (part G). Consider the reaction graphs G_2, G_3 in Figure 1 and mass-action kinetics. Focusing on the node 3 with label $3X_2$, a positive node balanced steady state with respect to G_2 fulfils

$$\kappa_2 x_1 x_2^2 + \kappa_5 x_1^3 = \kappa_6 x_2^3 + \kappa_3 x_2^3. \tag{11}$$

For nodes 3 and 6, both with label $3X_2$, a positive node balanced steady state with respect to G_3 fulfills

$$\kappa_2 x_1 x_2^2 = \kappa_6 x_2^3, \qquad \text{and} \qquad \kappa_5 x_1^3 = \kappa_3 x_2^3. \tag{12}$$

If these equations hold, then so does (11). The equations for the other nodes are the same for both G_2 and G_3. Therefore a node balanced steady state with respect to G_3 is also a node balanced steady state with respect to G_2. We knew this already from Proposition 5 since $G_2 \preceq G_3$. The reverse statement is also true in this case. It follows from the fact that the deficiencies of the two reaction graphs agree. The proof will be given below.

3.2 Main results

In this section we only consider reaction networks with mass-action kinetics and weakly reversible reaction graphs. Given a network $\mathcal{N}$, an associated reaction graph G and a vector $\kappa \in \mathbb{R}^p_{>0}$, we say that $(\mathcal{N}, G, \kappa)$ is *node balanced* if there exists a *positive* node balanced steady state of $\mathcal{N}$ with respect to G for mass-action kinetics with reaction rate constants κ. The proofs of the three theorems below are given in Section 6.

The first theorem is akin to Theorem 6A of [15].

Theorem 1 (Uniqueness and asymptotic stability). *Assume $\mathcal{N}$ is a reaction network with mass-action kinetics with reaction rate constants $\kappa \in \mathbb{R}^p_{>0}$, and let G be a weakly reversible reaction graph. If $(\mathcal{N}, G, \kappa)$ is node balanced, then any positive steady state of $\mathcal{N}$ is node balanced with respect to G. Furthermore, there is one such steady state in each stoichiometric compatibility class and it is locally asymptotically stable relatively to the class.*

The next main result tells us that there are δ_G equations in $\kappa \in \mathbb{R}^p_{>0}$ that determine whether $(\mathcal{N}, G, \kappa)$ is node balanced or not. The link between deficiency and the existence of complex balanced steady states was first explored by Horn and Feinberg [6, 14] (see also [8], and [4, 9] concerning detailed balancing). We follow the approach of [3] for complex balanced steady states, which applies to general reaction graphs.

For a node $i \in V_G$, let $\Theta_{G,i}$ be the set of spanning trees of the connected component i belongs to, rooted at i (that is, i is the only node with no outgoing edge). Given such a tree τ, let κ^τ be the product of the reaction rate constants corresponding to the edges of τ. Define

$$K_{G,i} = \sum_{\tau \in \Theta_{G,i}} \kappa^\tau \qquad \text{and} \qquad K_G = (K_{G,1}, \ldots, K_{G,m_G}). \tag{13}$$

The following theorem is a consequence of [3, Theorem 9], adapted to our setting. Recall that the kernel of the map Ψ_G given in (9) has dimension δ_G (Proposition 3).

Theorem 2 (**Existence of node balanced steady states).** *Let $\mathcal{N}$ be a reaction network, $\kappa \in \mathbb{R}^p_{>0}$, and G an associated weakly reversible reaction graph. Let $u_1, \dots, u_{\delta_G} \in \mathbb{Z}^{m_G}$ be a basis of* $\ker \Psi_G$. *Then the following holds.*

(i) $(\mathcal{N}, G, \kappa)$ is node balanced if and only if

$$(K_G)^{u_i} = \prod_{j=1}^{m_G} K_{G,j}^{u_{ij}} = 1, \qquad \text{for all} \quad i = 1, \dots, \delta_G.$$

(ii) $x \in \mathbb{R}^n_{>0}$ is a node balanced steady state of $\mathcal{N}$ with respect to G if and only if

$$K_{G,i} x^{Y_i} - K_{G,j} x^{Y_j} = 0 \qquad \text{for all} \quad (i,j) \in E_G.$$

By Theorem 2(i), there are δ_G relations in the reaction rate constants for which $(\mathcal{N}, G, \kappa)$ is node balanced. In fact, more is true. As proven in [3] for complex balanced steady states, these δ_G equations imply that the set of reaction rate constants $\kappa \in \mathbb{R}^p_{>0}$ for which a positive node balanced steady state exists forms a positive variety of codimension δ_G in $\mathbb{R}^p_{>0}$. The conditions given in (i) for complex balanced or detailed balanced steady states are equivalent to the conditions given in Proposition 1 and 4 of [4].

The next result tells us how to obtain the relations in Theorem 2(i) from the relations for complex balanced steady states.

Theorem 3 (**Node balancing and inclusion of reaction graphs).** *Let G', G be two weakly reversible reaction graphs such that $G' \preceq G$ and $m_G = m_{G'} + 1$. Further, consider the associated morphism $\varphi\colon G \to G'$ in Lemma 3, and let i_1, i_2 be the only pair of nodes of G such that $\varphi(i_1) = \varphi(i_2) = k$ with $k \in V_{G'}$. Let $\kappa \in \mathbb{R}^p_{>0}$.*

(i) If i_1, i_2 do not belong to the same connected component of G, then $(\mathcal{N}, G, \kappa)$ is node balanced if and only if $(\mathcal{N}, G', \kappa)$ is.

(ii) If i_1, i_2 belong to the same connected component of G, then $(\mathcal{N}, G, \kappa)$ is node balanced if and only if $(\mathcal{N}, G', \kappa)$ is node balanced and further $K_{G,i_1} = K_{G,i_2}$.

We obtain the following corollary.

Corollary 1. *Let $G' \preceq G$ be two weakly reversible reaction graphs associated with a reaction network. Assume mass-action kinetics with $\kappa \in \mathbb{R}^p_{>0}$.*

(i) If $\delta_G = \delta_{G'}$, then x^* is a positive node balanced steady state with respect to G' if and only if it is a positive node balanced steady state with respect to G.

(ii) Any set of $\delta_{G'}$ equations in κ for the existence of positive node balanced steady states with respect to G' (as in Theorem 2) can be extended to a set of equations in κ for the existence of positive node balanced steady states with respect to G by adding $\delta_G - \delta_{G'}$ equations.

Proof. (i) The reverse implication is Proposition 5(ii). If x^* is a positive node balanced steady state with respect to G', then by Theorem 3(i) and Proposition 4(i), $(\mathcal{N}, G, \kappa)$ is also node balanced. By Theorem 1, this means that all positive steady states of $\mathcal{N}$ with reaction rate constants κ are node balanced with respect to G, thus in particular x^* is.

(ii) It follows from Theorem 3(ii) and Proposition 4(iii). □

As a consequence of Corollary 1 and Proposition 4(i), we recover the following well-known result relating complex and detailed balanced steady states [4, 9]. Assume the network is reversible. If a complex reaction graph has no simple cycles (that is, with no repeated nodes) other than those given by pairs of reversible reactions, then a steady state is complex balanced if and only if it is detailed balanced.

By letting G' be a complex reaction graph in Corollary 1(ii), we conclude that the equations for the existence of positive complex balanced steady states can be extended to equations for the existence of positive node balanced steady states for any weakly reversible reaction graph. The extra conditions, obtained by applying Theorem 3(ii) iteratively in conjunction with Proposition 4, generalize the so-called cycle conditions [9], or formal balancing conditions [4], that relate conditions for the existence of complex and detailed balancing steady states.

If $\delta_G = \delta_{G'}$ but neither $G \preceq G'$ nor $G' \preceq G$, all possibilities might occur. The sets of reaction rate constants $\kappa \in \mathbb{R}^p_{>0}$ for which $(\mathcal{N}, G, \kappa)$ and $(\mathcal{N}, G', \kappa)$ are node balanced can be disjoint, have a proper intersection or coincide. Instances of the first two cases are given in Example 1 (part I) and Example 4 below. For what concerns the latter, we have the following corollary, which is a consequence of Theorem 3.

Corollary 2. *Let G, G' be two weakly reversible reaction graphs with the same deficiency $\delta_G = \delta_{G'}$. If either of the following conditions are fulfilled,*

(i) $\delta_G = \delta_{[G]\wedge[G']}$.

(ii) $[G] \vee [G']$ *is weakly reversible and* $\delta_G = \delta_{[G]\vee[G']}$,

then $(\mathcal{N}, G, \kappa)$ is node balanced if and only if $(\mathcal{N}, G', \kappa)$ is.

Example 3. Consider a reaction network with reactions $X_1 \rightleftharpoons X_2$, $X_2 \rightleftharpoons X_3$ and $X_3 \rightleftharpoons X_4$, and the following associated equivalence classes of reaction graphs (shown without the numbering of the nodes).

$\mathcal{G}_1$:	$X_1 \rightleftharpoons X_2 \rightleftharpoons X_3 \rightleftharpoons X_4$
$\mathcal{G}_2$:	$X_1 \rightleftharpoons X_2 \qquad X_2 \rightleftharpoons X_3 \rightleftharpoons X_4$
$\mathcal{G}_3$:	$X_1 \rightleftharpoons X_2 \rightleftharpoons X_3 \qquad X_3 \rightleftharpoons X_4$
$\mathcal{G}_4$:	$X_1 \rightleftharpoons X_2 \qquad X_2 \rightleftharpoons X_3 \qquad X_3 \rightleftharpoons X_4$

Neither $\mathcal{G}_2 \preceq \mathcal{G}_3$ nor $\mathcal{G}_3 \preceq \mathcal{G}_2$. Moreover, $\mathcal{G}_2 \wedge \mathcal{G}_3 = \mathcal{G}_1$, $\mathcal{G}_2 \vee \mathcal{G}_3 = \mathcal{G}_4$, and the reaction graphs in these classes have all the same deficiency. Hence, by Corollary 2, the sets of reaction rate constants for which $\mathcal{N}$ admits positive node balanced steady states with respect to any of the above equivalence classes coincide.

