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Sherali–Adams relaxations of graph isomorphism polytopes

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ABSTRACT

We investigate the Sherali–Adams lift & project hierarchy applied to a graph isomorphism polytope whose integer points encode the isomorphisms between two graphs. In particular, the Sherali–Adams relaxations characterize a new vertex classification algorithm for graph isomorphism, which we call the *generalized vertex classification algorithm*. This algorithm generalizes the classic vertex classification algorithm and generalizes the work of Tinhofer on polyhedral methods for graph automorphism testing. We establish that the Sherali–Adams lift & project hierarchy when applied to a graph isomorphism polytope of a graph with n vertices needs $\Omega(n)$ iterations in the worst case before converging to the convex hull of integer points. We also show that this generalized vertex classification algorithm is also strongly related to the well-known Weisfeiler–Lehman algorithm, which we show can also be characterized in terms of the Sherali–Adams relaxations of a semi-algebraic set whose integer points encode graph isomorphisms.

1. Introduction

Classical combinatorial optimization problems have been traditionally approached by means of linear programming relaxations. Recently, there has been significant interest in understanding *lift-and-project* techniques for constructing hierarchies of such relaxations for combinatorial problems. These lift-and-project methods lift relaxations to refined systems of polynomial equations and inequalities, and project back to the original space, offering tighter approximations of the convex hull in question. Such lift-and-project procedures have been proposed by Lovász and Schrijver [1], Lasserre [2], Sherali–Adams [3], among many others. The key computational interest in these relaxations is that linear optimization over the kth relaxation can be done in polynomial time for fixed k.

Many relaxations of combinatorial problems have been investigated using these methods. These methods have been shown not to converge in polynomial time for various NP-hard problems. For example, Schoenebeck et al. [4] prove that for Vertex Cover, the integrality gap is at least $2-\epsilon$ after $\Omega_\epsilon(n)$ rounds of Lovász–Schrijver, where n is the number of vertices, and also, they show that for Max Cut, the integrality gap is at least $\frac{1}{2}-\epsilon$ after $\Omega_\epsilon(n)$ rounds of Lovász–Schrijver. Schoenebeck in [5] further proved that for Vertex Cover, the integrality gap is at least $\frac{7}{6}-\epsilon$ after $\Omega_\epsilon(n)$ rounds of the Lasserre hierarchy. Moreover, for the matching problem, a polynomial-time solvable problem, the Lift-and-Project hierarchies have been shown to not give polynomial time algorithms (see [6–8]). See also [9] for a discussion of the integrality gaps of the Sherali–Adams relaxations.

The problems of determining whether a simple undirected graph has a non-trivial automorphism (graph automorphism problem) and whether two simple undirected graphs are isomorphic (graph isomorphism problem) are interesting problems

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in complexity theory as it is not known whether they are in P or NPC. The combinatorial approaches such as the Weisfeiler–Lehman method [10] do not give a polynomial time algorithm for graph automorphism or graph isomorphism [11]. It is then natural to study lift-and-project techniques to approach the graph isomorphism and automorphism problems applied to algebraic sets of points encoding graph automorphism and isomorphism. In [12], the authors investigated semidefinite relaxations of sets of points encoding the graph isomorphism and automorphism problems. In this paper, we investigate the application of the Sherali–Adams technique to sets of points that encode the graph isomorphism and automorphism problems towards the ultimate goal of better understanding the Sherali–Adams technique and the complexity of these problems.

Specifically, we show that the Sherali–Adams relaxations of a well-known polytope encoding of graph isomorphism do not converge after $\Omega(n)$ steps in the worst case. In order to do this, we show that the Sherali–Adams relaxations of this polytope correspond to an algorithm for graph isomorphism that is strongly related to the famous Weisfeiler–Lehman algorithm; this result can be thought of as a k-dimensional analogue of the work of Tinhofer [13]. Lastly, we also give a semi-algebraic set encoding of graph isomorphism whose Sherali–Adams relaxations correspond to the Weisfeiler–Lehman algorithm. There is thus a surprisingly strong correspondence between combinatorial approaches and polyhedral approaches to graph isomorphism.

1.1. Background

In this section, we introduce some notation and some standard algorithms to deal with the graph isomorphism and automorphism problems.

We consider simple undirected graphs with vertex set $V = \{1, 2, \dots, n\}$. We denote the set of edges of a graph G by E_G and the adjacency matrix of G by A_G. The neighbours of a vertex $u \in V$ are the vertices in the set $\delta_G(u) = \{v \in V : \{u, v\} \in E_G\}$. An *isomorphism* from a graph G to a graph H is a bijection $\psi : V \to V$ that is adjacency preserving. That is, $\{u, v\} \in E_G$ if and only if $\{\psi(u), \psi(v)\} \in E_H$. When $G = H$, we call ψ an *automorphism* of G. We denote the set of automorphisms of a graph G as $AUT(G)$ and the set of isomorphisms from graphs G to H as $ISO(G, H)$.

A standard combinatorial approach for the graph automorphism and isomorphism problems is the classic vertex classification algorithm (see e.g. [14–16]) (C-V-C algorithm). In the C-V-C automorphism algorithm, the vertex set V of a graph G is partitioned into equivalence classes $\{V_1, V_2, \dots, V_m\}$ that are invariant under automorphisms, that is, for all automorphisms $\psi \in AUT(G)$, we have $\psi(V_i) = \{\psi(v) : v \in V_i\} = V_i$ for all $1 \le i \le m$. If the C-V-C algorithm returns a complete partition, that is, $|V_i| = 1$ for $1 \le i \le m$, then G is asymmetric (i.e. has no non-trivial automorphism). The C-V-C algorithm starts from the trivial vertex partition $\{V\}$ and proceeds by iteratively refining the vertex partition based on the equivalence classes of the neighbours of a given vertex. In particular, given a vertex partition $\{V_1, V_2, \dots, V_m\}$, the vertices $u, v \in V_i$ for $1 \le i \le m$ are in the same refined equivalence class in the next iteration if $|\delta_G(u) \cap V_j| = |\delta_G(v) \cap V_j|$ for $1 \le j \le m$. This process is repeated until the partition stabilizes, which happens in at most n iterations.

For the isomorphism problem, the C-V-C isomorphism algorithm partitions the vertex sets of graphs G and H into equivalence classes $(V_1, \dots, V_m)$ and $(W_1, \dots, W_m)$ respectively such that for all isomorphisms $\psi \in ISO(G, H)$ we have $\psi(V_i) = W_i$. If $|V_i| \ne |W_i|$ for some $1 \le i \le m$, then there is no isomorphism from G to H, and also, if there exists $u \in V_s$ and $v \in W_s$ such that $|\delta_G(u) \cap V_j| \ne |\delta_H(v) \cap W_j|$ for some $1 \le j \le m$, then again there is no isomorphism from G to H. The sequences $(V_1, \dots, V_m)$ and $(W_1, \dots, W_m)$ are each constructed separately using the C-V-C automorphism algorithm with the modification that the sets in the partition are ordered at each stage in a way that is invariant under isomorphism (see Section 2.2.1.3 for details).

Despite the simplicity of the C-V-C algorithm, it works well in practice as has been theoretically justified (see [17–19]), and the algorithm is the basis of implementations of graph isomorphism and graph automorphism testing including the `nauty` package of McKay [16]. Notably, a slight variant of the C-V-C algorithm gives a linear-time graph isomorphism algorithm that works for almost all graphs [19]. The C-V-C algorithm does not work at all for some of the most important classes of graphs, namely regular graphs, in which case, the C-V-C algorithm returns the trivial partition. Despite this, the algorithm is used in graph isomorphism algorithms in order to reduce the search space of candidates isomorphisms and automorphisms, and the algorithm can be combined with backtracking technique in order to have a complete algorithm (see e.g., [16]).

The ineffectiveness of the C-V-C algorithm on regular graphs motivated the creation of the Weisfeiler–Lehman algorithm [20,10] (W–L algorithm). The aim of the k-dim W–L algorithm is to partition the set of k-tuples of vertices, $V^k = \{(u_1, \dots, u_k) : u_1, \dots, u_k \in V\}$, into equivalence classes $\{V_1^k, \dots, V_m^k\}$ that are invariant under automorphism meaning that $\psi(V_i^k) = \{(\psi(u_1), \dots, \psi(u_k)) : u \in V_i^k\} = V_i^k$ for all $\psi \in AUT(G)$. If the partition is complete, that is, $|V_i^k| = 1$ for $i = 1, \dots, m$, then the graph G is asymmetric. In the k-dim W–L algorithm, we start with a partition $\{V_1^k, \dots, V_m^k\}$ of k-tuples of vertices into subgraph type, that is, $u \equiv v$ if and only if $u_i = u_j \Leftrightarrow v_i = v_j$ and $\{u_i, u_j\} \in E_G \Leftrightarrow \{v_i, v_j\} \in E_G$ for all $1 \le i < j \le n$, or in other words, the ordered subgraphs of G induced by the ordered sets of vertices $\{u_1, \dots, u_k\}$ and $\{v_1, \dots, v_k\}$ are identical. Then, analogous to the C-V-C algorithm, we iteratively refine the partition as follows: the vertices $u, v \in V_i^k$ for $1 \le i \le m$ are in the same refined equivalence class in the next iteration if there exists a bijection $\psi : V \to V$ such that for all $w \in V$, we have $(u_1, \dots, u_{r-1}, w, u_{r+1}, \dots, u_k) \equiv (v_1, \dots, v_{r-1}, \psi(w), v_{r+1}, \dots, v_k)$ for all $1 \le r \le k$. Note that the n-dim W–L algorithm is trivially necessary and sufficient due to the conditions on the initial partition.

For the isomorphism problem, analogous to the C-V-C algorithm, the k-dim W–L algorithm partitions V^k into two sequences of equivalence classes $(V_1^k, \ldots, V_m^k)$ for G and $(W_1^k, \ldots, W_m^k)$ for H such that $\psi(V_i^k) = W_i^k$ for all $\psi \in ISO(G, H)$. The partitions are constructed in a similar manner to the automorphism case (see Section 2.2.2 for details).

The k-dim W–L algorithm does not give a polynomial time algorithm for the graph isomorphism problem as established in [11] where they constructed a class of pairs of non-isomorphic graphs (G_n, H_n) with $O(n)$ vertices such that the W–L algorithm needs $\Omega(n)$ iterations to distinguish the graphs. The graphs (G_n, H_n) are presented in [11].

Isomorphisms of graphs can naturally be represented by permutation matrices: an isomorphism $\psi \in ISO(G, H)$ can be represented by the n by n matrix $X_\psi = (X_{uv})_{1\le u,v\le n}$ with $X_{uv} = 1$ if $\psi(u) = v$, and $X_{uv} = 0$ otherwise. We define $\Psi_{G,H} \subseteq \{0, 1\}^{n\times n}$ to be the set of permutation matrices representing $ISO(G, H)$, and we define $\Psi_G = \Psi_{G,G}$ as the set of permutation matrices representing $AUT(G)$. The isomorphism problem is thus the same problem as determining if $\Psi_{G,H} \neq \emptyset$, and the automorphism problem is the same problem as determining if $\Psi_G \neq \{\mathcal{I}_n\}$ where $\mathcal{I}_n$ is the identity matrix. It is then natural to consider polyhedral relaxations of the sets $\Psi_{G,H}$ and Ψ_G and determine under what conditions the relaxations answer the isomorphism and automorphism problems.

Tinhofer [13] examined the following polyhedral relaxation of $\Psi_{G,H}$:

$$\mathcal{T}_{G,H} = \{X \in [0, 1]^{n\times n} : XA_G = A_H X, Xe = X^T e = e\}$$

where e is the n-dimensional column vector of 1's. Note that the graphs G and H are isomorphic if and only if there exists a permutation matrix $X \in \{0, 1\}^{n\times n}$ such that $XA_G = A_H X$. Thus $\Psi_{G,H}$ is precisely the integer points in the polytope $\mathcal{T}_{G,H}$, i.e. $\Psi_{G,H} = \mathcal{T}_{G,H} \cap \{0, 1\}^{n\times n}$. In [13], Tinhofer showed that $\mathcal{T}_{G,H} = \emptyset$ if and only if the C-V-C algorithm determines that G and H are not isomorphic, and that $\mathcal{T}_G = \{\mathcal{I}_n\}$ if and only if the C-V-C algorithm determines that G is asymmetric.

Tinhofer also established a strong relationship between $\mathcal{T}_{G,H}$ and the C-V-C algorithm. If $\{V_1, \ldots, V_m\}$ is the partition of the vertices of G given by the C-V-C algorithm, then for all $u, v \in V$, we have $u \not\equiv v$ if and only if $X_{uv} = 0$ for all $X \in \mathcal{T}_G$. Analogously, if $(V_1, \ldots, V_m)$ is a partition of the vertices of G and $(W_1, \ldots, W_m)$ is a partition of the vertices of H returned by the C-V-C algorithm, then for all $u \in V_s$, $v \in W_t$, we have $s \neq t$ if and only if $X_{uv} = 0$ for all $X \in \mathcal{T}_{G,H}$. In other words, Tinhofer showed that the polyhedral relaxations $\mathcal{T}_{G,H}$ and $\mathcal{T}_G$ are geometric analogues of the C-V-C algorithm for the isomorphism and automorphism problems respectively.

In this paper, we examine Sherali–Adams relaxations of $\mathcal{T}_{G,H}$ and $\mathcal{T}_G$. In general, given a semi-algebraic set

$$P = \{x \in [0, 1]^n \mid f_1(x) = 0, \ldots, f_s(x) = 0, g_1(x) \ge 0, \ldots, g_t(x) \ge 0\}$$

where the $f_j(x)$ and $g_j(x)$ are polynomials in $\mathbb{R}[x_1, \ldots, x_n]$, the Sherali–Adams relaxations of P are linear inequality descriptions of relaxations of $\mathrm{conv}(P \cap \{0, 1\}^n)$, the convex hull of the integer points P. In particular, the Sherali–Adams hierarchy of relaxations $[0, 1]^n \supseteq P^1 \supseteq \cdots \supseteq P^n = \mathrm{conv}(P \cap \{0, 1\}^n)$ is a hierarchy of polytope relaxations of $P \cap \{0, 1\}^n$ obtained by lifting P to a non-linear polynomial system of equations and inequalities, linearizing the system giving an extended formulation and projecting back down.

The kth relaxation P^k is obtained as follows. First, we generate a set of polynomial inequalities given by

$$\prod_{i\in I} x_i f_j(x) = 0 \qquad \forall I \subseteq \{1, \ldots, n\}, |I| \le k-1, 1 \le j \le s \tag{1}$$

$$\prod_{i\in I} x_i \prod_{i\in J\setminus I} (1 - x_i) g_j(x) \ge 0 \qquad \forall I \subseteq J \subseteq \{1, \ldots, n\}, |J| \le k-1, 1 \le j \le t, \tag{2}$$

$$\prod_{i\in I} x_i \prod_{i\in J\setminus I} (1 - x_i) \ge 0 \qquad \forall I \subseteq J \subseteq \{1, \ldots, n\}, |J| \le k. \tag{3}$$

All of these polynomial equations and inequalities, which include the original set of equations and inequalities, are satisfied on P. We then expand the polynomials and make all monomials square-free by replacing any occurrence of x_i^2 by x_i because $x_i^2 - x_i = 0$ is valid on $P \cap \{0, 1\}^n$. Next, we *linearize* the system of equations by replacing each monomial $\prod_{i\in I} x_i$ where $I \subseteq \{1, \ldots, n\}$ and $|I| \ge 1$ with a new variable y_I. The result is a set of linear inequalities describing a polyhedron $\hat{P}^k$ in extended y space. To achieve P^k, we finally project the extended polyhedron $\hat{P}^k$ onto the space of $x_i = y_{\{i\}}$ variables, that is, $P^k = \{x : x_i = y_{\{i\}}\ \forall 1 \le i \le n, y \in \hat{P}^k\}$. Note that at most n iterations are needed before the Sherali–Adams relaxations converge to the convex hull, that is, $P^n = \mathrm{conv}(P \cap \{0, 1\}^n)$ (see e.g. [21]).

1.2. Our contribution

We generalize Tinhofer's work by studying the *Sherali–Adams* relaxations of the polytopes $\mathcal{T}_{G,H}$ and $\mathcal{T}_G$. First, we introduce a combinatorial algorithm, called the *generalized vertex classification algorithm* or *k-dimensional vertex classification algorithm* (k-dim C-V-C algorithm), whose relationship with $\mathcal{T}_G^k$ and $\mathcal{T}_{G,H}^k$ is analogous to the relationship between the C-V-C algorithm for the automorphism and isomorphism problem and $\mathcal{T}_G$ and $\mathcal{T}_{G,H}$ respectively.

For the automorphism problem, analogous to the C-V-C automorphism algorithm and the k-dim W–L automorphism algorithm, the k-dim C-V-C automorphism algorithm partitions V^k into equivalence classes $\{V_1^k, \ldots, V_m^k\}$ such that $\psi(V_i^k) =$

V_i^k for all $\psi \in AUT(G)$ (see Section 2.2.1.3 for details). For the isomorphism problem, analogous to the C-V-C algorithm and the k-dim W–L algorithm, the k-dim C-V-C algorithm partitions V^k into two sequences of equivalence classes $(V_1^k, \ldots, V_m^k)$ for G and $(W_1^k, \ldots, W_m^k)$ for H such that $\psi(V_i^k) = W_i^k$ for all $\psi \in ISO(G, H)$. The partitions are constructed in a similar manner to the automorphism case (see Section 2.2.1.3).

The following theorem summarizes the relationship between the k-dim C-V-C algorithm for the automorphism and isomorphism problem to the corresponding kth Sherali–Adams relaxations $\mathcal{T}_G^k$ and $\mathcal{T}_{G,H}^k$ respectively.

Theorem 1.1. *Let $k \geq 1$. The polytope $\mathcal{T}_G^k = \{\mathcal{I}_n\}$ if and only if the k-dim C-V-C algorithm determines that G is asymmetric. The polytope $\mathcal{T}_{G,H}^k = \emptyset$ if and only if the k-dim C-V-C algorithm determines that G and H are not isomorphic.*

We will actually prove a more general and stronger result than the above theorem that illustrates that the polytopes $\mathcal{T}_G^k$ and $\mathcal{T}_{G,H}^k$ are geometric analogues of the k-dim C-V-C automorphism and isomorphism algorithms respectively (see Section 4).

Above, we introduced a vertex classification algorithm that corresponds to the Sherali–Adams relaxations of a given polytope. Somewhat surprisingly, we also found a relaxation of $\Psi_{G,H}$ whose Sherali–Adams relaxations naturally correspond to the W–L algorithm. Consider the following semi-algebraic set $\mathcal{Q}_{G,H}$:

$$\begin{aligned} X_{u_1v_1}X_{u_2v_2} &= 0 \quad \forall\{u_1, u_2\} \in E_G, \{v_1, v_2\} \notin E_H, \\ X_{u_1v_1}X_{u_2v_2} &= 0 \quad \forall\{u_1, u_2\} \notin E_G, \{v_1, v_2\} \in E_H, \\ Xe = X^Te &= e, \quad X \in [0, 1]^{n\times n}. \end{aligned}$$

Note that $\mathcal{Q}_{G,H} \cap \{0, 1\}^{n\times n} = \Psi_{G,H}$ because the equations $X_{u_1v_1}X_{u_2v_2} = 0$ enforce that edges must map onto edges and non-edges (2-vertex independent sets) must map onto non-edges. We define $\mathcal{Q}_G = \mathcal{Q}_{G,G}$, and $\mathcal{Q}_{G,H}^k$ (respectively $\mathcal{Q}_G^k$) as the kth Sherali–Adams relaxations of $\mathcal{Q}_{G,H}$ (respectively $\mathcal{Q}_G$). The following theorem summarizes the relationship between the W–L algorithm and the Sherali–Adams relaxations of $\mathcal{Q}_{G,H}$.

Theorem 1.2. *Let $k > 1$. The polytope $\mathcal{Q}_G^{k+1} = \{\mathcal{I}_n\}$ if and only if the k-dim W–L algorithm determines that G is asymmetric. The polytope $\mathcal{Q}_{G,H}^{k+1} = \emptyset$ if and only if the k-dim W–L algorithm determines that G and H are not isomorphic.*

Again, we will actually prove a more general and stronger result than the above theorem that illustrates that the polytopes $\mathcal{Q}_G^k$ and $\mathcal{Q}_{G,H}^k$ are geometric analogues of the k-dim W–L automorphism and isomorphism algorithms respectively (see Section 4).

The C-V-C algorithm and the W–L algorithm are strongly related: the k-dim W–L algorithm is stronger than the k-dim C-V-C algorithm, but the $(k+1)$-dim C-V-C algorithm is stronger than the k-dim W–L algorithm. This relationship is summarized in the following lemma, which compares the corresponding Sherali–Adams relaxations:

Lemma 1.3. *The inclusions $\mathcal{Q}_G^{k+1} \subseteq \mathcal{T}_G^k \subseteq \mathcal{Q}_G^k$ and $\mathcal{Q}_{G,H}^{k+1} \subseteq \mathcal{T}_{G,H}^k \subseteq \mathcal{Q}_{G,H}^k$ hold.*

Together with Theorems 1.1 and 1.2, Lemma 1.3 implies that if the k-dim C-V-C algorithm determines that G and H are not isomorphic, then the k-dim W–L algorithm also determines that G and H are not isomorphic, and if the k-dim W–L algorithm determines that G and H are not isomorphic, then the $(k+1)$-dim C-V-C algorithm determines that G and H are not isomorphic. Analogous statements hold for automorphism.

Combining Theorems 1.1 and 1.2 and Lemma 1.3 and the result established by [11] on the complexity of the W–L algorithm, we arrive at the following complexity results for the Sherali–Adams relaxations of the graph isomorphism polytopes $\mathcal{T}_{G,H}^k$ and $\mathcal{Q}_{G,H}^k$.

Corollary 1.4. *There exists a class of pairs of non-isomorphic graphs (G_n, H_n) where G_n and H_n have $O(n)$ vertices such that the Sherali–Adams procedure applied to the sets $\mathcal{T}_{G,H}$ and $\mathcal{Q}_{G,H}$ needs $\Omega(n)$ iterations to converge to* $\mathrm{conv}(\Psi_{G_n,H_n}) = \emptyset$.

Our paper is organized as follows. In Section 2, we give a detailed description of the combinatorial algorithms for graph automorphism and isomorphism. In Section 3, we describe the Sherali–Adams relaxation of the sets $\mathcal{T}_{G,H}$ and $\mathcal{Q}_{G,H}$. Section 4 shows that Sherali–Adams relations are geometric analogues of the corresponding combinatorial algorithms thus proving Theorems 1.1 and 1.2.

2. Combinatorial algorithms

In this section, we first present the combinatorial algorithms for automorphism and how they compare to each other, and second, we present the combinatorial algorithms for graph isomorphism and how they compare to each other.

2.1. Automorphism algorithms

In this section, we present in detail three combinatorial algorithms for the graph automorphism problem: the k-dim W–L algorithm, the k-dim C-V-C algorithm, and a new combinatorial algorithm that will prove useful for comparing the k-dim W–L algorithm and the k-dim C-V-C algorithm.

We will first present a general framework for an automorphism algorithm using the notion of a *vertex classification equivalence relation* in order to prove general results that apply to all of the graph automorphism algorithms in this paper and thus avoid having to prove analogous results. Then, we will present algorithms that we are interested in, and finally, we will compare the three algorithms.

First, we give some necessary definitions and background. We denote by Π^k the set of all partitions of V^k. For any partition $\pi \in \Pi^k$, we say two sets u, v are equivalent with respect to π if they lie in the same cell of π. This is denoted by $u \equiv_\pi v$. Given $\pi, \tau \in \Pi^k$, we write $\pi \leq \tau$ if $u \equiv_\pi v$ implies $u \equiv_\tau v$ for all $u, v \in V^k$, in other words, π is a refinement of τ. It is well known that $\leq$ is a partial order on Π^k and that Π^k forms a complete lattice under $\leq$ (see for example [16]).

Let $\mathcal{G}$ be the set of all simple undirected graphs with vertex set $V = \{1, \dots, n\}$. Let $\psi : V \to V$ be a bijection. For a k-tuple $u \in V^k$, we define $\psi(u) = (\psi(u_1), \dots, \psi(u_k))$, and for a set of k-tuples $W \subseteq V^k$, we define $\psi(W) = \{\psi(u) : u \in W\}$. Given a graph $G \in \mathcal{G}$, a partition $\pi = \{\pi_1, \dots, \pi_m\}$ and a bijection $\psi : V \to V$, we define $AUT(G, \pi) = \{\psi \in AUT(G) : \psi(\pi_i) = \pi_i \; \forall 1 \leq i \leq m\}$. In this paper, we address the more general graph automorphism question of whether $|AUT(G, \pi)| = 1$ for a given partition $\pi \in \Pi^k$, which is useful when using a backtracking algorithm for solving the automorphism problem (see for example [16]). We denote by $\theta_G^k(\pi) \in \Pi^k$, the k-dimensional orbit partition of graph G with respect to π: the partition where $u \equiv_{\theta_G^k(\pi)} v$ if there exists $\psi \in AUT(G, \pi)$ such that $\psi(u) = v$. We write θ_G^k for the orbit partition of G.