Finding K_G. We conclude this section by expanding on how to find the relations in Theorem 2(i) in practice and with further examples. Let $G_1, \ldots, G_{\ell_G}$ be the connected components of a weakly reversible reaction graph G. To determine the kernel of Ψ_G, we consider the associated $(n + \ell_G) \times m_G$ Cayley matrix A_G [3]. It is a block matrix with upper block Y $(n \times m_G)$ and lower block $(\ell_G \times m_G)$, where the i-th row has 1 in entry j if node j belongs to component G_i, and otherwise is zero. Since A_G is an integer matrix, then $\ker(\Psi_G)$ has a basis with integer entries as well.

The form of $K_{G,i}$ is a consequence of the Matrix-Tree Theorem [21, 22]. Specifically, let $L_\kappa \in \mathbb{R}^{m_G \times m_G}$ be the Laplacian of G with off-diagonal (k, j)-th entry equal to κ_ℓ, if $j \to k \in E_G$

and the edge corresponds to the reaction r_ℓ, and zero otherwise. Let L'_κ be the submatrix of L_κ obtained by selecting the rows and columns with indices in the node set of the connected component G' of G that contains node i. Let $(L'_\kappa)_{(i)}$ denote the minor corresponding to the submatrix obtained from L'_κ by removing the i-th column and the last row. Then

$$K_{G,i} = (-1)^i (L'_\kappa)_{(i)}. \tag{14}$$

In fact $(-1)^i (L'_\kappa)_{(i)}$ also agrees with $(-1)^{m'+1+i+j}$ times the minor obtained from L'_κ by removing the i-th column and the j-th row, where m' is the number of nodes of G'.

In practice, this is often the way to find K_G, rather than finding the trees. However, the description of K_G in terms of trees is a useful interpretation of K_G.

Example 1 (part H). The reaction graph G_4 in Figure 1 has one connected component. The map Ψ_G has matrix

$$A_G = \begin{pmatrix} 3 & 1 & 0 & 2 & 3 \\ 0 & 2 & 3 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix} \in \mathbb{Z}^{3\times 5}.$$

The first two rows of A_G are the column vectors encoded by the labels (complexes) of the nodes of the graph. Since $\delta_G = 3$, we find three linearly independent vectors in the kernel with integer entries, $u_1 = (-1, 0, 0, 0, 1), u_2 = (-1, -1, 0, 2, 0), u_3 = (1, -3, 2, 0, 0)$. Furthermore, we have $K_G = \big(\kappa_2\kappa_3\kappa_4\kappa_5,\ \kappa_1\kappa_3\kappa_4\kappa_5,\ \kappa_1\kappa_2\kappa_4\kappa_5,\ \kappa_1\kappa_2\kappa_3\kappa_5,\ \kappa_1\kappa_2\kappa_4\kappa_6\big)$. By Theorem 2, $(\mathcal{N}, G, \kappa)$ is node balanced if and only if

$$K_{G,1}^{-1} K_{G,5} = 1, \qquad K_{G,1}^{-1} K_{G,2}^{-1} K_{G,4}^2 = 1, \qquad K_{G,1} K_{G,2}^{-3} K_{G,3}^2 = 1.$$

This reduces to three algebraic relations

$$\kappa_1\kappa_6 = \kappa_3\kappa_5, \qquad \kappa_1\kappa_2 = \kappa_4^2, \qquad \kappa_1\kappa_3^2 = \kappa_2^3. \tag{15}$$

We find analogously relations for positive node balanced steady states with respect to the complex balanced reaction graph G_1,

$$(\kappa_1 + \kappa_5)^2 \kappa_2^3 = (\kappa_3 + \kappa_6)^2 \kappa_1^3, \qquad \kappa_2\kappa_3^2(\kappa_1 + \kappa_5)^2 = (\kappa_3 + \kappa_6)^2 \kappa_4^2 \kappa_1 \tag{16}$$

The relation $K_{G_4,1} = K_{G_4,5}$ is $\kappa_3\kappa_5 = \kappa_1\kappa_6$. By isolating κ_6 from this equation and inserting it into (16), we obtain after simplification the set of equations in (15), in accordance with Theorem 3(ii).

Example 1 (part I). Since $G_2 \preceq G_3$ and the reaction graphs have the same deficiency (Table 1), it follows from Corollary 1, that a steady state is node balanced with respect to G_2 if and only if it is with respect to G_3. This implies that equation (12) and (11) have the same solutions. Similarly, a positive steady state is node balanced with respect to G_5 if and only if it is with respect to G_4. In this example, $G_2 \preceq G_3$ and $G_4 \preceq G_5$.

The reaction graphs G_2 and G_4 which are not related by inclusion, have deficiency 3. However, the values of κ for which positive node balanced steady states exist differ. As in Example 1 (part H), we find the relations for G_2 (identical to those for G_3)

$$\kappa_1\kappa_3 = \kappa_5\kappa_6, \qquad \kappa_1\kappa_2\kappa_3^2 = \kappa_4^2\kappa_6^2, \qquad \kappa_2^3 = \kappa_1\kappa_6^2. \tag{17}$$

These equations and the equations for G_4 in equation (15) in Example 1 (part H) define different sets with non-empty intersection. For example, $\kappa = (1, \ldots, 1)$ fulfils both (15) and (17), but $\kappa = (1, 1, 1, 1, 2, 2)$ fulfils only (15). Note however that the matrix A_G is the same for both reaction graphs.

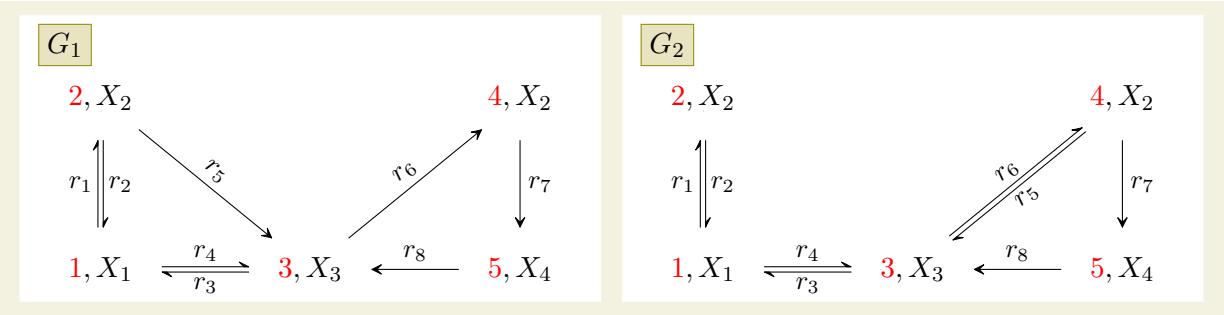


Figure 2: Reaction graphs for the network in Example 4.

Example 4. Consider a reaction network with reactions $X_1 \rightleftharpoons X_2$, $X_2 \rightleftharpoons X_3$, $X_1 \rightleftharpoons X_3$ and $X_2 \to X_4 \to X_3$, and the associated reaction graphs, depicted in Figure 2.

We have $\delta_{G_1} = \delta_{G_2} = 1$, but neither $G_1 \preceq G_2$ nor $G_2 \preceq G_1$. If x^* were a positive node balanced steady state with respect to both G_1 and G_2, it would follow from (10), applied to node 2, that $v_{X_2 \to X_3}(x^*) = 0$, which contradicts that $v(x) \in \mathbb{R}^p_{>0}$. Hence $(\mathcal{N}, G_1, \kappa)$ and $(\mathcal{N}, G_2, \kappa)$ cannot be node balanced for the same choice of reaction rate constants.

A different route to reach the same conclusion consists in finding the set of reaction rate constants κ for which $(\mathcal{N}, G_1, \kappa)$ and $(\mathcal{N}, G_2, \kappa)$ are node balanced. The complex balanced reaction graph associated with the network has deficiency zero and thus $\mathcal{N}$ is complex balanced for all κ. A complex balanced reaction graph can be obtained from either reaction graph, G_1 or G_2, by joining the nodes 2 and 4. In view of Theorem 3(ii), it is enough to find the label of the trees rooted at 2 and 4 for each reaction graph. We obtain that $(\mathcal{N}, G_1, \kappa)$ is node balanced if and only if

$$\begin{aligned} K_{G_1,2} = K_{G_1,4} \quad &\iff \quad \kappa_1\kappa_3\kappa_7\kappa_8 = \kappa_1\kappa_5\kappa_6\kappa_8 + \kappa_4\kappa_5\kappa_6\kappa_8 + \kappa_2\kappa_4\kappa_6\kappa_8 \\ &\iff \quad \kappa_1\kappa_3\kappa_7 = \kappa_1\kappa_5\kappa_6 + \kappa_4\kappa_5\kappa_6 + \kappa_2\kappa_4\kappa_6. \end{aligned} \tag{18}$$

Similarly, $(\mathcal{N}, G_2, \kappa)$ is node balanced if and only if

$$\begin{aligned} K_{G_2,2} = K_{G_2,4} \quad &\iff \quad \kappa_1\kappa_3\kappa_7\kappa_8 + \kappa_1\kappa_3\kappa_5\kappa_8 = \kappa_2\kappa_4\kappa_6\kappa_8 \\ &\iff \quad \kappa_1\kappa_3\kappa_7 + \kappa_1\kappa_3\kappa_5 = \kappa_2\kappa_4\kappa_6. \end{aligned} \tag{19}$$

By (19), if $(\mathcal{N}, G_2, \kappa)$ is node balanced, then $\kappa_1\kappa_3\kappa_7 - \kappa_2\kappa_4\kappa_6 < 0$, while by (18), if $(\mathcal{N}, G_1, \kappa)$ is node balanced, then $\kappa_1\kappa_3\kappa_7 - \kappa_2\kappa_4\kappa_6 > 0$. This shows that there does not exist κ such that $\mathcal{N}$ is node balanced with respect to both reaction graphs.

4 Horn and Jackson's symmetry conditions

Horn and Jackson studied steady states in general and complex and detailed balanced steady states in particular [15]. They showed that there exist certain symmetry conditions on the *rate matrix* such that the detailed and complex balanced steady states, and the steady states in general, are precisely the points fulfilling these symmetry conditions. We revisit these symmetry conditions in the light of the theory developed here.

Given a kinetics $v(x)$, the $m \times m$ *rate matrix* $\rho(x)$ is such that the (i, j)-th entry is $v_k(x)$ if the k-th reaction is $r_k \colon y_j \to y_i$, and zero otherwise. Say a function Ω on $\mathbb{R}^{m \times m}$ is *symmetric*

at x if

$$\Omega(\rho(x)) = \Omega(\rho^T(x)), \tag{20}$$

where ρ^T denotes the transpose matrix of ρ. Define the functions

$$\Omega_d(\rho(x)) = \rho(x), \qquad \Omega_c(\rho(x)) = \rho(x)e, \qquad \Omega_e(\rho(x)) = Y_c\rho(x)e$$

where $e = (1, \dots, 1) \in \mathbb{R}^m$ and Y_c is the labeling matrix of the canonical complex reaction graph. Then any detailed balanced steady state x^* of $\mathcal{N}$ is characterized by the symmetry condition for Ω_d, any complex balanced steady state x^* of $\mathcal{N}$ is characterized by the symmetry condition for Ω_c and finally any steady state x^* of $\mathcal{N}$ is characterized by the symmetry condition for Ω_e [15]. We might straightforwardly extend this to node balanced steady states in the following way.

Given a reaction graph G, we define a function $\iota_G \colon \mathbb{R}^{m\times m} \to \mathbb{R}^{m_G\times m_G}$ entry-wise by $\iota_G(z)_{i_1,i_2} = z_{j_1,j_2}$ if $i_2 \to i_1 \in E_G$ and $R_{i_2\to i_1} = y_{j_2} \to y_{j_1}$, and 0 otherwise. Then $\iota_G(\rho(x))$ is simply the rate matrix in terms of the nodes of the reaction graph G. Now define

$$\Omega_G(\rho(x)) = \iota_G(\rho(x))e_G \ \in \ \mathbb{R}^{m_G}, \tag{21}$$

where $e_G = (1, \dots, 1) \in \mathbb{R}^{m_G}$. The i-th entry of the vector in (21) is the sum of the rate functions of the edges with target i in G. Using (10), note that

$$\Omega_G(\rho(x)) - \Omega_G(\rho^T(x)) = C_G v(x),$$

which is zero if and only if x is a node balanced steady state with respect to G, and if and only if the symmetry condition is fulfilled for Ω_G at x.

If G is the canonical complex reaction graph, then ι_G is the identity map and $\Omega_G(\rho(x)) = \rho(x)e = \Omega_c(\rho(x))$. If G is a detailed reaction graph, then there is only one element in each row of $\iota_G(\rho(x))$. Hence the vector $\iota_G(\rho(x))e_G$, up to a permutation of the entries, agrees with $\Omega_d(\rho(x))$.

Horn and Jackson speculated that there would be other types of steady states fulfilling similar symmetry conditions as they verified for detailed and complex balanced steady state [15]. The analysis above confirms that this is indeed the case and that the function Ω_G in (21) perhaps is the natural function to study in this context.

5 Steady states of subnetworks

In this section we present an application of our theory of reaction graphs and node balanced steady states to determine whether a node balanced steady state of a network is also node balanced for a subnetwork, and *vice versa*.

Given a reaction network $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$, the network generated by a subset of reactions $\mathcal{R}' \subseteq \mathcal{R}$ is called a *subnetwork* of $\mathcal{N}$. Any kinetics of $\mathcal{N}$ naturally induces a kinetics of a subnetwork.

Let $\mathcal{N}_1, \dots, \mathcal{N}_\ell$ be subnetworks generated by disjoint subsets of reactions $\mathcal{R}_1, \dots, \mathcal{R}_\ell \subseteq \mathcal{R}$, respectively. Let $\mathcal{R}_{\ell+1} = \mathcal{R} \backslash \bigcup_{i=1}^{\ell} \mathcal{R}_i$ and let $\mathcal{N}_{\ell+1}$ be the subnetwork generated by $\mathcal{R}_{\ell+1}$, called the *complementary subnetwork*. Observe that $\mathcal{R}_1, \dots, \mathcal{R}_{\ell+1}$ form a partition of $\mathcal{R}$.

Consider a reaction graph G associated with $\mathcal{N}$. For $i = 1, \dots, \ell+1$, let $G_i = (V_i, E_i)$ be the subgraph induced by the edges corresponding to the reactions of $\mathcal{R}_i$, and let m_{G_i} denote the number of nodes of G_i. After renumbering the nodes by means of a bijection between

$\{1, \ldots, m_{G_i}\}$ and V_i, the graph G_i becomes a reaction graph associated with $\mathcal{N}_i$, denoted by $G_{\mathcal{N}_i}$. We say that $G_{\mathcal{N}_i}$ is a *reaction graph associated with $\mathcal{N}_i$ induced by G*. That is, G_i and $G_{\mathcal{N}_i}$ are isomorphic digraphs, but G_i is a subgraph of G, while $G_{\mathcal{N}_i}$ is a reaction graph associated with $\mathcal{N}_i$.

One might construct a new reaction graph G' by taking the disjoint union of $G_1, \ldots, G_{\ell+1}$, or equivalently, the disjoint union of $G_{\mathcal{N}_1}, \ldots, G_{\mathcal{N}_{\ell+1}}$, up to a numbering of the nodes. Specifically, let $\mathcal{P}$ be the partition defining $[G]$. We define a new partition $\mathcal{P}'$ as follows: $j \sim_{\mathcal{P}'} k$ if and only if $j \sim_{\mathcal{P}} k$ and further, the edge involving j and the edge involving k in G_{sp} correspond to reactions of the same subset $\mathcal{R}_i$ (equivalently, the corresponding edges of G belong to the same subgraph G_i).

Clearly, $\mathcal{P}' \leqslant \mathcal{P}$ and any reaction graph G' with partition $\mathcal{P}'$ fulfills $G \preceq G'$. Any such G' is called a reaction graph *induced by G and the subnetworks $\mathcal{N}_1, \ldots, \mathcal{N}_\ell$*.

Let n_i be the number of species of $\mathcal{N}_i$ and π_i denote the projection from $\mathbb{R}^n$ to $\mathbb{R}^{n_i}$, obtained by selecting the indices of the species in $\mathcal{N}_i$.

Proposition 6. *Consider a reaction network $\mathcal{N}$ and subnetworks $\mathcal{N}_1, \ldots, \mathcal{N}_\ell$ with complementary subnetwork $\mathcal{N}_{\ell+1}$. Let G be a reaction graph, $G_{\mathcal{N}_i}$ the reaction graph associated with $\mathcal{N}_i$ induced by G, for all $i = 1, \ldots, \ell+1$, and G' a reaction graph induced by G and the subnetworks $\mathcal{N}_1, \ldots, \mathcal{N}_\ell$. Assume $\mathcal{N}$ is equipped with mass-action kinetics for some choice of reaction rate constants.*

Let $x^* \in \mathbb{R}^n_{\geqslant 0}$. The following statements are equivalent:

(i) x^* is a node balanced steady state of $\mathcal{N}$ with respect to G, and $\pi_i(x^*)$ is a node balanced steady state of $\mathcal{N}_i$ with respect to $G_{\mathcal{N}_i}$ for all $i = 1, \ldots, \ell$.

(ii) x^* is a node balanced steady state of $\mathcal{N}$ with respect to G'.

(iii) $\pi_i(x^*)$ is a node balanced steady state of $\mathcal{N}_i$ with respect to $G_{\mathcal{N}_i}$ for all $i = 1, \ldots, \ell+1$.

Proof. After renumbering the elements of the set of reactions, there is a choice of G'' with $[G''] = [G']$ such that $C_{G''}$ is a block matrix with $\ell+1$ blocks. Since the statements are independent of the choice of representative of the equivalence class of G', we assume $G' = G''$.