We now define an equivalence relation that provides a general framework for graph automorphism.

Definition 2.1. An equivalence relation α on $\mathcal{G} \times \Pi^k \times V^k$ is a *vertex classification (V-C) equivalence relation* if it has the following properties for all $G \in \mathcal{G}, \pi \in \Pi^k$ and $u, v \in V^k$:

1. $(G, \pi, u) \equiv_\alpha (G, \pi, v)$ implies $u \equiv_\pi v$;
2. $(G, \pi, u) \equiv_\alpha (G, \pi, v)$ implies $(G, \pi', v) \equiv_\alpha (G, \pi', u)$ for all $\pi' \in \Pi^k$ where $\pi \leq \pi'$; and
3. $(G, \pi, u) \equiv_\alpha (G, \pi, \psi(u))$ for all automorphisms $\psi \in AUT(G, \pi)$.

Using a V-C equivalence relation, we construct a function that refines partitions as follows.

Definition 2.2. Let α be a V-C equivalence relation, and let $G \in \mathcal{G}$. We define $\alpha_G : \Pi^k \to \Pi^k$ where $u \equiv_{\alpha_G(\pi)} v$ if $(G, \pi, u) \equiv_\alpha (G, \pi, v)$ for all $\pi \in \Pi^k$ and $u, v \in \Pi^k$. We say that a partition is α_G-stable if $\alpha_G(\pi) = \pi$, and we denote by $\alpha_G^*(\pi)$ as the fixed point given by recursively applying α_G to π, and specifically, we define $\alpha_G^k = \alpha_G^*(\{V^k\})$ where $\{V^k\}$ is the trivial partition.

Some useful properties of α_G are as follows.

Lemma 2.3. *Let α be a V-C equivalence relation. Let $G \in \mathcal{G}$, and let $\pi, \pi' \in \Pi^k$.*

1. $\pi \geq \alpha_G(\pi) \geq \alpha_G^*(\pi)$.
2. $\pi \geq \pi'$ *implies* $\alpha_G(\pi) \geq \alpha_G(\pi')$.
3. $AUT(G, \pi) = AUT(G, \alpha_G(\pi)) = AUT(G, \alpha_G^*(\pi))$.
4. $\alpha_G^*(\pi)$ *is the unique coarsest α_G-stable partition finer than π.*
5. $\theta_G^k(\pi)$ *is α_G-stable and* $\alpha_G^*(\pi) \geq \theta_G^k(\pi)$.

Proof. (1) $\pi \geq \alpha_G(\pi)$ follows by construction, which applied recursively gives $\alpha_G(\pi) \geq \alpha_G^*(\pi)$. (2) If $\pi' \geq \pi$, then $\alpha_G(\pi') \geq \alpha_G(\pi)$ since $(G, \pi, u) \equiv_\alpha (G, \pi, v)$ implies $(G, \pi', u) \equiv_\alpha (G, \pi', v)$ by definition. (3) Since $u \equiv_{\alpha_G(\pi)} \psi(u)$ for all $\psi \in AUT(G, \pi)$ and for all $u \in V^k$ by definition, it follows that $AUT(G, \pi) = AUT(G, \alpha_G(\pi))$, which applied recursively gives $AUT(G, \alpha_G(\pi)) = AUT(G, \alpha_G^*(\pi))$. (4) Assume that $\pi \geq \pi'$ and that π' is α_G-stable. By property (2), we have $\alpha_G(\pi) \geq \alpha_G(\pi') = \pi'$, which applied recursively gives $\alpha_G^*(\pi) \geq \pi'$. If we also have $\alpha_G^*(\pi) \leq \pi'$, then $\alpha_G^*(\pi) = \pi'$ since $\leq$ is a partial order, and thus, $\alpha_G^*(\pi)$ is the unique coarsest α_G-stable partition finer than π. (5) The orbit partition $\theta_G^k(\pi)$ is α_G-stable since $u \equiv_{\alpha_G(\pi)} \psi(u)$ for all $\psi \in AUT(G, \pi)$ and for all $u \in V^k$ by definition. Thus, $\alpha_G^*(\pi) \geq \theta_G^k(\pi)$ since $\alpha_G^*(\pi)$ is the unique coarsest α_G-stable partition finer than π. □

Given $\pi \in \Pi^k$ and $G \in \mathcal{G}$ and a V-C equivalence relation α, we define the k-dimensional α-Vertex Classification algorithm (or k-dim α-V-C algorithm for short) as computing $\alpha^*(\pi)$. Since $\pi \geq \alpha_G^*(\pi) \geq \theta_G^k(\pi)$, if $\alpha_G^*(\pi)$ is a complete partition, we have shown that $|AUT(G, \pi)| = 1$. If $\alpha_G^*(\pi)$ is not the complete partition, then we have hopefully at least reduced the search space of possible automorphisms.

Given two vertex classification equivalence relations α and κ, we are interested in sufficient conditions for when the k-dim α-V-C algorithm is at least as strong as the k-dim κ-V-C algorithm, that is, $\alpha_G^*(\pi) \leq \kappa_G^*(\pi)$ for all $\pi \in \Pi^k$, in which case, we say that k-dim α implies k-dim κ. The lemma below gives such a sufficient condition.

Lemma 2.4. *Let $G \in \mathcal{G}$. Let α and κ be two V-C equivalence relations such that for all $\pi \in \Pi^k$ where $\alpha_G(\pi) = \pi$, we have $\kappa_G(\pi) = \pi$. Then, for all $\pi \in \Pi^k$, we have $\alpha_G^*(\pi) \leq \kappa_G^*(\pi)$.*

Proof. Since $\alpha_G^*(\pi)$ is α_G-stable, it is κ_G-stable by assumption, and since $\kappa_G^*(\pi)$ is the unique maximal κ_G-stable subpartition of π, we must have $\alpha_G^*(\pi) \leq \kappa_G^*(\pi)$. □

2.1.1. V-C equivalence relations

In this section, we define all the V-C equivalence relations that we need.

2.1.1.1. Symmetric equivalence relation. A simple but useful equivalence relation is the symmetric equivalence relation $\mathcal{S}$, which we use to ensure partitions are invariant under permutation of tuple components, meaning the following. Let $\sigma \in \mathcal{S}_k$ be a permutation where $\mathcal{S}_k$ is the symmetric group on k elements. For all tuples $u \in V^k$, we define $\sigma(u)$ as the permutation of the tuples components, that is, $\sigma(u)_i = u_{\sigma(i)}$ for all $1 \leq i \leq k$. We also define $\sigma(\pi) = \{\sigma(\pi_1), \ldots, \sigma(\pi_m)\}$ where $\sigma(\pi_i) = \{\sigma(u) : u \in \pi_i\}$ for all $1 \leq i \leq m$. We say a partition $\pi \in \Pi^k$ is $\mathcal{S}_k$-invariant, that is, invariant under permutation of tuple components, if $\sigma(\pi) = \pi$ for all $\sigma \in \mathcal{S}_k$ or equivalently $\sigma(u) \equiv_\pi \sigma(v)$ for all $\sigma \in \mathcal{S}_k$ (or equivalently $u \equiv_{\sigma(\pi)} v$ for all $\sigma \in \mathcal{S}_k$).

Now, we define the symmetric equivalence relation $\mathcal{S}$ on $\Pi^k \times V^k$. First, let $\Sigma_k = \{\sigma_1, \sigma_2\} \subset \mathcal{S}_k$ be a generating set of $\mathcal{S}_k$; we need only two permutations to generate $\mathcal{S}_k$: a two cycle and a k-cycle.

Definition 2.5. We define the symmetric equivalence relation $\mathcal{S}$ on $\Pi^k \times V^k$ where for all $\pi \in \Pi^k$ and $u, v \in V^k$, we write $(\pi, u) \equiv_{\mathcal{S}} (\pi, v)$ if $u \equiv_\pi v$ and $\sigma_i(u) \equiv_\pi \sigma_i(v)$ for all $\sigma_i \in \Sigma_k$.

This equivalence relation induces a V-C equivalence relation on $\mathcal{G} \times \Pi^k \times V^k$ where for all $G \in \mathcal{G}$, $\pi \in \Pi^k$ and $u, v \in V^k$, we write $(G, \pi, u) \equiv_{\mathcal{S}} (G, \pi, v)$ if $(\pi, u) \equiv_{\mathcal{S}} (\pi, v)$. It is straight-forward to show that this is indeed a V-C equivalence relation. As in Definition 2.2, we define the partition refinement function $\mathcal{S} : \Pi^k \to \Pi^k$, and a partition $\pi \in \Pi^k$ is *$\mathcal{S}$-stable* if $\mathcal{S}(\pi) = \pi$, and we denote by $\mathcal{S}^*(\pi)$ the unique coarsest $\mathcal{S}$-stable partition that is finer than π. It is straight-forward to show that π is $\mathcal{S}$-stable if and only if π is $\mathcal{S}_k$-invariant, and thus, $\mathcal{S}^*(\pi)$ is $\mathcal{S}_k$-invariant; thus, $\mathcal{S}^*(\pi)$ is the coarsest $\mathcal{S}_k$-invariant subpartition of π.

2.1.1.2. Combinatorial equivalence relation. Another simple but useful V-C equivalence relation is the *combinatorial* equivalence relation $\mathcal{C}$. This equivalence relation has simple and useful properties that we want all V-C equivalence relations to have, and so we will use it as a basis for the other equivalence relations.

First, we define $\mathcal{C}$ as a combinatorial equivalence relation on V^k where $u \equiv_{\mathcal{C}} v$ if $u_i = u_j \Leftrightarrow v_i = v_j$ for all $1 \leq i, j \leq k$. Also, we define $\mathcal{C}$ as an equivalence relation on $\mathcal{G} \times V^k$: For all $G \in \mathcal{G}$ and $u, v \in V^k$, we define $(G, u) \equiv_{\mathcal{C}} (G, v)$ if $u \equiv_{\mathcal{C}} v$ and $\{u_i, u_j\} \in E_G \Leftrightarrow \{v_i, v_j\} \in E_G$ for all $1 \leq i, j \leq k$. We can now define the combinatorial equivalence relation.

Definition 2.6. We define the combinatorial equivalence relation $\mathcal{C}$ on $\Pi^k \times V^k \times V^k$ where for all $G \in \mathcal{G}$, $\pi \in \Pi^k$ and $u, v \in V^k$, we write $(G, \pi, u) \equiv_{\mathcal{C}} (G, \pi, v)$ if $(\pi, u) \equiv_{\mathcal{S}} (\pi, v)$ and $(G, u) \equiv_{\mathcal{C}} (H, v)$.

It is straight-forward to show that this is indeed a V-C equivalence relation. As in Definition 2.2, we define the partition refinement function $\mathcal{C}_G : \Pi^k \to \Pi^k$, and a $\mathcal{C}_G$-stable partition is thus a partition $\pi \in \Pi^k$ where $\mathcal{C}_G(\pi) = \pi$. Note that k-dim $\mathcal{C}$ implies k-dim $\mathcal{S}$ by construction.

2.1.1.3. Classic equivalence relation. In this section, we define the V-C equivalence relation underlying the C-V-C automorphism algorithm.

Definition 2.7. For $u \in V^k$, we define $\delta_G^i(u) = \{\phi_i(u, w) : w \in \delta_G(u)\}$.

We then define the V-C equivalence relation δ as follows.

Definition 2.8. We define the equivalence relation δ on $\mathcal{G} \times \Pi^k \times V^k$ where for all $G \in \mathcal{G}$, $\pi \in \Pi^k$ and $u, v \in V^k$, we write $(G, \pi, u) \equiv_\delta (G, \pi, v)$ if $(G, \pi, u) \equiv_{\mathcal{C}} (G, \pi, v)$ and

$$|\delta_G^i(u) \cap \pi_s| = |\delta_G^i(v) \cap \pi_s| \quad \text{and} \quad |\bar{\delta}_G^i(u) \cap \pi_s| = |\bar{\delta}_G^i(v) \cap \pi_s|$$

for all $\pi_s \in \pi$ and $1 \leq i \leq k$.