The i-th block of $C_{G'}$ is precisely the incidence matrix of $G_{\mathcal{N}_i}$, for the induced numberings. Let v be the kinetics of $\mathcal{N}$ and v_i the kinetics induced on $\mathcal{N}_i$. Let p_i be the cardinality of $\mathcal{R}_i$, and let ρ denote the projection from $\mathbb{R}^p$ to $\mathbb{R}^{p_i}$, obtained by selecting the indices of the reactions in $\mathcal{R}_i$. Note that

$$v_i(\pi_i(x^*)) = \rho_i(v(x^*)).$$

(ii) $\Leftrightarrow$ (iii): We have x^* is node balanced with respect to G' if and only if

$$C_{G_{\mathcal{N}_i}} v_i(\pi_i(x^*)) = C_{G_{\mathcal{N}_i}} \rho_i(v(x^*)) = 0, \qquad \text{for all } i = 1, \ldots, \ell+1,$$

if and only if $\pi_i(x^*)$ is a node balanced steady state of $\mathcal{N}_i$ with respect to $G_{\mathcal{N}_i}$ for all $i = 1, \ldots, \ell+1$.

(iii) $\Rightarrow$ (i): If (iii) holds, then clearly the second part of (i) holds. Further, since we have proven (ii) $\Leftrightarrow$ (iii), x^* is a node balanced steady state of $\mathcal{N}$ with respect to G', which, since $G \preceq G'$, also is a node balanced steady state of $\mathcal{N}$ with respect to G. This shows that (iii) implies the first part of (i).

(i) $\Rightarrow$ (ii): If (i) holds, then $C_G v(x^*) = 0$ and

$$C_{G'} v(x^*) = \left(0, \ldots, 0, C_{G_{\mathcal{N}_{\ell+1}}} v_{\ell+1}(\pi_{\ell+1}(x^*))\right),$$

where the zeroes cover the first $m_1 + \cdots + m_\ell$ entries. By Proposition 2(iii), there exists an $(m_G \times m_{G'})$-matrix B such that $C_G = BC_{G'}$. Write $B = (B_1|\ldots|B_{\ell+1})$ such that each block B_i has m_i columns. Then, by hypothesis we have

$$B_{\ell+1} C_{G_{\mathcal{N}_{\ell+1}}} v_{\ell+1}(\pi_{\ell+1}(x^*)) = 0. \tag{22}$$

Let $\varphi\colon V_{G'} \to V_G$ be the morphism defining the inclusion $G \preceq G'$. By construction (see the proof of Proposition 2(iii)), the j-th column of B has one non-zero entry, equal to one, in the $\varphi(j)$-th row. By definition of G', φ is injective on each V_{G_i}. In particular, $B_{\ell+1}$ has $m_{\ell+1}$ non-zero rows, which define a permutation matrix. Thus, (22) implies $C_{G_{\mathcal{N}_{\ell+1}}} v_{\ell+1}(\pi_{\ell+1}(x^*)) = 0$. Hence $C_{G'} v(x^*) = 0$. □

Note that if $\delta_G = \delta_{G'}$, then any node balanced steady state with respect to G automatically fulfills the three equivalent statements in Proposition 6.

An interesting consequence of Proposition 6 and Theorem 1 is that, given a reaction graph G, either all or none of the positive steady states of $\mathcal{N}$ are node balanced with respect to G and fulfil that $\pi_i(x^*)$ is a node balanced steady state of $\mathcal{N}_i$ with respect to $G_{\mathcal{N}_i}$ for $i = 1, \ldots, \ell$. Indeed, either all or none the positive steady states of $\mathcal{N}$ are node balanced with respect to G'.

In the particular setting of complex balanced steady states, the reaction graphs induced by a complex reaction graph are complex reaction graphs associated with the subnetworks. Proposition 6 says that the set of complex balanced steady states that are also complex balanced for a set of disjoint subnetworks agree with the set of node balanced steady states for a specific reaction graph defined from the subnetworks. Therefore, the properties of node balanced steady states derived from Theorem 1, 2 and 3 also apply in this case. In particular, positive steady states of this type can only exist if the reaction networks $\mathcal{N}_1, \ldots, \mathcal{N}_\ell$, as well as the complementary subnetwork, are weakly reversible. Moreover, conditions on the reaction rate constants κ for which such steady states exist are given in Theorem 2. Finally, if there exists a positive complex balanced steady state of $\mathcal{N}$ that is also complex balanced for a subnetwork, then so is any positive steady state of $\mathcal{N}$.

Example 1 (part J). Consider the following subsets of $\mathcal{R}$:

$$\mathcal{R}_1 = \{r_1, r_2, r_6\}, \qquad \mathcal{R}_2 = \{r_3, r_4, r_5\}.$$

Let respectively $\mathcal{N}_1, \mathcal{N}_2$ denote the subnetworks generated by $\mathcal{R}_1, \mathcal{R}_2$. Consider the complex balanced reaction graph G_1 in Figure 1. Then G_3 is a reaction graph induced by G_1 and $\mathcal{N}_1$. By Proposition 6, x^* is a complex balanced steady state for $\mathcal{N}$ and $\mathcal{N}_1$, if and only if x^* is a node balanced steady state with respect to G_3. In this case, it is also a complex balanced steady state for $\mathcal{N}_2$.

Example 1 (part K). Let $\mathcal{N}'$ be the subnetwork generated by $\mathcal{R}' = \{r_1, r_2, r_5, r_6\}$. Both $\mathcal{N}$ and $\mathcal{N}'$ are weakly reversible, but the complementary subnetwork, with reactions r_3, r_4, is not. Thus there does not exist reaction rate constants for which there exists a positive complex balanced steady state for both $\mathcal{N}$ and $\mathcal{N}'$.

If the sets of reactions $\mathcal{R}_1, \ldots, \mathcal{R}_\ell$ are not disjoint, then there is not a general unambiguous answer similar to that of Proposition 6.

6 Proofs

6.1 Proof of Theorems 1 and 2

To ease the notation, we use $[k] = \{1, \dots, k\}$ for $k \in \mathbb{N}$.

One way to prove Theorem 1 and 2 would be to reproduce the arguments of the original results for complex balanced steady states. Indeed, the original arguments work line by line because it is not explicitly used in the proofs that the complexes (node labels of the reaction graph) are different from each other. This is not even stated as a requirement in [3, 4]. The reader familiar with these results will readily see that this is the case. However, we take a different route here.

For a given network $\mathcal{N}$, we construct another network $\mathcal{N}'$, such that their steady states agree. Further, the complex balanced steady states of $\mathcal{N}'$ are in one-to-one correspondence with the node balanced steady states of $\mathcal{N}$. Hence, we can lift the (known) results for complex balanced steady states such that they hold for node balanced steady states as well.

Let G be a reaction graph associated with $\mathcal{N}$. We start with the construction of the network $\mathcal{N}' = (\mathcal{S}', \mathcal{C}', \mathcal{R}')$. To this end, we define the species set as $\mathcal{S}' = \mathcal{S} \times V_G = \{(X_i, j) \mid X_i \in \mathcal{S},\ j \in V_G\}$, and define

$$\epsilon = 1 + \max_{y \in \mathcal{C}} \sum_{i=1}^{n} y_i, \quad \text{and} \quad y^j = \sum_{i=1}^{n} (Y_j)_i \, (X_i, j). \tag{23}$$

Since Y_j is the label of the node j, then $(Y_j)_i \in \mathbb{N}$ is the coefficient of Y_j in species X_i in the original network. The reaction set $\mathcal{R}'$ is defined as

$$\mathcal{R}' = \{y^i \to y^j \mid i \to j \in E_G\} \cup \{\epsilon(X_i, j) \to \epsilon(X_i, j') \mid (X_i, j), (X_i, j') \in \mathcal{S}'\}, \tag{24}$$

and the complex set as

$$\mathcal{C}' = \{y^1, \dots, y^{m_G}\} \cup \left\{\epsilon(X_i, j) \mid \ (X_i, j) \in \mathcal{S}'\right\}.$$

This set has cardinality $m_G + n\, m_G = m_G(n+1)$. We number the set $\mathcal{C}'$ according to the order

$$y^1, \dots, y^{m_G}, \epsilon(X_1, 1), \dots, \epsilon(X_1, m_G), \dots, \epsilon(X_n, 1), \dots, \epsilon(X_n, m_G), \tag{25}$$

and the species set analogously: $(X_1, 1), \dots, (X_1, m_G), \dots, (X_n, 1), \dots, (X_n, m_G)$. Reactions are numbered such that the reactions $1, \dots, p$ correspond to the reactions in $\mathcal{R}$ (first set in (24), and the rest of the reactions are ordered increasingly in i and arbitrarily within the subsets of reactions involving (X_i, j), $j = 1, \dots, m_G$. The complex reaction graph G'_c of $\mathcal{N}'$ will refer to this numbering.

There is a graph isomorphism from G and the subgraph of G'_c induced by the nodes $1, \dots, m_G$ (those with label $y^1, \dots, y^{m_G}$) that maps $i \in V_G$ to i. The coefficient ϵ ensures that the source and target of the reactions in (24) are not one of y^j in (23). Thus the reaction graph G'_c has n extra connected components, one for each X_i, whose nodes are labeled by $\epsilon(X_i, j)$, $j = 1, \dots, m_G$. These components are complete digraphs since there is a directed edge from every node to every other node.

For example, for the reaction graph

$$1, X_1 + X_2 \to 2, 3X_1,$$

we have $\epsilon = 4$ and the reaction network $\mathcal{N}'$ consists of the reactions

$$(X_1, 1) + (X_2, 1) \to 3(X_1, 2), \qquad 4(X_1, 1) \rightleftharpoons 4(X_1, 2), \qquad 4(X_2, 1) \rightleftharpoons 4(X_2, 2).$$

The species set has $n\, m_G$ elements. We identify $\mathbb{R}^{n\, m_G}$ with $\mathbb{R}^{n \times m_G}$ and index the concentration of the species (X_i, j) as x_{ij}. Consider the linear map $\pi\colon \mathbb{R}^{n \times m_G} \to \mathbb{R}^n$ and the injective linear map $g\colon \mathbb{R}^n \to \mathbb{R}^{n \times m_G}$ defined by

$$\begin{aligned} \pi(x)_i &= \sum_{j=1}^{m_G} x_{ij}, && i \in [n], \qquad \text{for all } x \in \mathbb{R}^{n \times m_G}, \\ g(x)_{ij} &= x_i, && i \in [n], j \in [m_G], \qquad \text{for all } x \in \mathbb{R}^n. \end{aligned}$$

Note that g maps positive vectors to positive vectors and that $\pi(g(x)) = m_G\, x$.

Lemma 4. *Let $s = \dim(S)$ and let S' be the stoichiometric subspace of $\mathcal{N}'$. Then $S = \pi(S')$. Further, S' has dimension $s + n(m_G - 1)$ and the deficiency of the network $\mathcal{N}'$ is δ_G.*

Proof. Let $e_{i,j\to j'} = (X_i, j') - (X_i, j)$ be the vector in $\mathbb{R}^{n \times m_G}$ that has two nonzero entries, the (i, j)-th, where it is equal to -1, and the (i, j')-th where it is equal to 1. Then

$$S' = \left\langle y^j - y^i \mid i \to j \in E_G \right\rangle + \left\langle e_{i,j\to j'} \mid i \in [n], j, j' \in [m_G] \right\rangle.$$

Let us show that $\pi(S') = S$. Observe that $\pi(S') \subseteq S$ since $\pi(e_{i,j\to j'}) = 0$ and $\pi(y^j - y^i) = Y_j - Y_i$. Furthermore, if $u \in S$, then

$$u = \sum_{i\to j \in E_G} \lambda_{ij}(Y_j - Y_i) = \sum_{i\to j \in E_G} \lambda_{ij}\pi(y^j - y^i) \;\in\; \pi(S'),$$

hence $\pi(S') = S$.

To determine $\dim S'$ we do the following. For $x \in \ker \pi$ we have $\sum_{j=1}^{m_G} x_{ij} = 0$ for all $i \in [n]$. Consider the vector

$$x' = \sum_{i=1}^{n} \sum_{j=2}^{m_G} x_{ij} e_{i,1\to j}.$$

Since the nonzero entries of $e_{i,1\to j}$ are $(e_{i,1\to j})_{i,j} = 1$ and $(e_{i,1\to j})_{i,1} = -1$, we have $x'_{k,k'} = x_{k,k'}$ if $k' \neq 1$. Further, using that $x \in \ker \pi$ by assumption, we have $x'_{k1} = -\sum_{j=2}^{m_G} x_{kj} = x_{k1}$. It follows that $x = x'$ and thus $\ker \pi = \langle e_{i,1\to j} \mid i \in [n], j \in [m_G] \rangle \subseteq S'$. For each $i \in [n]$, the vectors $e_{i,1\to j}$ are the columns of the incidence matrix of a connected graph with m_G nodes, which has rank $m_G - 1$. It follows that $\dim \ker \pi = n(m_G - 1)$. Now, by the first isomorphism theorem

$$\dim S' = \dim \ker \pi + \dim \pi(S') = s + n(m_G - 1).$$

Since C' has $\ell_G + n$ connected components and $m_G(n + 1)$ nodes, the deficiency of $\mathcal{N}'$ is

$$\delta_{\mathcal{N}'} = m_G(n + 1) - s - n(m_G - 1) - \ell_G - n = m_G - s - \ell_G = \delta_G.$$

□

Proof of Theorem 1. In order to prove Theorem 1 we use that the theorem holds for complex balanced steady states [15, Theorem 6A]. Since a positive node balanced steady state is in particular complex balanced, any positive node balanced steady state is asymptotically stable. Further, if there is one positive node balanced steady state with respect to G, then the network $\mathcal{N}$ admits exactly one positive steady state within every stoichiometric compatibility class, which is complex balanced. Therefore, to prove the theorem all we need is to show that if there is one positive node balanced steady state with respect to G, then all positive steady states are node balanced with respect to G.

We endow $\mathcal{N}'$ with mass-action kinetics, such that the reaction rate constant $\kappa_{i\to j}$ of $y^i \to y^j$ is that of $Y_i \to Y_j$ for any $i \to j \in E_G$. This implies that the reaction rate constants of the reaction $R_{i\to j}$ in G and G'_c agree. The reaction rate constant of $\epsilon(X_i, j) \to \epsilon(X_i, j')$ is set to $\kappa_{i,j\to j'} = 1$.

By (23), for any complex of the form $y^k \in \mathcal{C}'$, the only nonzero entries are $y^k_{ik} = (Y_k)_i$, $i = 1, \dots, n$. This gives

$$g(x)^{y^k} = \prod_{(i,j)\in[n]\times[m_G]} g(x)_{ij}^{y^k_{ij}} = \prod_{i\in[n]} x_i^{(Y_k)_i} = x^{Y_k}, \qquad g(x)^{\epsilon(X_i,k)} = x_i^{\epsilon}. \tag{26}$$

Denote the kinetics of $\mathcal{N}$ by v and that of $\mathcal{N}'$ by v'. Then, by the choice of reaction rate constants we have,

$$v'(g(x)) = (v(x), (x_1^{\epsilon}, \dots, x_1^{\epsilon}), \dots, (x_n^{\epsilon}, \dots, x_n^{\epsilon})), \tag{27}$$

where for all $i \in [n]$ the vector $(x_i^{\epsilon}, \dots, x_i^{\epsilon})$ has length $m_G(m_G - 1)$.

The incidence matrix of the canonical complex reaction graph of $\mathcal{N}'$, denoted by C', is block diagonal with the first block equal to C_G, and the remaining blocks $2, \dots, n+1$ equal to the incidence matrix of a complete digraph with m_G nodes. We have the following key lemma.

Lemma 5. *(i)* $C'\, v'(g(x)) = (C_G\, v(x), 0, \dots, 0) \in \mathbb{R}^{m_G + n\, m_G}$.

(ii) $x \in \mathbb{R}^n_{>0}$ *is a positive node balanced steady state of* $\mathcal{N}$ *with respect to* G *if and only if* $g(x) \in \mathbb{R}^{n\times m_G}_{>0}$ *is a positive complex balanced steady state for* $\mathcal{N}'$.

(iii) If $x' \in \mathbb{R}^{n\times m_G}_{>0}$ *is a positive complex balanced steady state of* $\mathcal{N}'$*, then there exists a unique* $x \in \mathbb{R}^n_{>0}$ *such that* $x' = g(x)$.

Proof. (i) By the block form of C' and (27), every column in the blocks $2, \dots, n+1$ appear with $+$ and with $-$ sign in the same block. Thus multiplication of $(i+1)$-th block with $(x_i^{\epsilon}, \dots, x_i^{\epsilon})$ is zero. The result follows now because the first block of C' is C_G and the first m_G entries of $v'(g(x))$ agree with $v(x)$.

(ii) follows directly from (i).

(iii) For fixed $i \in [n]$, consider the incidence matrix of the complete digraph corresponding to the nodes (i, j) for all $j \in [m_G]$. Each row of the matrix has exactly $m_G - 1$ entries equal to -1 and $m_G - 1$ entries equal to one, since there are $m_G - 1$ edges with target j and $m_G - 1$ edges with source j. For the edges with source j, the rate function is $(x')^{\epsilon(X_i,j)} = (x')^{\epsilon}_{ij}$. Thus complex balancing implies

$$(m_G - 1)(x')^{\epsilon}_{ij} = \sum_{j'\in[m_G], j'\neq j} (x')^{\epsilon}_{ij'}, \qquad \text{for all } j \in [m_G].$$

For distinct $j_1, j_2 \in [m_G]$ this gives

$$(m_G - 1)((x')^\epsilon_{ij_1} - (x')^\epsilon_{ij_2}) = \sum_{j' \in V_G, j' \neq j_1} (x')^\epsilon_{ij'} - \sum_{j' \in V_G, j' \neq j_2} (x')^\epsilon_{ij'} = (x')^\epsilon_{ij_2} - (x')^\epsilon_{ij_1}.$$

This gives $0 = m_G((x')^\epsilon_{ij_1} - (x')^\epsilon_{ij_2})$. Since x' is positive, we obtain $x'_{ij_1} = x'_{ij_2}$ for all pairs j_1, j_2 and all $i \in [n]$. As a consequence, x' is in the image of g. Unicity follows because g is injective. □

By Lemma 5(ii), if $\mathcal{N}$ admits a positive node balanced steady state x^* with respect to G, then $g(x^*)$ is a positive complex balanced steady state of $\mathcal{N}'$ and it follows that all positive steady states of $\mathcal{N}'$ are complex balanced. Let now x^{**} be another positive steady state of $\mathcal{N}$. The stoichiometric compatibility class of $\mathcal{N}'$ containing $g(x^{**})$ has one positive steady state x', which is complex balanced. By Lemma 5(iii), there exists $x'' \in \mathbb{R}^n_{>0}$ such that $x' = g(x'')$, and by Lemma 5(ii), it follows that x'' is a node balanced steady state with respect to G. Let us show that $x'' = x^{**}$. We have that $g(x'' - x^{**}) \in S'$, since x' and $g(x^{**})$ belong to the same stoichiometric compatibility class of $\mathcal{N}'$. By Lemma 4, it follows that $x'' - x^{**} = \frac{1}{m_G}\pi(g(x' - x^{**})) \in S$. Thus x'' and x^{**} are in the same stoichiometric compatibility class of $\mathcal{N}$ and they are both positive steady states. Since there is a unique positive (complex balanced) steady state in each class, they must coincide. This concludes the proof of Theorem 1. □

Proof of Theorem 2. Consider the labeling matrix Y' of the canonical complex reaction graph of $\mathcal{N}'$ with numbering of complexes given in (25). We let a vector $u \in \mathbb{R}^{m_G + n\, m_G}$ be indexed as

$$u = (u_1, \ldots, u_{m_G}, u_{11}, \ldots, u_{1m_G}, \ldots, u_{n1}, \ldots, u_{nm_G})$$

and use the same indexing for the columns of Y'. The matrix Y' has one or two nonzero entries in each row: if (X_i, j) is part of y^j, then the row corresponding to this species has two nonzero entries: $(Y_j)_i$ in column j and ϵ in column (i, j). If (X_i, j) is not part of y^j, then the row corresponding to this species has one nonzero entry: ϵ in column (i, j).