It is straight-forward to show that the relation δ is a V-C equivalence relation. Then, as in Definition 2.2, we define the function $\delta_G : \Pi^k \to \Pi^k$, the concept of δ_G-stable, and the partitions $\delta_G^*(\pi)$ and δ_G^k. Note that by construction, $\delta_G(\pi) = \pi$ implies $\mathcal{C}_G(\pi) = \pi$ where $\pi \in \Pi^k$. Given a partition $\pi \in \Pi^k$, the k-dim δ-V-C automorphism algorithm (or k-dim C-V-C algorithm) is thus to compute $\delta_G^*(\pi)$. Note that k-dim δ implies k-dim $\mathcal{C}$ by construction.

In the 1-dim case, for all $\pi \in \Pi$, we trivially have that $\mathcal{C}_G(\pi) = \pi$, and moreover, $|\delta_G^i(u) \cap \pi_s| = |\delta_G^i(v) \cap \pi_s|$ implies that $|\bar{\delta}_G^i(u) \cap \pi_s| = |\bar{\delta}_G^i(v) \cap \pi_s|$ for all $\pi_s \in \pi$ and $1 \leq i \leq k$. Thus, in this case, the δ-V-C automorphism algorithm is the same as the C-V-C algorithm in the literature where a δ_G-stable partition is referred to as an *equitable* partition with respect to G (in e.g., [16]).

2.1.1.4. Weisfeiler–Lehman equivalence relation. In this section, we define the V-C equivalence relation underlying the k-dimensional Weisfeiler–Lehman automorphism algorithm (see e.g., [20,10,11]). First, we need the following definition.

Definition 2.9. Given $u \in V^k$ and $v \in V$, we define $\phi_i(u, v) = (u_1, \dots, u_{i-1}, v, u_{i+1}, \dots, u_k)$.

We can now define the V-C equivalence relation ω for the W–L algorithm.

Definition 2.10. We define the equivalence relation ω on $\mathcal{G} \times \Pi^k \times V^k$ where for all $G \in \mathcal{G}$, $\pi \in \Pi^k$ and $u, v \in V^k$, we write $(G, \pi, u) \equiv_\omega (G, \pi, v)$ if $(G, \pi, u) \equiv_{\mathcal{C}} (G, \pi, v)$ and there exists a bijection $\psi : V \to V$ such that $\phi_i(u, w) \equiv_\pi \phi_i(v, \psi(w))$ for all $1 \le i \le k$ and for all $w \in V$.

It is straight-forward to verify that ω is a V-C equivalence relation, and that ω implies $\mathcal{C}$ by construction. Then, as in Definition 2.2, we define the function $\omega_G : \Pi^k \to \Pi^k$, and a partition $\pi \in \Pi^k$ is ω_G-stable if $\omega_G(\pi) = \pi$, and we denote by $\omega_G^*(\pi)$ the unique coarsest ω-stable partition that is finer than π. Also, we define ω_G^k as the unique coarsest ω_G-stable partition, that is, $\omega_G^k = \omega_G^*(\{V^k\})$. So, given a partition $\pi \in \Pi^k$, the k-dim ω-V-C automorphism algorithm (or k-dim W–L algorithm) is thus to compute $\omega_G^*(\pi)$.

The k-dim W–L algorithm as presented in the literature is to compute $\omega_G'^*(\mathcal{C}_G^k)$ (see e.g., [11]) where ω' is a V-C equivalence relation defined as follows: for all $G \in \mathcal{G}$, $\pi \in \Pi^k$ and $u, v \in V^k$, we write $(G, \pi, u) \equiv_{\omega'} (G, \pi, v)$ if $u \equiv_\pi v$ and there exists a bijection $\psi : V \to V$ such that $\phi_i(u, w) \equiv_\pi \phi_i(v, \psi(w))$ for all $1 \le i \le k$ and for all $w \in V$. It is straight-forward to show that $\omega_G'^*(\mathcal{C}_G^k) = \omega_G^k$, and so the k-dim W–L algorithm is equivalent to the ω-V-C automorphism algorithm; in this paper, we consider the more general case of arbitrary starting partitions, so we defined ω so that it implies $\mathcal{C}$.

2.1.1.5. Δ equivalence relation. In this section, we define the Δ V-C equivalence relation. We will see that the k-dim Δ V-C algorithm is strongly related to the $(k-1)$-dim W–L algorithm and thus useful in proving results about the k-dim W–L algorithm.

Definition 2.11. For $u \in V^k$, we define $\Delta^i(u) = \{\phi_i(u, w) : w \in V\}$.

Definition 2.12. We define the equivalence relation Δ on $\mathcal{G} \times \Pi^k \times V^k$ where for all $G \in \mathcal{G}$, $\pi \in \Pi^k$ and $u, v \in V^k$, we write $(G, \pi, u) \equiv_\Delta (G, \pi, v)$ if $(G, \pi, u) \equiv_{\mathcal{C}} (G, \pi, v)$ and $|\Delta^i(u) \cap \pi_s| = |\Delta^i(v) \cap \pi_s|$ for all $\pi_s \in \pi$ and $1 \le i \le k$.

The equivalence relation Δ is a V-C equivalence relation, which implies $\mathcal{C}$. As in Definition 2.2, we define the function $\Delta_G : \Pi^k \to \Pi^k$, the concept of Δ_G-stable, and the partitions $\Delta_G^*(\pi)$ and Δ_G^k.

2.1.2. Comparison of combinatorial automorphism algorithms

In this section, we compare the different combinatorial approaches for graph automorphism. In particular, we show that the k-dim ω-V-C algorithm is at least as strong as the k-dim δ-V-C algorithm, which is at least as strong as the k-dim Δ-V-C algorithm, and finally, we show that the k-dim Δ-V-C algorithm is as strong as the $(k-1)$-dim ω-V-C algorithm. Some of the longer proofs of results in this section are omitted as the results here are implied by more general and analogous results for isomorphism algorithms in Section 2.2.2.

We now show that k-dim δ implies k-dim Δ.

Lemma 2.13. *Let $G \in \mathcal{G}$, and let $\pi \in \Pi^k$. If $\delta_G(\pi) = \pi$, then $\Delta_G(\pi) = \pi$. Moreover, $\delta_G^*(\pi) \le \Delta_G^*(\pi)$.*

Proof. Since $\Delta^i(u) = \delta_G^i(u) \cup \bar{\delta}_G^i(u)$, we have $\delta_G(\pi) = \pi$ implies $\Delta_G(\pi) = \pi$. The second part follows from Lemma 2.4. □

Below is the result that k-dim ω implies k-dim δ.

Lemma 2.14. *Let $G \in \mathcal{G}$, and let $\pi \in \Pi^k$. If $\omega_G(\pi) = \pi$, then $\delta_G(\pi) = \pi$. Moreover, $\omega_G^*(\pi) \le \delta_G^*(\pi)$.*

Proof. The first part follows from the Lemma 2.33 for isomorphism algorithms. The second part follows from Lemma 2.4. □

We next show that the k-dim Δ implies $(k-1)$-dim ω. First, we need a way of mapping a k-tuple onto an $(k-1)$-tuple and a $(k-1)$-tuple onto a k tuple. Also, we need a way of mapping a k-dimensional partition onto a $(k-1)$-dimensional partition.

Definition 2.15. We define the map $\rho : V^k \to V^{k-1}$ where $\rho(u) = (u_1, \dots, u_{k-1})$ for all $u \in V^k$, and we define the map $\nu : V^{k-1} \to V^k$ where $\nu(u') = (u'_1, \dots, u'_{k-1}, u'_{k-1})$ for all $u' \in V^{k-1}$. We define the map $\rho : \Pi^k \to \Pi^{k-1}$ such that for $\pi \in \Pi^k$ and for $u', v' \in V^{k-1}$, we have $u' \equiv_{\rho(\pi)} v'$ if and only if $\nu(u') \equiv_\pi \nu(v')$.

Now, we present the result that k-dim Δ implies $(k-1)$-dim ω. See the analogous result Lemma 2.35 for isomorphism algorithms for a proof.

Lemma 2.16. *Let $G \in \mathcal{G}$, and let $\pi \in \Pi^k$. If $\Delta_G(\pi) = \pi$, then $\omega_G(\rho(\pi)) = \rho(\pi)$. Moreover, we have $\rho(\Delta_G^*(\pi)) \le \omega_G^*(\rho(\pi))$.*

Next, we show that k-dim ω implies $(k+1)$-dim Δ. First, we show that k-dim ω implies $(k+1)$-dim Δ where $k > 1$. In order to show this, we need a way of mapping a k-dimensional partition to a $(k+1)$-dimensional partition.

Definition 2.17. We define the map $\nu : \Pi^k \to \Pi^{k+1}$ such that for $\pi \in \Pi^k$ and for $u, v \in V^{k+1}$, we have $u \equiv_{\nu(\pi)} v$ if $\rho(u) \equiv_\pi \rho(v)$ and $\phi_i(\rho(u), u_{k+1}) \equiv_\pi \phi_i(\rho(v), v_{k+1})$ for all $1 \le i \le k$.

Lemma 2.18 below shows that k-dim ω implies $(k+1)$-dim Δ. For the proof of this lemma, see Lemma 2.37 for the analogous result for isomorphism algorithms.

Lemma 2.18. *Let $G \in \mathcal{G}$, and let $\pi \in \Pi^k$ where $k > 1$. If $\omega_G(\pi) = \pi$, then $\Delta_G(\nu(\pi)) = \nu(\pi)$. Moreover, $\nu(\omega^*_G(\pi)) \le \Delta^*_G(\nu(\pi))$.*

Specifically, we have $\nu(\omega^k_G) \le \Delta^{k+1}_G$ since $\nu(\{V^k\}) = \{V^{k+1}\}$.

Corollary 2.19. *Let $k > 1$ and let $G \in \mathcal{G}$. Let $\pi \in \Pi^k$. Then, $\rho(\Delta^*_G(\nu(\pi))) = \omega^*_G(\pi)$.*

Proof. By Lemma 2.18, we have $\nu(\omega^*(\pi)) \le \Delta^*_G(\nu(\pi))$, and since $\omega^*(\pi)$ is Δ-stable, we have $\omega^*(\pi) \le \rho(\Delta^*_G(\nu(\pi))$ since $\rho(\nu(\omega^*(\pi))) = \omega^*(\pi)$ by Corollary A.6. By Lemma 2.16, we have $\omega^*(\rho(\nu(\pi))) \ge \rho(\Delta^*_G(\nu(\pi))$, but $\omega^*(\rho(\nu(\pi))) \le \omega^*(\pi)$ since $\rho(\nu(\pi)) \le \pi$ from Corollary A.6. Therefore, $\omega^*(\pi) = \rho(\Delta^*_G(\nu(\pi))$. $\square$

This implies that for all $\pi \in \Pi^k$, we have $\omega^*_G(\pi)$ is a complete partition if and only if $\Delta^*_G(\nu(\pi))$ is a complete partition, and so, the algorithms are essentially equivalent. Specifically, ω^k_G is a complete partition if and only if Δ^{k+1}_G is a complete partition, and moreover, $\rho(\Delta^{k+1}_G) = \omega^k_G$.

2.2. Isomorphism algorithms

In this section, we present in detail combinatorial algorithms for the graph isomorphism problem and how they compare to each other. The isomorphisms algorithms are analogous to the automorphism algorithms.

As we did for automorphisms, we first present a general framework using the notion of a *vertex classification preorder* in order to prove general results that apply to all of the graph isomorphism algorithms. Then, we will present isomorphism algorithms, and finally, we will compare the three algorithms.

First, we give some necessary definitions and background. For isomorphism, we need to work with ordered partitions. We denote by $\vec{\Pi}^k$ the set of all ordered partitions of V^k, that is, $\vec{\Pi}^k = \{(\pi_1, \dots, \pi_m) : \{\pi_1, \dots, \pi_m\} \in \Pi^k\}$. For an ordered partition $\vec{\pi} \in \vec{\Pi}^k$, we denote $\vec{\pi}_i$ as the ith set in the partition. For a partition $\vec{\pi} = (\vec{\pi}_1, \dots, \vec{\pi}_m) \in \vec{\Pi}^k$ and a bijection $\psi : V \to V$, we define $\psi(\vec{\pi}) = (\psi(\vec{\pi}_1), \dots, \psi(\vec{\pi}_m))$. We define $ISO(G, \vec{\pi}, H, \vec{\tau}) = \{\psi \in ISO(G, H) : \psi(\vec{\pi}) = \vec{\tau}\}$. Analogous to the automorphism algorithm, we address the more general graph isomorphism question of whether $ISO(G, \vec{\pi}, H, \vec{\tau}) = \emptyset$ for given partitions $\vec{\pi}, \vec{\tau} \in \Pi^k$, which is useful when using a backtracking algorithm for solving the isomorphism problem as in the automorphism case (see for example [16]).