Let Ψ' be the map (9) for the canonical complex reaction graph of $\mathcal{N}'$. We start by giving an explicit isomorphism between $\ker \Psi'$ and $\ker \Psi_G$, which exists since both vector subspaces have dimension δ_G (cf. Lemma 4, Proposition 3). Consider the projection map

$$\rho \colon \mathbb{R}^{m_G + nm_G} \to \mathbb{R}^{m_G}, \qquad \rho(x) = (x_1, \ldots, x_{m_G}).$$

Lemma 6. *The linear map ρ induces an isomorphism from $\ker \Psi'$ to $\ker \Psi_G$.*

Proof. We first show that $\rho(x) \in \ker \Psi_G$ for $x \in \ker \Psi'$. Using the form of the labeling matrix Y', we have that if $x \in \ker \Psi'$, then

$$(Y_j)_i\, x_j = -\epsilon x_{ij}, \qquad \text{for all } i \in [n], j \in [m_G]. \tag{28}$$

Thus, for every $i \in [n]$ we have

$$\sum_{j=1}^{m_G} (Y_j)_i x_j = -\epsilon \sum_{j=1}^{m_G} x_{ij} = 0,$$

by definition of Ψ', since the nodes $(i, 1), \ldots, (i, m_G)$ form a connected component of C'. By the correspondence between connected components of C' and G, $\sum_{i \in G_k} x_i = 0$ for all $k \in [\ell_G]$. This shows that $\rho(x) \in \ker \Psi_G$.

Let us find the kernel of ρ restricted to $\ker \Psi'$. We have $\rho(x) = 0$ if and only if $x_j = 0$ for all $j = 1, \dots, m_G$. By (28), it follows that also $x_{ij} = 0$ for all i and j. As a consequence $x = 0$. Therefore ρ is an injective linear map between two vector spaces of the same dimension, $\ker \Psi'$ and $\ker \Psi_{\mathcal{N}_G}$, and it is thus an isomorphism. □

By Theorems 7 and 9 in [3], there exists a positive complex balanced steady state for $\mathcal{N}'$ with a vector of reaction rate constants κ' if and only if Theorem 2(i) holds, that is,

$$(K')^u = 1, \qquad \text{for all } u \in \ker \Psi',$$

where K' is computed from the spanning trees in C' with labels given by κ'. For the particular choice of reaction rate constants we have made,

$$K'_{ij} = K'_{ij'} \qquad \text{for all } i \in [n], j, j' \in [m_G]. \tag{29}$$

Indeed, the reaction rate constants of any spanning tree rooted at $\epsilon(X_i, j)$ or $\epsilon(X_i, j')$ (in the corresponding connected component) are equal to one. Moreover $\epsilon(X_i, j)$ and $\epsilon(X_i, j')$ are in the same connected component, which is a complete digraph. Hence the number of spanning trees rooted at $\epsilon(X_i, j)$ and $\epsilon(X_i, j')$ is the same.

Further, using that G and the subgraph of C' with nodes $1, \dots, m_G$ are isomorphic and preserve the reaction rate constants, it holds that

$$K_G = \rho(K'). \tag{30}$$

If $u \in \ker \Psi'$, then $\sum_{j=1}^{m_G} u_{ij} = 0$. Therefore

$$(K')^u = \rho(K')^{\rho(u)} \prod_{i=1}^{n} \prod_{j=1}^{m_G} (K'_{ij})^{u_{ij}} = \rho(K')^{\rho(u)} \prod_{i=1}^{n} (K'_{i1})^{\sum_{j=1}^{m_G} u_{ij}} = \rho(K')^{\rho(u)} = K_G^{\rho(u)}.$$

Since ρ is an isomorphism between $\ker \Psi'$ and $\ker \Psi_G$, we conclude that

$$(K')^u = 1, \qquad \text{for all } u \in \ker \Psi', \qquad \Leftrightarrow \qquad K_G^u = 1, \qquad \text{for all } u \in \ker \Psi_G. \tag{31}$$

Consequently, we have $K_G^u = 1$ for all $u \in \ker \Psi_G$ if and only if $\mathcal{N}'$ admits a positive complex balanced steady state for a choice of reaction rate constants κ' such that $\kappa'_{i,j\to j'} = 1$ for all $i \in [n]$, $j, j' \in [m_G]$ and $\kappa'_{i\to j} = \kappa_{i\to j}$ for all $i \to j \in E_{C'}$, if and only if $\mathcal{N}$ admits a positive node balanced steady state with respect to G for the corresponding choice of reaction rate constants κ (Lemma 5(ii)). This proves (i).

The proof of part (ii) follows the same line of arguments. We use the same notation for reaction rate constants κ of $\mathcal{N}$ and κ' of $\mathcal{N}'$. By [4, Eq (21)], (ii) holds for complex balanced steady states of $\mathcal{N}'$. That is, $x' \in \mathbb{R}^{n\times m_G}_{>0}$ is a complex balanced steady state of $\mathcal{N}'$ if and only if

$$\begin{aligned} K'_i (x')^{y^i} - K'_j (x')^{y^j} &= 0, \quad \forall (i,j) \in E_G, \qquad \textit{and} \\ K'_{ij} \, (x')^{\epsilon(X_i,j)} - K'_{ij'} \, (x')^{\epsilon(X_i,j')} &= 0, \qquad \forall i \in [n], j, j' \in [m_G]. \end{aligned}$$

Let $x' = g(x)$. By (26) and (29), the equations in the second row are satisfied. According to (26) and (30), the equations in the first row are equal to $K_i x^{Y_i} - K_j x^{Y_j} = 0$. This gives the following: x is a positive node balanced steady state of $\mathcal{N}$ with respect to G, if and only if $g(x)$ is a positive complex balanced steady state of $\mathcal{N}'$ (Lemma 5(ii)), if and only if $K_i x^{Y_i} - K_j x^{Y_j} = 0$ for all $(i, j) \in E_G$. Thus (ii) holds and the theorem is proven. □

6.2 Proof of Theorem 3

To simplify the notation, we let K denote K_G and K' denote $K_{G'}$ throughout the subsection.

(i) The nodes i_1, i_2 do *not* belong to the same connected component of G. In this case, $\delta_G = \delta_{G'}$ by Proposition 4. We will show that the two sets of equations in κ for which $(\mathcal{N}, G, \kappa)$ and $(\mathcal{N}, G', \kappa)$ are node balanced can be chosen to be the same. Let G_{p_1} and G_{p_2} be the connected components of G containing i_1, i_2 respectively, and G'_q be the connected component of G' containing k. The morphism φ is a bijection between $V_G \backslash \{i_1, i_2\}$ and $V'_G \backslash \{k\}$ and induces an isomorphism between the subgraph of G obtained by removing G_{p_1}, G_{p_2} and the subgraph of G' obtained by removing G'_q. Let V_i (resp. V'_i) denote the set of nodes of the i-th connected component of G (resp. G').

We define two linear maps $\alpha\colon \mathbb{R}^{m_G} \to \mathbb{R}^{m'_G}$, and $\beta\colon \mathbb{R}^{m'_G} \to \mathbb{R}^{m_G}$ by

$$\alpha(x)_i = \begin{cases} x_{\varphi^{-1}(i)} & \text{if } i \neq k \\ x_{i_1} + x_{i_2} & \text{if } i = k, \end{cases} \qquad \beta(x)_i = \begin{cases} x_{\varphi(i)} & \text{if } i \neq i_1, i_2 \\ \sum_{j \in V_{p_2}} x_{\varphi(j)} & \text{if } i = i_1 \\ \sum_{j \in V_{p_1}} x_{\varphi(j)} & \text{if } i = i_2. \end{cases}$$

Proposition 7. *The morphisms α and β induce isomorphisms between* $\ker \Psi_G$ *and* $\ker \Psi_{G'}$.

Proof. We first show that $\alpha \circ \beta(x) = x$ if $x \in \ker \Psi_{G'}$. For $i \neq k$, we have $\varphi^{-1}(i) \neq i_1, i_2$ and this gives

$$\alpha \circ \beta(x)_i = \beta(x)_{\varphi^{-1}(i)} = x_{\varphi \circ \varphi^{-1}(i)} = x_i.$$

For $i = k$, using that $x \in \ker \Psi_{G'}$, we have

$$\alpha \circ \beta(x)_k = \beta(x)_{i_1} + \beta(x)_{i_2} = \sum_{j \in V_{p_2}} x_{\varphi(j)} + \sum_{j \in V_{p_1}} x_{\varphi(j)} = x_k + \sum_{j \in V'_q} x_j = x_k.$$

This proves that $\alpha \circ \beta(x) = x$. In particular, β is injective.