For a k-tuple $u \in V^k$ and an ordered partition $\vec{\pi} \in \vec{\Pi}^k$, we denote the index of the equivalence class of $u \in V^k$ as $[u]_{\vec{\pi}} = i$ where $u \in \vec{\pi}_i$. For ordered partitions $\vec{\pi} = (\pi_1, \dots, \pi_m) \in \vec{\Pi}^k$, there is a natural preorder $\leqq_{\vec{\pi}}$ on V^k extending the equivalence $\equiv_{\vec{\pi}}$ relation as follows: for $u \in \vec{\pi}_s$, $v \in \vec{\pi}_t$, we write $u \leqq_{\vec{\pi}} v$ if $s \le t$. In the following, let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$. We write $\vec{\pi} \le \vec{\tau}$ if $u \equiv_{\vec{\pi}} v \Rightarrow u \equiv_{\vec{\tau}} v$ for all $u, v \in V^k$, and we write $\vec{\pi} \simeq \vec{\tau}$ if $u \equiv_{\vec{\pi}} v \Leftrightarrow u \equiv_{\vec{\tau}} v$ for all $u, v \in V^k$. We write $\vec{\pi} \preceq \vec{\tau}$ if $u \leqq_{\vec{\pi}} v$ implies $u \leqq_{\vec{\tau}} v$ for all $u, v \in V^k$. So, $\vec{\pi} \preceq \vec{\tau}$ implies that $\vec{\pi} \le \vec{\tau}$. We write $\vec{\pi} \approx \vec{\tau}$ if $|\vec{\pi}| = |\vec{\tau}|$ and $|\vec{\pi}_i| = |\vec{\tau}_i|$ for all $1 \le i \le |\vec{\pi}|$. We write $(\vec{\pi}, \vec{\tau}) \le (\vec{\pi}', \vec{\tau}')$ if $\vec{\pi} \approx \vec{\tau}$ and $[u]_{\vec{\pi}} = [v]_{\vec{\tau}} \Rightarrow [u]_{\vec{\pi}'} = [v]_{\vec{\tau}'}$ for all $u, v \in V^k$, and we write $(\vec{\pi}, \vec{\tau}) \simeq (\vec{\pi}', \vec{\tau}')$ if $[u]_{\vec{\pi}} = [v]_{\vec{\tau}} \Leftrightarrow [u]_{\vec{\pi}'} = [v]_{\vec{\tau}'}$ for all $u, v \in V^k$. Note that $(\vec{\pi}, \vec{\tau}) \le (\vec{\pi}', \vec{\tau}')$ implies $\vec{\pi} \le \vec{\pi}'$, $\vec{\tau} \le \vec{\tau}'$ and $\vec{\tau}' \approx \vec{\pi}'$.

Definition 2.20. We call a total preorder $\vec{\alpha}$ on $\mathcal{G} \times \vec{\Pi}^k \times V^k$ a *vertex classification (V-C) preorder* if $\vec{\alpha}$ has the following properties for all $G, H \in \mathcal{G}$, $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ and $u, v \in V^k$:

1. $(G, \vec{\pi}, u) \leqq_{\vec{\alpha}} (H, \vec{\tau}, v)$ implies $[u]_{\vec{\pi}} \le [v]_{\vec{\tau}}$;
2. $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (H, \vec{\tau}, v)$ implies $(G, \vec{\pi}', v) \equiv_{\vec{\alpha}} (H, \vec{\tau}', u)$ for all $\vec{\pi}', \vec{\tau}' \in \vec{\Pi}^k$ where $(\vec{\pi}, \vec{\tau}) \le (\vec{\pi}', \vec{\tau}')$; and
3. $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (\psi(G), \psi(\vec{\pi}), \psi(u))$ for all bijections $\psi : V \to V$.

Using a V-C preorder, we can construct an ordered partition function that refines ordered partitions.

Definition 2.21. Let $\vec{\alpha}$ be a V-C preorder, and let $G \in \mathcal{G}$. We define $\vec{\alpha}_G : \vec{\Pi}^k \to \vec{\Pi}^k$ where for all $\vec{\pi} \in \vec{\Pi}^k$ and $u, v \in V^k$, we have $u \leqq_{\vec{\alpha}_G(\vec{\pi})} v$ if $(G, \vec{\pi}, u) \leqq_{\vec{\alpha}} (G, \vec{\pi}, v)$. We say that a partition $\vec{\pi}$ is $\vec{\alpha}_G$-stable if $\vec{\alpha}_G(\vec{\pi}) = \vec{\pi}$, and we denote by $\vec{\alpha}^*_G(\vec{\pi})$ the fixed point reached by recursively applying $\vec{\alpha}$ to $\vec{\pi}$, and specifically, we define $\vec{\alpha}^k_G = \vec{\alpha}^*_G((V^k))$ where (V^k) is the trivial ordered partition.

The function $\vec{\alpha}_G$ has the properties that $\vec{\pi} \succeq \vec{\alpha}_G(\vec{\pi})$, and crucially, $\psi(\vec{\alpha}_G(\vec{\pi})) = \vec{\alpha}_{\psi(G)}(\psi(\vec{\pi}))$ since $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (G, \vec{\pi}, v)$ implies $(\psi(G), \psi(\vec{\pi}), \psi(v)) \equiv_{\vec{\alpha}} (\psi(G), \psi(\vec{\pi}), \psi(v))$ by property (3).

The concept of a V-C preorder is analogous to the concept of a V-C equivalence relation from before. Specifically, a V-C preorder $\vec{\alpha}$ induces a V-C equivalence relation α on $\mathcal{G} \times \Pi^k \times V^k$ where we define $(G, \pi, u) \equiv_\alpha (G, \pi, v)$ if $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (G, \vec{\pi}, v)$ for all $\vec{\pi} \simeq \pi$. By property (2) above, $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (G, \vec{\pi}, v)$ if and only if $(G, \vec{\pi}', u) \equiv_{\vec{\alpha}} (G, \vec{\pi}', v)$ for all $\vec{\pi}' \simeq \vec{\pi}$. Thus, given $\vec{\pi} \simeq \pi$, we have $\vec{\alpha}_G(\vec{\pi}) \simeq \alpha_G(\pi)$ and $\vec{\alpha}^*_G(\vec{\pi}) \simeq \alpha^*_G(\pi)$, and also, the partition $\vec{\pi}$ is $\vec{\alpha}_G$-stable if and only if π is α_G-stable. This is useful since it means that proving results for $\vec{\alpha}$ implies results for α.

Before describing the algorithm for graph isomorphism, we need to define an equivalence relation on $\mathcal{G} \times \vec{\Pi}^k$. This equivalence condition will serve as a useful necessary but not sufficient condition for isomorphism.

Definition 2.22. Given a V-C preorder $\vec{\alpha}$, we define an equivalence relation $\equiv_{\vec{\alpha}}$ on $\mathcal{G} \times \vec{\Pi}^k$ where for all $G, H \in \mathcal{G}, \vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ and $u, v \in V^k$, we have $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$ if $\vec{\alpha}_G(\vec{\pi}) \approx \vec{\alpha}_H(\vec{\tau})$ and $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (H, \vec{\tau}, v) \Leftrightarrow [u]_{\vec{\alpha}_G(\vec{\pi})} = [v]_{\vec{\alpha}_H(\vec{\tau})}$.

In other words, $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$ if and only if there exists a bijection of tuples $\gamma : V^k \to V^k$ where for all $u \in V^k$, we have $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (H, \vec{\tau}, \gamma(u))$. The equivalence relation $\equiv_{\vec{\alpha}}$ has analogous properties to those defining the preorder $\vec{\alpha}$. Note that we always have $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (G, \vec{\pi})$.

Lemma 2.23. *Let $\vec{\alpha}$ be a vertex classification preorder on $\mathcal{G} \times \vec{\Pi}^k \times V^k$. Then, for all $G, H \in \mathcal{G}$ and $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$, we have the following:*

(1) $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$ *implies* $(\vec{\alpha}_G(\vec{\pi}), \vec{\alpha}_H(\vec{\tau})) \leq (\vec{\pi}, \vec{\tau})$ *and* $\vec{\pi} \approx \vec{\tau}$;
(2) $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$ *implies* $(G, \vec{\pi}') \equiv_{\vec{\alpha}} (H, \vec{\tau}')$ *and* $(\vec{\alpha}_G(\vec{\pi}), \vec{\alpha}_H(\vec{\tau})) \leq (\vec{\alpha}_G(\vec{\pi}'), \vec{\alpha}_H(\vec{\tau}'))$ *for all* $\vec{\pi}', \vec{\tau}' \in \vec{\Pi}^k$ *where* $(\vec{\pi}, \vec{\tau}) \leq (\vec{\pi}', \vec{\tau}')$;
(3) $(G, \vec{\pi}) \not\equiv_{\vec{\alpha}} (H, \vec{\tau})$ *implies* $ISO(G, \vec{\pi}, H, \vec{\tau}) = \emptyset$; *and*
(4) $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$ *implies* $ISO(G, \vec{\pi}, H, \vec{\tau}) = ISO(G, \vec{\alpha}_G(\vec{\pi}), H, \vec{\alpha}_H(\vec{\tau}))$.

Proof. (1) Assume $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$. Since $\vec{\alpha}_G(\vec{\pi}) \approx \vec{\alpha}_H(\vec{\tau})$ and since $[u]_{\vec{\alpha}_G(\vec{\pi})} = [v]_{\vec{\alpha}_H(\vec{\tau})}$ implies $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (H, \vec{\tau}, v)$ and thus $[u]_{\vec{\pi}} = [v]_{\vec{\tau}}$, we have $(\vec{\alpha}_G(\vec{\pi}), \vec{\alpha}_H(\vec{\tau})) \leq (\vec{\pi}, \vec{\tau})$, which implies $\vec{\pi} \approx \vec{\tau}$.

(2) Again assume $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$. We have $(\vec{\pi}', \vec{\tau}') \geq (\vec{\pi}, \vec{\tau})$ implies $(\vec{\alpha}_G(\vec{\pi}'), \vec{\alpha}_H(\vec{\tau}')) \geq (\vec{\alpha}_G(\vec{\pi}), \vec{\alpha}_H(\vec{\tau}))$. This follows since $[u]_{\vec{\alpha}_G(\vec{\pi})} = [v]_{\vec{\alpha}_H(\vec{\tau})}$ implies $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (G, \vec{\tau}, v)$, which by Definition 2.20 implies that $(G, \vec{\pi}', u) \equiv_{\vec{\alpha}} (H, \vec{\tau}', v)$, and therefore, $[u]_{\vec{\alpha}_G(\vec{\pi}')} = [v]_{\vec{\alpha}_H(\vec{\tau}')}$ as required. Second, since $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$, there exists a tuple bijection $\gamma : V^k \to V^k$ such that $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (H, \vec{\tau}, \gamma(u))$ for all $u \in V^k$ implying that $(G, \vec{\pi}', u) \equiv_{\vec{\alpha}} (H, \vec{\tau}', \gamma(u))$ for all $u \in V^k$ by property of Definition 2.20. Hence, $(G, \vec{\pi}') \equiv_{\vec{\alpha}} (H, \vec{\tau}')$.

(3) We prove the contrapositive. Assume $ISO(G, \vec{\pi}, H, \vec{\tau}) \neq \emptyset$. Let $\psi \in ISO(G, \vec{\pi}, H, \vec{\tau})$. Then, from property (3) of Definition 2.20, we have $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (H, \vec{\tau}, \psi(u))$ for all $u \in V^k$, and thus, $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (G, \tau)$ as required.

(4) This follows from property (3) of Definition 2.20, which says that if $(G, \vec{\pi}, u) \not\equiv_{\vec{\alpha}} (H, \vec{\tau}, v)$, then there does not exist $\psi \in ISO(G, \vec{\pi}, H, \vec{\tau})$ such that $\psi(u) = v$. Then, it follows from the definition of $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$ that $ISO(G, \vec{\pi}, H, \vec{\tau}) = ISO(G, \vec{\alpha}_G(\vec{\pi}), H, \vec{\alpha}_H(\vec{\tau}))$. Hence, if $(G, \vec{\alpha}_G(\vec{\pi})) \not\equiv_{\vec{\alpha}} (H, \vec{\alpha}_H(\vec{\tau}))$, then $ISO(G, \vec{\alpha}_G(\vec{\pi}), H, \vec{\alpha}_H(\vec{\tau})) = \emptyset = ISO(G, \vec{\pi}, H, \vec{\tau})$. □

We show below in Lemma 2.24 that under the condition that $\vec{\pi} \approx \vec{\tau}$, we have $ISO(G, \vec{\pi}, H, \vec{\tau}) = ISO(G, \alpha^*_G(\vec{\pi}), H, \alpha^*_H(\vec{\tau}))$. So, if $(G, \vec{\alpha}^*_G(\vec{\pi})) \not\equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}))$, then $ISO(G, \alpha^*_G(\vec{\pi}), H, \alpha^*_H(\vec{\tau})) = \emptyset$, and therefore, $ISO(G, \vec{\pi}, H, \vec{\tau}) = \emptyset$.