We show now that $\beta(\ker \Psi_{G'}) \subseteq \ker \Psi_G$. Recall that $Y'_{\varphi(i)} = Y_i$ for all $i \in [m_G]$. Consider the labeling matrices Y, Y' and the linear maps induced by Y, Y' in $\mathbb{R}^{m_G}$ and $\mathbb{R}^{m'_G}$, respectively. We will show that $Y = Y' \circ \alpha$ in $\mathbb{R}^{m_G}$. For $x \in \mathbb{R}^{m_G}$ we have

$$\begin{aligned} Y' \circ \alpha(x) &= \sum_{i=1}^{m'_G} \alpha(x)_i Y'_i = (x_{i_1} + x_{i_2}) Y'_k + \sum_{i=1, i \neq k}^{m'_G} x_{\varphi^{-1}(i)} Y'_i \\ &= x_{i_1} Y_{i_1} + x_{i_2} Y_{i_2} + \sum_{j=1, j \neq i_1, i_2}^{m'_G} x_j Y_{\varphi(j)} = \sum_{j=1}^{m_G} x_j Y_j = Yx. \end{aligned}$$

Let $x \in \ker \Psi_{G'}$. For $j \neq p_1, p_2$, let $G'_{t(j)}$ be the connected component of G' isomorphic to G_j by φ. Then

$$\begin{aligned} &Y \circ \beta(x) = Y' \circ \alpha \circ \beta(x) = Y'x = 0 \\ &\sum_{i \in V_j} \beta(x)_i = \sum_{i \in V_j} x_{\varphi(i)} = \sum_{i \in V'_{t(j)}} x_i = 0, \qquad j \neq p_1, p_2, \\ &\sum_{i \in V_{p_1}} \beta(x)_i = \beta(x)_{i_1} + \sum_{i \in V_{p_1}, i \neq i_1} x_{\varphi(i)} = \sum_{i \in V_{p_2}} x_{\varphi(i)} + \sum_{i \in V_{p_1}, i \neq i_1} x_{\varphi(i)} = \sum_{i \in V'_q} x_i = 0. \end{aligned}$$

The last equation with the roles of p_1 and p_2 interchanged holds analogously. Thus $\Psi_G(\beta(x)) = 0$ and $\beta(x) \in \ker \Psi_G$. Since $\dim \ker \Psi_{G'} = \delta_{G'} = \delta_G = \dim \ker \Psi_G$ and β is injective, β is an isomorphism and so is α. In particular $\alpha(\ker \Psi_G) \subseteq \ker \Psi_{G'}$. □

The proposition shows how the morphism β can be used to find a basis of $\ker \Psi_G$ from a basis of $\ker \Psi_{G'}$, provided that G' is obtained from G by joining one pair of nodes and G' has one fewer connected components than G.

Proposition 8. *Let $u \in \ker \Psi_{G'}$. Then*

$$K'^u = K^{\beta(u)}.$$

Proof. If i is a node of G that does not belong to G_{p_1} nor G_{p_2}, then $K_i = K'_{\varphi(i)}$. If $i \in V_{p_1}$, then any spanning tree rooted at $\varphi(i)$ in G'_q consists of the image by φ of the union of a spanning tree rooted at i in G_{p_1} and one tree rooted at i_2 in G_{p_2}. Thus $K'_{\varphi(i)} = K_i K_{i_2}$. If $i \in V_{p_2}$, then we obtain analogously that $K'_{\varphi(i)} = K_i K_{i_1}$. Note that if $i = i_1$ or i_2 and $\varphi(i) = k$, then the two equations agree, $K'_k = K_{i_1} K_{i_2}$. Using the definition of β, this gives:

$$(K')_{\varphi(i)}^{u_{\varphi(i)}} = \begin{cases} K_i^{\beta(u)_i} & \text{if } i \notin V_{p_1} \cup V_{p_2} \\ K_i^{\beta(u)_i} K_{i_2}^{u_{\varphi(i)}} & \text{if } i \in V_{p_1} \backslash \{i_1\} \\ K_i^{\beta(u)_i} K_{i_1}^{u_{\varphi(i)}} & \text{if } i \in V_{p_2} \backslash \{i_2\} \\ K_{i_1}^{u_{\varphi(i_1)}} K_{i_2}^{u_{\varphi(i_2)}} & \text{if } i = i_1, i_2. \end{cases}$$

Thus

$$\begin{aligned} K'^u &= \prod_{j=1}^{m_{G'}} (K')_j^{u_j} = (K')_k^{u_k} \prod_{i \in [m_G] \backslash \{i_1, i_2\}} (K')_{\varphi(i)}^{u_{\varphi(i)}} = \left[\prod_{i \in [m_G] \backslash \{i_1, i_2\}} K_i^{\beta(u)_i} \right] \left[\prod_{i \in V_{p_1}} K_{i_2}^{u_{\varphi(i)}} \prod_{i \in V_{p_2}} K_{i_1}^{u_{\varphi(i)}} \right] \\ &= \left[\prod_{i \in [m_G] \backslash \{i_1, i_2\}} K_i^{\beta(u)_i} \right] K_{i_2}^{\beta(u)_{i_2}} K_{i_1}^{\beta(u)_{i_1}} = K^{\beta(u)}. \end{aligned}$$

This concludes the proof. □

We are ready to prove Theorem 3(i). Using Theorem 2(i), $(\mathcal{N}, G', \kappa)$ is node balanced if and only if $K'^u = 1$ for all $u \in \ker \Psi_{G'}$. By Proposition 8, this is equivalent to $K^{\beta(u)} = 1$ for all $u \in \ker \Psi_{G'}$, which in turn is equivalent to $K^u = 1$ for all $u \in \ker \Psi_G$, because β is an isomorphism. Using Theorem 2(i), the later condition is equivalent to $(\mathcal{N}, G, \kappa)$ being node balanced. This concludes the proof of Theorem 3(i). □

Case 2: The nodes i_1, i_2 belong to the same connected component of G. In this situation, we have $\delta_{G'} = \delta_G - 1$ and $m_G = m'_G + 1$. Let G_p be the connected component of G containing i_1, i_2, and G'_q the connected component of G' that contains k. Again, we have that φ induces an isomorphism between G and G' outside the connected components G_p and G'_q.

Consider the linear and injective morphism $\gamma \colon \mathbb{R}^{m'_G} \to \mathbb{R}^{m_G}$ defined for $i \in [m_G]$ by

$$\gamma(x)_i = \begin{cases} x_{\varphi(i)} & \text{if } i \neq i_2 \\ 0 & \text{if } i = i_2. \end{cases}$$

(All constructions could be done alternatively by replacing i_2 with i_1).

Proposition 9. *Let $\delta(i_1,i_2)\in\mathbb{R}^{m_G}$ be the vector with $\delta(i_1,i_2)_{i_1}=1$, $\delta(i_1,i_2)_{i_2}=-1$ and the rest of entries equal to zero. Let $\{u_1,\dots,u_{\delta_{G'}}\}$ be a basis of $\ker\Psi_{G'}$. Then*

$$\big\{\gamma(u_1),\dots,\gamma(u_{\delta_{G'}}),\delta(i_1,i_2)\big\}$$

is a basis of $\ker\Psi_G$.

Proof. Since the i_2-th component of $\gamma(u_j)$ is zero for all $j\in[\delta_{G'}]$, the vector $\delta(i_1,i_2)$ does not belong to $\langle\gamma(u_1),\dots,\gamma(u_{\delta_G})\rangle$. Since γ is injective, the vectors $\gamma(u_1),\dots,\gamma(u_{\delta_{G'}}),\delta(i_1,i_2)$ are linearly independent and generate a vector space of dimension $\delta_{G'}+1=\delta_G=\dim\ker\Psi_G$. Thus all we need is to show that $\delta(i_1,i_2),\gamma(u)\in\ker\Psi_G$ for all $u\in\ker\Psi_{G'}$.

We have

$$Y\delta(i_1,i_2)=Y_{i_1}-Y_{i_2}=Y'_k-Y'_k=0.$$

Since i_1 and i_2 belong to the same connected component of G, we have $\sum_{i\in G_j}\delta(i_1,i_2)_i=0$ for all connected components G_j of G. Thus $\delta(i_1,i_2)\in\ker\Psi_G$.

For a connected component G_j of G, let $G'_{t(j)}$ be the corresponding connected component of G' under the morphism φ, such that $t(p)=q$. For $u\in\ker\Psi_{G'}$ and $j\in[\ell_G]$, we have

$$Y\gamma(u)=\sum_{i=1}^{m_G}\gamma(u)_iY_i=\sum_{i=1,i\neq i_2}^{m_G}u_{\varphi(i)}Y_i=\sum_{i=1,i\neq i_2}^{m_G}u_{\varphi(i)}Y'_{\varphi(i)}=\sum_{j=1}^{m_{G'}}u_jY'_j=Y'u=0,$$
$$\sum_{i\in G_j}\gamma(u)_i=\sum_{i\in G_j,i\neq i_2}u_{\varphi(i)}=\sum_{i\in G'_{t(j)}}u_i=0.$$

This shows that $\gamma(u)\in\ker\Psi_G$, which concludes the proof. □

Proposition 10. *Assuming $K^{\delta(i_1,i_2)}=1$, then for all $u\in\ker\Psi_{G'}$ it holds*

$$K^{\gamma(u)}=K'^u.$$

Proof. Because γ induces an isomorphism of digraphs outside G_p and G'_q, we can without loss of generality restrict the proof to the case, where G,G' are strongly connected. For simplicity, we let $m=m_{G'}$ such that $V_G=[m+1]$ and $V_{G'}=[m]$, and assume that φ is the identity on $\{1,\dots,m\}$ and sends $m+1$ to 1 (so $i_1=1,i_2=m+1,k=1$). In this setting, $K^{\delta(i_1,i_2)}=1$ is equivalent to $K_1=K_{m+1}$.