Lemma 2.24. *Let $G, H \in \mathcal{G}$. Let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$. Then, $ISO(G, \vec{\pi}, H, \vec{\tau}) = ISO(G, \alpha^*_G(\vec{\pi}), H, \alpha^*_H(\vec{\tau}))$.*

Proof. Recall that for all $\vec{\pi}', \vec{\tau}' \in \vec{\Pi}^k$, if $(G, \vec{\pi}') \equiv_{\vec{\alpha}} (H, \vec{\tau}')$, then $ISO(G, \vec{\pi}', H, \vec{\tau}') = ISO(G, \vec{\alpha}_G(\vec{\pi}'), H, \vec{\alpha}_H(\vec{\tau}'))$, and if $(G, \vec{\pi}') \not\equiv_{\vec{\alpha}} (H, \vec{\tau}')$, then $ISO(G, \vec{\pi}', H, \vec{\tau}') = \emptyset$. Firstly, assume $(G, \alpha^*_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \alpha^*_H(\vec{\tau}))$. Then, by Corollary A.2, for all $r \geq 0$, we have $(G, \vec{\alpha}^r_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^r_H(\vec{\tau}))$ implying that $ISO(G, \alpha^r_G(\vec{\pi}), H, \alpha^r_H(\vec{\tau})) = ISO(G, \vec{\alpha}^{r+1}_G(\vec{\pi}'), H, \vec{\alpha}^{r+1}_H(\vec{\tau}'))$. Thus, $ISO(G, \vec{\pi}, H, \vec{\tau}) = ISO(G, \alpha^*_G(\vec{\pi}), H, \alpha^*_H(\vec{\tau}))$.

Secondly, assume $(G, \alpha^*_G(\vec{\pi})) \not\equiv_{\vec{\alpha}} (H, \alpha^*_H(\vec{\tau}))$. Then, $ISO(G, \alpha^*_G(\vec{\pi}), H, \alpha^*_H(\vec{\tau})) = \emptyset$. There exists $r \geq 0$ such that $(G, \vec{\alpha}^r_G(\vec{\pi})) \not\equiv_{\vec{\alpha}} (H, \vec{\alpha}^r_H(\vec{\tau}))$ and $(G, \vec{\alpha}^{\bar{r}}_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^{\bar{r}}_H(\vec{\tau}))$ for all $\bar{r} < r$. Then, we have $ISO(G, \alpha^r_G(\vec{\pi}), H, \alpha^r_H(\vec{\tau})) = \emptyset$ since $(G, \vec{\alpha}^r_G(\vec{\pi})) \not\equiv_{\vec{\alpha}} (H, \vec{\alpha}^r_H(\vec{\tau}))$, and also, we have $ISO(G, \vec{\pi}, H, \vec{\tau}) = ISO(G, \alpha^r_G(\vec{\pi}), H, \alpha^r_H(\vec{\tau}))$ since $ISO(G, \alpha^{\bar{r}}_G(\vec{\pi}), H, \alpha^{\bar{r}}_H(\vec{\tau})) = ISO(G, \vec{\alpha}^{\bar{r}+1}_G(\vec{\pi}'), H, \vec{\alpha}^{\bar{r}+1}_H(\vec{\tau}'))$ for all $\bar{r} < r$. Thus, again $ISO(G, \vec{\pi}, H, \vec{\tau}) = ISO(G, \alpha^*_G(\vec{\pi}), H, \alpha^*_H(\vec{\tau}))$ as required. □

We can now present the k-dim $\vec{\alpha}$-V-C algorithm for isomorphism given $G, H \in \mathcal{G}$ and $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$: first, we compute $\vec{\alpha}^*_G(\vec{\pi})$; second, we compute $\vec{\alpha}^*_H(\vec{\tau})$; and finally, we check if $(G, \vec{\alpha}^*_G(\vec{\pi})) \not\equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}))$, and if so, then we have shown that $ISO(G, \vec{\pi}, H, \vec{\tau}) = \emptyset$. We may assume without loss of generality that $\vec{\pi} \approx \vec{\tau}$ since it is easily verifiable and if $\vec{\pi} \not\approx \vec{\tau}$, then trivially $ISO(G, \vec{\pi}, H, \vec{\tau}) = \emptyset$. If $(G, \vec{\alpha}^*_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}))$, then although we have not shown that G and H are not isomorphic, we have hopefully at least reduced the search space of isomorphisms from G to H.

There is one more definition we will use, which we define for notational convenience.

Definition 2.25. Given a V-C preorder $\vec{\alpha}$, we define the equivalence relation $\equiv_{\vec{\alpha}^*}$ on $\mathcal{G} \times \vec{\Pi}^k$ where for all $G, H \in \mathcal{G}$ and $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$, we have $(G, \vec{\pi}) \equiv_{\vec{\alpha}^*} (H, \vec{\tau})$ if $\vec{\alpha}_G(\vec{\pi}) = \vec{\pi}, \vec{\alpha}_H(\vec{\tau}) = \vec{\tau}$ and $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$.

Next, we consider the general case of comparing two different vertex classification preorders $\vec{\alpha}$ and $\vec{\kappa}$. Lemma 2.26 below presents a sufficient condition for when the k-dim $\vec{\alpha}$-V-C algorithm is at least as strong as the k-dim $\vec{\kappa}$-V-C algorithm, in which case, we say that k-dim $\vec{\alpha}$ implies k-dim $\vec{\kappa}$.

Lemma 2.26. *Let $G, H \in \mathcal{G}$. Let $\vec{\alpha}$ and $\vec{\kappa}$ be two V-C preorders where for all $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$, if $(G, \vec{\pi}) \equiv_{\vec{\alpha}^*} (H, \vec{\tau})$, then $(G, \vec{\pi}) \equiv_{\vec{\kappa}^*} (H, \vec{\tau})$. Then, for all $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$, $(G, \vec{\alpha}^*_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}))$ implies $(G, \vec{\kappa}^*_G(\vec{\pi})) \equiv_{\vec{\kappa}} (H, \vec{\kappa}^*_H(\vec{\tau}))$ and $(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_H(\vec{\tau})) \leq (\vec{\kappa}^*_G(\vec{\pi}), \vec{\kappa}^*_H(\vec{\tau}))$.*

Proof. Assume $(G, \vec{\alpha}^*_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}))$. Using Corollary A.2, we have $(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_H(\vec{\tau})) \leq (\vec{\pi}, \vec{\tau})$. By assumption, we have that $(G, \vec{\alpha}^*_G(\vec{\pi})) \equiv_{\vec{\kappa}} (H, \vec{\alpha}^*_H(\vec{\tau}))$. Then, using Lemma A.1, we have $(G, \vec{\kappa}^*_G(\vec{\pi})) \equiv_{\vec{\kappa}} (H, \vec{\kappa}^*_H(\vec{\tau}))$ and $(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_H(\vec{\tau})) \leq (\vec{\kappa}^*_G(\vec{\pi}), \vec{\kappa}^*_H(\vec{\tau}))$ as required. □

Note that Lemma 2.26 implies the analogous result for automorphism (Lemma 2.4) meaning that if k-dim $\vec{\alpha}$ implies k-dim $\vec{\kappa}$, then k-dim α implies k-dim κ where α and κ are the induced V-C equivalence relations on $\mathcal{G} \times \Pi^k \times V^k$ for $\vec{\alpha}$ and $\vec{\kappa}$ respectively. This follows since $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (G, \vec{\pi}, v)$ if and only if $(G, \pi, u) \equiv_{\alpha} (G, \pi, v)$ where $\vec{\pi} \simeq \pi$ and similarly for $\vec{\kappa}$ and κ, and thus, if $(G, \vec{\pi}) \equiv_{\vec{\alpha}^*} (H, \vec{\tau})$ implies $(G, \vec{\pi}) \equiv_{\vec{\kappa}^*} (H, \vec{\tau})$ for all $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$, then $\alpha_G(\pi) = \pi$ implies $\kappa_G(\pi) = \pi$ for all $\pi \in \Pi^k$.

2.2.1. V-C preorders

In this section, we define all the V-C preorders that we need.

2.2.1.1. Symmetric preorder. Analogous to the unordered case, a useful property of pairs ordered partitions is invariance under permutation of tuple components, defined as follows. Let $\vec{\pi} \in \vec{\Pi}^k$. We define $\sigma(\vec{\pi}) = (\sigma(\vec{\pi}_1), \ldots, \sigma(\vec{\pi}_m))$ for all $\sigma \in \mathcal{S}_k$. Given $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$, we say that the pair $(\vec{\pi}, \vec{\tau})$ is $\mathcal{S}_k$-invariant, that is, invariant under permutation of tuple components, if $(\vec{\pi}, \vec{\tau}) \simeq (\sigma(\vec{\pi}), \sigma(\vec{\tau}))$ for all $\sigma \in \mathcal{S}_k$, that is, for all $u, v \in V^k$, we have $[u]_{\vec{\pi}} = [v]_{\vec{\tau}} \Leftrightarrow [u]_{\sigma(\vec{\pi})} = [v]_{\sigma(\vec{\tau})}$ for all $\sigma \in \mathcal{S}_k$ (or equivalently $[u]_{\vec{\pi}} = [v]_{\vec{\tau}} \Leftrightarrow [\sigma(u)]_{\vec{\pi}} = [\sigma(v)]_{\vec{\tau}}$ for all $\sigma \in \mathcal{S}_k$).

If we are given partitions $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ such that $(\vec{\pi}, \vec{\tau})$ is not $\mathcal{S}_k$-invariant, then we can construct such initial partitions using a V-C preorder analogous to the symmetric equivalence relations as follows. Let $\Sigma_k = \{\sigma_1, \sigma_2\}$ be a generating set of $\mathcal{S}_k$ as before. For all $\vec{\pi} \in \vec{\Pi}^k$ and $u \in V^k$, we define $\vec{\mathcal{S}}_{\vec{\pi}}(u) = ([\sigma_1(u)]_{\vec{\pi}}, [\sigma_2(u)]_{\vec{\pi}})$. Analogous to $\mathcal{S}$, we define the *symmetric* V-C preorder as follows.

Definition 2.27. We define the preorder $\vec{\mathcal{S}}$ on $\vec{\Pi}^k \times V^k$ where for all $G, H \in \mathcal{G}$, $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ and $u, v \in V^k$, we write $(\vec{\pi}, u) \leqq_{\vec{\mathcal{S}}} (\vec{\tau}, v)$ if $[u]_{\vec{\pi}} < [v]_{\vec{\tau}}$ or $[u]_{\vec{\pi}} = [v]_{\vec{\tau}}$ and $\vec{\mathcal{S}}_{\vec{\pi}}(u) \leq_{lex} \vec{\mathcal{S}}_{\vec{\tau}}(v)$.

Here, $\leq_{lex}$ is the lexicographical order. The preorder $\vec{\mathcal{S}}$ induces a preorder on $\mathcal{G} \times \vec{\Pi}^k \times V^k$ where for all $G, H \in \mathcal{G}$, $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^r$ and $u, v \in V^k$, we write $(G, \vec{\pi}, u) \leqq_{\vec{\mathcal{S}}} (G, \vec{\tau}, v)$ if $(\vec{\pi}, u) \leqq_{\vec{\mathcal{S}}} (\vec{\tau}, v)$. It is straight-forward to verify that $\vec{\mathcal{S}}$ is a V-C preorder, which induces the V-C equivalence relation $\mathcal{S}$. Then, as in Definition 2.21, we define the function $\vec{\mathcal{S}} : V^k \to V^k$, the concept of $\vec{\mathcal{S}}$-stable, and the partition $\vec{\mathcal{S}}^*(\vec{\pi})$. Also, as in Definition 2.22, we define the $\vec{\mathcal{S}}$ equivalence relation on $\vec{\Pi}^k$ inducing an equivalence relation on $\mathcal{G} \times \vec{\Pi}^k$. Furthermore, it is straight-forward to show that for all $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$, the pair $(\vec{\pi}, \vec{\tau})$ is $\mathcal{S}_k$-invariant if and only if $\vec{\pi} \equiv_{\vec{\mathcal{S}}^*} \vec{\tau}$.

2.2.1.2. Combinatorial preorder. We define the *combinatorial* preorder $\vec{\mathcal{C}}$ on $\mathcal{G} \times \vec{\Pi}^k \times V^k$, which is analogous to the combinatorial V-C equivalence relation $\mathcal{C}$. The combinatorial preorder has some useful basic properties that we want V-C preorders to possess, so we will use it as a basis for other preorders. First, we define the matrix $\vec{\mathcal{C}}_G(u) \in \mathbb{R}^{k\times k}$ where $\vec{\mathcal{C}}_G(u)_{ij} = 0$ if $u_i = u_j$ and $\vec{\mathcal{C}}_G(u)_{ij} = 1$ if $\{u_i, u_j\} \in E_G$ and $\vec{\mathcal{C}}_G(u)_{ij} = -1$ otherwise.

Definition 2.28. We define the preorder $\vec{\mathcal{C}}$ on $\mathcal{G} \times \vec{\Pi}^k \times V^k$ where for all $G, H \in \mathcal{G}$, $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ and $u, v \in V^k$, we write $(G, \vec{\pi}, u) \leqq_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$ if $(\vec{\pi}, u) <_{\vec{\mathcal{S}}} (\vec{\tau}, v)$ or $(\vec{\pi}, u) \equiv_{\vec{\mathcal{S}}} (\vec{\tau}, v)$ and $\vec{\mathcal{C}}_G(u) \leq_{lex} \vec{\mathcal{C}}_G(v)$.

It is straight-forward to verify that $\vec{\mathcal{C}}$ is a V-C preorder, which induces $\mathcal{C}$ and implies $\vec{\mathcal{S}}$. Then, as in Definition 2.21, we define the function $\vec{\mathcal{C}}_G : V^k \to V^k$, and we say $\vec{\pi}$ is $\vec{\mathcal{C}}_G$-stable if $\vec{\mathcal{C}}_G(\vec{\pi}) = \vec{\pi}$, and we denote by $\vec{\mathcal{C}}^*_G(\vec{\pi})$ the fixed point reached by recursively applying $\vec{\mathcal{C}}_G$ to $\vec{\pi}$. As in Definition 2.22, we define the $\vec{\mathcal{C}}$ equivalence relation on $\mathcal{G} \times \vec{\Pi}^k$. Lastly, we define $\vec{\mathcal{C}}^k_G = \vec{\mathcal{C}}^*_G((V^k))$.

2.2.1.3. Classic preorder. In this section, we give the V-C preorder underlying the k-dimensional C-V-C algorithm for the isomorphism problem. First, we need the following definitions. For all $\vec{\pi} = (\vec{\pi}_1, \ldots, \vec{\pi}_m) \in \vec{\Pi}^k$, $1 \leq i \leq k$, and $u \in V^k$, we define

$$\vec{\delta}^i_{G,\vec{\pi}}(u) = (|\delta^i_G(u) \cap \vec{\pi}_1|, \ldots, |\delta^i_G(u) \cap \vec{\pi}_m|, |\bar{\delta}^i_G(u) \cap \vec{\pi}_1|, \ldots, |\bar{\delta}^i_G(u) \cap \vec{\pi}_m|),$$

and also, we define $\vec{\delta}_{G,\vec{\pi}}(u) = (\vec{\delta}^1_{G,\vec{\pi}}(u), \ldots, \vec{\delta}^k_{G,\vec{\pi}}(u))$.

Definition 2.29. We define $\vec{\delta}$ a preorder on $\mathcal{G} \times \vec{\Pi}^k \times V^k$ where for all $G, H \in \mathcal{G}$, $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ and $u, v \in V^k$, we write $(G, \vec{\pi}, u) \leqq_{\vec{\delta}} (H, \vec{\tau}, v)$ if $(G, \vec{\pi}, u) <_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$ or $(G, \vec{\pi}, u) \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$ and $\vec{\delta}_{G,\vec{\pi}}(u) \leq_{lex} \vec{\delta}_{H,\vec{\tau}}(v)$.

The preorder $\vec{\delta}$ is a V-C preorder, which is straight-forward to check. Note that $\vec{\delta}$ induces δ and that k-dim $\vec{\delta}$ implies k-dim $\vec{\mathcal{C}}$ by construction. Then, as in Definition 2.21, we define the function $\vec{\delta}_G : V^k \to V^k$, the concept of $\vec{\delta}_G$-stable, and the partitions $\vec{\delta}^*_G(\vec{\pi})$ and $\vec{\delta}^k_G$. Also, as in Definition 2.22, we define the $\vec{\delta}$ equivalence relation on $\mathcal{G} \times \vec{\Pi}^k$. Again, in the 1-dim case, the $\vec{\delta}$-V-C algorithm simplifies to the C-V-C algorithm for isomorphism.

2.2.1.4. Weisfeiler–Lehman preorder. In this section, we introduce the V-C preorder $\vec{\omega}$ underlying the k-dimensional Weisfeiler–Lehman isomorphism algorithm where $k > 1$ (see e.g., [20,10,11]). First, given $\vec{\pi} \in \Pi^k$, $u \in V^k$ and $w \in V$, we define

$$\vec{\omega}_{\vec{\pi}}(u, w) = ([\phi_1(u, w)]_{\vec{\pi}}, [\phi_2(u, w)]_{\vec{\pi}}, \ldots, [\phi_k(u, w)]_{\vec{\pi}}),$$

and we define $\vec{\omega}_{\vec{\pi}}(u) = (\vec{\omega}_{\vec{\pi}}(u, w_1), \ldots, \vec{\omega}_{\vec{\pi}}(u, w_n))$ where $\{w_1, \ldots, w_n\} = V$ and $\vec{\omega}_{\vec{\pi}}(u, w_i) \leq_{lex} \vec{\omega}_{\vec{\pi}}(u, w_j)$ for all $i < j$. Note that $\vec{\omega}_{\vec{\pi}}(u) = \vec{\omega}_{\vec{\tau}}(v)$ means that there exists a bijection $\psi : V \to V$ such that $[\phi_i(u, w)]_{\vec{\pi}} = [\phi_i(v, \psi(w))]_{\vec{\tau}}$ for all $1 \leq i \leq k$ and for all $w \in V$.

Definition 2.30. We define $\vec{\omega}$ a preorder on $\mathcal{G} \times \vec{\Pi}^k \times V^k$ where for all $G, H \in \mathcal{G}$, $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ and $u, v \in V^k$, we write $(G, \vec{\pi}, u) \leq_{\vec{\omega}} (H, \vec{\tau}, v)$ if $(G, \vec{\pi}, u) <_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$ or $(G, \vec{\pi}, u) \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$ and $\vec{\omega}_{\vec{\pi}}(u) \leq_{lex} \vec{\omega}_{\vec{\tau}}(v)$.

It is straight-forward to verify that $\vec{\omega}$ is a V-C preorder, which induces ω and implies $\vec{\mathcal{C}}$. As in Definition 2.21, we define the function $\vec{\omega}_G : \vec{\Pi}^k \to \vec{\Pi}^k$, and we say that a partition $\vec{\pi} \in \vec{\Pi}^k$ is $\vec{\omega}_G$-stable if $\vec{\omega}_G(\vec{\pi}) = \vec{\pi}$. Also, we define $\vec{\omega}^*_G(\vec{\pi})$ as the fixed point reach by recursively applying $\vec{\omega}_G$, and specifically, we define $\vec{\omega}^k_G = \vec{\omega}^*_G((V^k))$. Also, analogous to Definition 2.22, we define the equivalence relation $\vec{\omega}$ on $\mathcal{G} \times \vec{\Pi}^k$. Given $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$, the k-dim $\vec{\omega}$-V-C algorithm is thus to compute $\vec{\omega}^*_G(\vec{\pi})$ and $\vec{\omega}^*_H(\vec{\tau})$ and then to check whether $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$.

The k-dim W–L isomorphism algorithm as presented in [11] is essentially to check whether $(G, \vec{\mathcal{C}}^k_G) \equiv_{\vec{\mathcal{C}}} (H, \vec{\mathcal{C}}^k_H)$, and then to check whether $(G, \vec{\omega}'^*_G(\vec{\mathcal{C}}^k_G)) \equiv_{\vec{\omega}'} (H, \vec{\omega}'^*_H(\vec{\mathcal{C}}^k_H))$ where $\vec{\omega}'$ a is V-C preorder on $\mathcal{G} \times \vec{\Pi}^k \times V^k$ defined as follows: for all $G, H \in \mathcal{G}$, $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ and $u, v \in V^k$, we write $(G, \vec{\pi}, u) \leq_{\vec{\omega}'} (H, \vec{\tau}, v)$ if $[u]_{\vec{\pi}} < [v]_{\vec{\tau}}$ or $[u]_{\vec{\pi}} = [v]_{\vec{\tau}}$ and $\vec{\omega}_{\vec{\pi}}(u) \leq_{lex} \vec{\omega}_{\vec{\tau}}(v)$. It is straight-forward to verify that $(G, \vec{\mathcal{C}}^k_G) \equiv_{\vec{\mathcal{C}}} (H, \vec{\mathcal{C}}^k_H)$ and $(G, \vec{\omega}'^*_G(\vec{\mathcal{C}}^k_G)) \equiv_{\vec{\omega}'} (H, \vec{\omega}'^*_H(\vec{\mathcal{C}}^k_H))$ if and only if $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$, and so, the k-dim W–L isomorphism algorithm is equivalent to the k-dim $\vec{\omega}$-V-C algorithm; however, we consider the more general case of arbitrary starting ordered partitions, so we defined $\vec{\omega}$ so that it implies $\vec{\mathcal{C}}$.

2.2.1.5. $\vec{\Delta}$ preorder. Here, we define the V-C preorder $\vec{\Delta}$. This preorder is useful in that the k-dim $\vec{\Delta}$-V-C algorithm is strongly related to the $(k-1)$-dim $\vec{\omega}$-V-C algorithm. First, we need the following definitions. For all $\vec{\pi} = (\vec{\pi}_1, \ldots, \vec{\pi}_m) \in \vec{\Pi}^k$, $1 \leq i \leq k$, and $u \in V^k$, we define

$$\vec{\Delta}^i_{\vec{\pi}}(u) = (|\Delta^i(u) \cap \vec{\pi}_1|, \ldots, |\Delta^i(u) \cap \vec{\pi}_m|),$$

and also, we define $\vec{\Delta}_{\vec{\pi}}(u) = (\vec{\Delta}^1_{\vec{\pi}}(u), \ldots, \vec{\Delta}^k_{\vec{\pi}}(u))$.

Definition 2.31. We define $\vec{\Delta}$ a preorder on $\mathcal{G} \times \vec{\Pi}^k \times V^k$ where for all $G, H \in \mathcal{G}$, $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ and $u, v \in V^k$, we write $(G, \vec{\pi}, u) \leq_{\vec{\Delta}} (H, \vec{\tau}, v)$ if $(G, \vec{\pi}, u) <_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$ or $(G, \vec{\pi}, u) \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$ and $\vec{\Delta}_{\vec{\pi}}(u) \leq_{lex} \vec{\Delta}_{\vec{\tau}}(v)$.

The preorder $\vec{\Delta}$ is a V-C preorder, which induces Δ and implies $\vec{\mathcal{C}}$. Then, we define the function $\vec{\Delta}_G : V^k \to V^k$, the concept of $\vec{\Delta}_G$-stable, and the partitions $\vec{\Delta}^*_G(\vec{\pi})$ and $\vec{\Delta}^k_G$ as in Definition 2.21. Also, we define the $\vec{\Delta}$ equivalence relation on $\mathcal{G} \times \vec{\Pi}^k$ as in Definition 2.22.

2.2.2. Comparison of combinatorial isomorphism algorithms

In this section, we compare the algorithms for graph isomorphism. Analogous to the automorphism case, we show that the k-dim $\vec{\omega}$-V-C algorithm is at least as strong as the k-dim $\vec{\delta}$-V-C algorithm, which is at least as strong as the k-dim $\vec{\Delta}$-V-C algorithm, and finally, we show that the k-dim $\vec{\Delta}$-V-C algorithm is as strong as the $(k-1)$-dim $\vec{\omega}$-V-C algorithm.

The lemma below shows that k-dim $\vec{\delta}$ implies k-dim $\vec{\Delta}$.