Assume that it holds

$$K_1K'_i-K_iK'_1=0,\qquad\text{for all } i=1,\dots,m. \tag{32}$$

Not that since the graphs are strongly connected, none of K_i,K'_i is zero. Then, using $K_1=K_{m+1}$, we have

$$K^{\gamma(u)}=\prod_{i=1}^{m}K_i^{u_i}=\prod_{i=1}^{m}K_1^{u_i}\frac{K_i^{u_i}}{K_1^{u_i}}=\left[\prod_{i=1}^{m}K_1^{u_i}\right]\prod_{i=1}^{m}\left[\frac{K'_i}{K'_1}\right]^{u_i}=\left[\frac{K_1}{K'_1}\right]^{\sum_{i=1}^m u_i}\prod_{i=1}^{m}(K')_i^{u_i}=(K')^u,$$

where we use $\sum_{i=1}^m u_i=0$ since $u\in\ker\Psi_{G'}$.

Thus, all we need is to show that (32) holds provided $K_1=K_{m+1}$. Below we use the indices k,ℓ generically. Let Θ'_j be the set of spanning trees of G' rooted at j. Given $F,B\subseteq[m+1]$ of cardinality M, let $\Theta(F,B)$ be the set of spanning forests of G with M connected components,

such that each component is a tree rooted at one element of B and contains exactly one element of F. Let

$$\Theta_{i,j} = \Theta(\{1, m+1\}, \{i, j\}).$$

If $\zeta \in \Theta_{i,m+1}$, then ζ is a spanning forest that consists of two trees ζ_i, ζ_{m+1} rooted respectively at i and $m+1$ such that 1 is a node of ζ_i. Analogously, $\zeta \in \Theta_{1,i}$ is a spanning forest that consists of two trees ζ_1, ζ_i rooted respectively at 1 and i such that $m+1$ is a node of ζ_i. Then, φ induces two one-to-one correspondences

$$\Theta'_i \longleftrightarrow \Theta_{i,m+1} \sqcup \Theta_{1,i} \qquad\qquad \Theta'_1 \longleftrightarrow \Theta_{1,m+1},$$

for $2 \leqslant i \leqslant m$. The one-to-one correspondence between E_G and $E_{G'}$ induces a bijective map $\widehat{\varphi}$ from the set of subgraphs of G to the set of subgraphs of G'. It is thus enough to show that $\widehat{\varphi}$ maps $\Theta_{i,m+1} \sqcup \Theta_{1,i}$ to Θ'_i and $\Theta_{1,m+1}$ to Θ'_1. First, observe that for any subgraph ζ of G, $\widehat{\varphi}(\zeta)$ contains an undirected cycle if and only if ζ contains an undirected cycle or an undirected path joining 1 and $m+1$. Hence, for ζ in $\Theta_{i,m+1}$, $\Theta_{1,i}$ or $\Theta_{1,m+1}$, $\widehat{\varphi}(\zeta)$ is acyclic. Moreover, $\widehat{\varphi}(\zeta)$ is connected because ζ consists of two disjoint trees, one containing 1 and the other containing $m+1$. Hence, $\widehat{\varphi}(\zeta)$ is a tree, and since ζ is a spanning forest, $\widehat{\varphi}(\zeta)$ is a spanning tree. Finally, if $\zeta \in \Theta_{i,m+1} \sqcup \Theta_{1,i}$, then ζ has no edge with source i, so $\widehat{\varphi}(\zeta) \in \Theta'_i$. Similarly, $\zeta \in \Theta_{1,m+1}$ has no edge with source 1 or $m+1$, so $\widehat{\varphi}(\zeta) \in \Theta'_1$, as desired.

By hypothesis, $K_1 = K_{m+1}$. Thus

$$K_1 K'_i = K_1 \left[\sum_{\zeta \in \Theta_{i,m+1}} \zeta^\kappa + \sum_{\zeta \in \Theta_{1,i}} \zeta^\kappa \right] = K_1 \left[\sum_{\zeta \in \Theta_{i,m+1}} \zeta^\kappa \right] + K_{m+1} \left[\sum_{\zeta \in \Theta_{1,i}} \zeta^\kappa \right]. \tag{33}$$

We make now use of the All-Minors Matrix-Tree theorem, which extends equation (14). Since we are assuming G is connected, the Laplacian matrix L is of size $(m+1) \times (m+1)$ (we omit reference to κ for simplicity). Recall that $L_{(j)}$ is the minor of L obtained by removing the row $m+1$ and columns j of L and taking the determinant. Let $L_{(j,k)}$ for $j < k$ be the minor of L obtained by removing rows $1, m+1$ and columns j, k. Then it holds that [17, Th 3.1]

$$L_{(j,k)} = (-1)^{j+k+1} \sum_{\zeta \in \Theta_{j,k}} \zeta^\kappa.$$

In view of (33) and (14), to prove (32) we need to show that

$$(-1)^{1+i+m+1+1} L_{(1)} L_{(i,m+1)} + (-1)^{m+1+i+1+1} L_{(m+1)} L_{(1,i)} = (-1)^{i+1+m+1+1} L_{(i)} L_{(1,m+1)},$$

that is, we have to show that it holds

$$L_{(1)} L_{(i,m+1)} + L_{(m+1)} L_{(1,i)} = L_{(i)} L_{(1,m+1)}. \tag{34}$$

We find $L_{(1)}$, $L_{(m+1)}$ and $L_{(i)}$ by expanding the corresponding submatrix of the Laplacian used for the computation of each of the minors along the first row. Then (34) is equivalent to

$$\sum_{j=2}^{m+1} (-1)^j L_{(1,j)} L_{(i,m+1)} + \sum_{j=1}^{m} (-1)^{j+1} L_{(j,m+1)} L_{(1,i)} = \sum_{j=1, j \neq i}^{m+1} (-1)^{\epsilon_j} L_{(i,j)} L_{(1,m+1)}. \tag{35}$$

where $\epsilon_j = j+1$ if $j < i$ and j if $j > i$.

Equation (35) has three sums, which we refer to as the first, second and third sum for simplicity, reading from left to right. The summand for $j = i$ in the first two sums is respectively $(-1)^i L_{(1,i)} L_{(i,m+1)}$ and $(-1)^{i+1} L_{(i,m+1)} L_{(1,i)}$, which cancel out. The two terms for $j = 1$ in the second and third sums agree, using that $\epsilon_1 = 2$. Finally, the summands for $j = m + 1$ in the first and the third sums agree since $\epsilon_{m+1} = m + 1$.

We consider now the three summands, one for each sum, corresponding to a fixed $j \in \{2, \ldots, m\}$, $j \neq i$. We will use the Plücker relations on the maximal minors of a rectangular matrix [16]. These are as follows. Consider a $d \times n$ matrix A, $d < n$. For a set $I \subseteq [n]$, let A_I be the minor obtained after removing the columns with index in I of A. Consider two sets I, K of cardinality $n - d + 1$ and $n - d - 1$, respectively. Then it holds that

$$\sum_{k \in I \setminus K} (-1)^{\bar{\epsilon}_k} A_{I \setminus k} A_{K \cup \{k\}} = 0,$$

with $\bar{\epsilon}_k = \#\{\ell \in I \mid k < \ell\} + \#\{\ell \in K \mid k < \ell\}$. (See for example [16]. Note that the formula given in [16] is stated in complementary notation, indicating the columns that are kept to construct the minor, and not those that are removed).

Let A be the $(m - 1) \times (m + 1)$ submatrix of L obtained by removing the first and last rows. We apply the Plücker relation to A with the sets $I = \{1, j, m + 1\}$, $K = \{i\}$ and obtain

$$(-1)^{\bar{\epsilon}_{m+1}} L_{(1,j)} L_{(i,m+1)} + (-1)^{\bar{\epsilon}_j} L_{(1,m+1)} L_{(i,j)} + (-1)^{\bar{\epsilon}_1} L_{(j,m+1)} L_{(1,i)} = 0.$$

We have $\bar{\epsilon}_{m+1} = 0$, $\bar{\epsilon}_1 = 2 + 1 = 3$, and $\bar{\epsilon}_j = 1$ if $j > i$, and $\bar{\epsilon}_j = 2$ if $j < i$. Thus, after rearranging the terms, we obtain

$$(-1)^j L_{(1,j)} L_{(i,m+1)} + (-1)^{j+1} L_{(j,m+1)} L_{(1,i)} - (-1)^{\epsilon_j} L_{(j,m+1)} L_{(1,m+1)} = 0.$$

This implies that (35) holds and concludes the proof. □

We are now ready to prove Theorem 3(ii). By Theorem 2(i) and Proposition 9, $(\mathcal{N}, G, \kappa)$ is node balanced if and only if $K^{\gamma(u)} = 1$ for all $u \in \ker \Psi_{G'}$ and $K^{\delta(i_1,i_2)} = 1$. By Proposition 10, this is equivalent to $K'^u = 1$ for all $u \in \ker \Psi_{G'}$ and $K_{i_1} = K_{i_2}$, which in turn is equivalent to $(\mathcal{N}, G', \kappa)$ being node balanced and $K_{i_1} = K_{i_2}$, by Theorem 2(i). This concludes the proof. □

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