Lemma 2.32. *Let $G, H \in \mathcal{G}$, and let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$. If $(G, \vec{\pi}) \equiv_{\vec{\delta}^*} (H, \vec{\tau})$, then $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$. Furthermore, if $(G, \vec{\delta}^*_G(\vec{\pi})) \equiv_{\vec{\delta}} (H, \vec{\delta}^*_H(\vec{\tau}))$, then $(G, \vec{\Delta}^*_G(\vec{\pi})) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\tau}))$ and $(\vec{\delta}^*_G(\vec{\pi}), \vec{\delta}^*_H(\vec{\tau})) \leq (\vec{\Delta}^*_G(\vec{\pi}), \vec{\Delta}^*_H(\vec{\tau}))$.*

Proof. The first part follows from the fact that $\Delta^i(u) = \delta^i_G(u) \cup \bar{\delta}^i_G(u)$. The second part follows from Lemma 2.26. □

The lemma below shows that k-dim $\vec{\omega}$ implies k-dim $\vec{\delta}$.

Lemma 2.33. *Let $G, H \in \mathcal{G}$, and let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$. If $(G, \vec{\pi}) \equiv_{\vec{\omega}^*} (H, \vec{\tau})$, then $(G, \vec{\pi}) \equiv_{\vec{\delta}^*} (H, \vec{\tau})$. Furthermore, if $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$, then $(G, \vec{\delta}^*_G(\vec{\pi})) \equiv_{\vec{\delta}} (H, \vec{\delta}^*_H(\vec{\tau}))$ and $(\vec{\omega}^*_G(\vec{\pi}), \vec{\omega}^*_H(\vec{\tau})) \leq (\vec{\delta}^*_G(\vec{\pi}), \vec{\delta}^*_H(\vec{\tau}))$.*

Proof. Let $\vec{\pi} = (\vec{\pi}_1, \ldots, \vec{\pi}_m)$ and $\vec{\tau} = (\vec{\tau}_1, \ldots, \vec{\tau}_m)$ where $(G, \vec{\pi}) \equiv_{\vec{\omega}^*} (H, \vec{\tau})$, and let $u, v \in V^k$ where $[u]_{\vec{\pi}} = [v]_{\vec{\tau}}$. We must show that $(G, \vec{\pi}, u) \equiv_{\delta} (H, \vec{\tau}, v)$ and the result follows.

Since $(G, \vec{\pi}, u) \equiv_{\vec{\omega}} (H, \vec{\tau}, v)$ by assumption, there exists a bijection $\psi : V \to V$ such that $[\phi_j(u, w)]_{\vec{\pi}} = [\phi_j(v, \psi(w))]_{\vec{\tau}}$ for all $1 \le j \le k$ and for all $w \in V$. Let $1 \le t \le m$, $1 \le i \le k$ and $w \in V$. We show that $\phi_i(u, w) \in \delta^i_G(u) \cap \vec{\pi}_t \Leftrightarrow \phi_i(v, \psi(w)) \in \delta^i_H(v) \cap \vec{\tau}_t$ and that $\phi_i(u, w) \in \bar{\delta}^i_G(u) \cap \vec{\pi}_t \Leftrightarrow \phi_i(v, \psi(w)) \in \bar{\delta}^i_H(v) \cap \vec{\tau}_t$ implying that $|\delta^i_G(u) \cap \vec{\pi}_t| = |\delta^i_H(v) \cap \vec{\tau}_t|$ and $|\bar{\delta}^i_G(u) \cap \vec{\pi}_t| = |\bar{\delta}^i_H(v) \cap \vec{\tau}_t|$ since ψ is a bijection, thereby proving that $(G, \vec{\pi}, u) \equiv_{\delta} (H, \vec{\tau}, v)$.

First, $\phi_i(u, w) \in \vec{\pi}_t \Leftrightarrow \phi_i(v, \psi(w)) \in \vec{\tau}_t$ since $[\phi_i(u, w)]_{\vec{\pi}} = [\phi_i(v, \psi(w))]_{\vec{\tau}}$ by assumption. Let $j \ne i$. Then, since $[\phi_j(u, w)]_{\vec{\pi}} = [\phi_j(v, \psi(w))]_{\vec{\tau}}$ and $(G, \vec{\pi}) \equiv_{\vec{\mathcal{C}}^*} (H, \vec{\tau})$, we have $(G, \phi_j(u, w)) \equiv_{\mathcal{C}} (H, \phi_j(v, \psi(w)))$. Thus, $w \in \delta_G(u_i) \Leftrightarrow \psi(w) \in \delta_H(v_i)$ implying $\phi_i(u, w) \in \delta^i_G(u) \Leftrightarrow \phi_i(v, \psi(w)) \in \delta^i_H(v)$ and $\phi_i(u, w) \in \bar{\delta}^i_G(u) \Leftrightarrow \phi_i(v, \psi(w)) \in \bar{\delta}^i_H(v)$ as required.

The second part follows from Lemma 2.26. $\square$

With the next few lemmas, we show that the k-dim $\vec{\Delta}$-V-C algorithm is as strong as the $(k-1)$-dim $\vec{\omega}$-V-C algorithm. In order to do this, we first show that k-dim $\vec{\Delta}$ implies $(k-1)$-dim $\vec{\omega}$, and second, we show that k-dim $\vec{\omega}$ implies $(k+1)$-dim $\vec{\Delta}$, and then we can show the equivalence.

First, we need a way of mapping ordered k-dim partitions onto $(k-1)$-dim partitions, analogous to ρ for ordered partitions.

Definition 2.34. We define the map $\vec{\rho} : \vec{\Pi}^k \to \vec{\Pi}^{k-1}$ such that for $\vec{\pi} \in \vec{\Pi}^k$ and for $u', v' \in V^{k-1}$, we have $u' \leqq_{\vec{\rho}(\vec{\pi})} v'$ if $\nu(u') \leqq_{\vec{\pi}} \nu(v')$.

The next lemma establishes that k-dim $\vec{\Delta}$ implies $(k-1)$-dim $\vec{\omega}$.

Lemma 2.35. *Let $G, H \in \mathcal{G}$. Let $k > 1$, and let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$. If $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$, then $(G, \vec{\rho}(\vec{\pi})) \equiv_{\vec{\omega}^*} (H, \vec{\rho}(\vec{\tau}))$. Furthermore, we have $(G, \vec{\Delta}^*_G(\vec{\pi})) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\tau}))$ implies $(G, \vec{\omega}^*(\rho(\vec{\pi}))) \equiv_{\vec{\omega}} (H, \vec{\omega}^*(\rho(\vec{\tau})))$ and $(\vec{\rho}(\vec{\Delta}^*_G(\vec{\pi})), \vec{\rho}(\vec{\Delta}^*_H(\vec{\tau}))) \le (\vec{\omega}^*_G(\vec{\rho}(\vec{\pi})), \vec{\omega}^*_H(\vec{\rho}(\vec{\tau})))$.*

Proof. Let $\vec{\pi}' = \vec{\rho}(\vec{\pi})$ and $\vec{\tau}' = \vec{\rho}(\vec{\tau})$. Firstly, assume $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$. We must show that $(G, \vec{\pi}', u') \equiv_{\vec{\omega}} (H, \vec{\tau}', v')$ for all $u', v' \in V^{k-1}$ where $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$. Then, since $\vec{\pi}' \approx \vec{\tau}'$ by Lemma A.9, it follows that $(G, \vec{\pi}') \equiv_{\vec{\omega}^*} (H, \vec{\tau}')$.

Let $u', v' \in V^{k-1}$ where $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$. By Lemma A.9, we have $(G, \vec{\pi}', u') \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}', v')$. It thus remains to show that there exists a bijection $\psi : V \to V$ such that $[\phi_i(u', w)]_{\vec{\pi}'} = [\phi_i(v', \psi(w))]_{\vec{\tau}'}$ for all $w \in V$ and $1 \le i \le k-1$.

Let $u = \vec{\nu}(u')$ and $v = \vec{\nu}(v')$. By Lemma A.9, we have $[u]_{\vec{\pi}} = [v]_{\vec{\tau}}$, and so by assumption, $(G, \vec{\pi}, u) \equiv_{\vec{\Delta}} (H, \vec{\tau}, v)$. Thus, we have $|\Delta^i(u) \cap \vec{\pi}_t| = |\Delta^i(v) \cap \vec{\tau}_t|$ for all $1 \le t \le m$ and $1 \le i \le k$ where $m = |\vec{\pi}|$. Let $U_t = \{w \in V : \phi_k(u, w) \in \vec{\pi}_t\}$ and let $W_t = \{w \in V : \phi_k(v, w) \in \vec{\tau}_t\}$ for all $1 \le t \le m$. Note that $\{U_1, \ldots, U_m\}$ and $\{W_1, \ldots, W_m\}$ are partitions of V such that $|\Delta^k(u) \cap \vec{\pi}_t| = |U_t| = |W_t| = |\Delta^k(v) \cap \vec{\tau}_t|$ for all $1 \le t \le m$. Let $\psi : V \to V$ be a bijection such that $\psi(U_t) = W_t$ for all $1 \le t \le m$. Let $w \in U_t$ and let $w' = \psi(w)$. Then, by construction, $[\phi_k(u, w)]_{\vec{\pi}} = [\phi_k(v, w')]_{\vec{\tau}}$, and since $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$, we also have $(G, \vec{\pi}, \phi_k(u, w)) \equiv_{\vec{\Delta}} (H, \vec{\tau}, \phi_k(v, w'))$. From Lemma A.3, we have $[\phi_i(\phi_k(u, w), w)]_{\vec{\pi}} = [\phi_i(\phi_k(v, w'), w')]_{\vec{\tau}}$ and moreover $(G, \vec{\pi}, \phi_i(\phi_k(u, w), w)) \equiv_{\vec{\Delta}} (H, \vec{\tau}, \phi_i(\phi_k(v, w'), w'))$ for all $1 \le i \le k-1$. Thus, $[\phi_i(u', w)]_{\vec{\pi}'} = [\phi_i(v', w')]_{\vec{\tau}'}$ for all $1 \le i \le k-1$ since $\rho(\phi_i(\phi_k(u, w), w)) = \phi_i(u', w)$ and $\rho(\phi_i(\phi_k(v, w'), w')) = \phi_i(v', w')$ as required.

Secondly, assume $(G, \vec{\Delta}^*_G(\vec{\pi})) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\tau}))$. Let $\vec{\pi}'' = \vec{\rho}(\vec{\Delta}^*_G(\vec{\pi}))$ and $\vec{\tau}'' = \rho(\vec{\Delta}^*_H(\vec{\tau}))$. From Corollary A.2, we have $(\vec{\Delta}^*_G(\vec{\pi}), \vec{\Delta}^*_H(\vec{\tau})) \le (\vec{\pi}, \vec{\tau})$ implying $(\vec{\pi}'', \vec{\tau}'') \le (\vec{\pi}', \vec{\tau}')$ by Lemma A.9. Then, from above, $(G, \vec{\pi}'') \equiv_{\vec{\omega}^*} (H, \vec{\tau}'')$, and by Lemma A.1, we have $(G, \vec{\omega}^*(\vec{\pi}')) \equiv_{\vec{\omega}} (H, \vec{\omega}^*(\vec{\tau}'))$ and $(\vec{\pi}'', \vec{\tau}'') \le (\vec{\omega}^*_G(\vec{\pi}'), \vec{\omega}^*_H(\vec{\tau}'))$ as required. $\square$

Next, we show that k-dim $\vec{\omega}$ implies $(k+1)$-dim $\vec{\Delta}$, but first we need a map from ordered partitions of k-tuples to ordered partitions of $(k+1)$-tuples.

Definition 2.36. Define $\vec{\nu} : \vec{\Pi}^k \to \vec{\Pi}^{k+1}$ where for all $\vec{\pi} \in \vec{\Pi}^k$ and $u, v \in V^{k+1}$, we have $u \leqq_{\vec{\nu}(\vec{\pi})} v$ if $\rho(u) \lneqq_{\vec{\pi}} \rho(v)$ or $\rho(u) \equiv_{\vec{\pi}} \rho(v)$ and $\vec{\omega}_{\vec{\pi}}(\rho(u), u_{k+1}) \le_{lex} \vec{\omega}_{\vec{\pi}}(\rho(v), v_{k+1})$.

The next lemma establishes that k-dim $\vec{\omega}$ implies $(k+1)$-dim $\vec{\Delta}$.

Lemma 2.37. *Let $G, H \in \mathcal{G}$. Let $k > 1$, and let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$. Then, $(G, \vec{\pi}) \equiv_{\vec{\omega}^*} (H, \vec{\tau})$ implies $(G, \vec{\nu}(\vec{\pi})) \equiv_{\vec{\Delta}^*} (H, \vec{\nu}(\vec{\tau}))$. Furthermore, $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$ implies $(G, \vec{\Delta}^*_G(\vec{\nu}(\vec{\pi})) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\nu}(\vec{\tau})))$ and $(\vec{\nu}(\vec{\omega}^*_G(\vec{\pi})), \vec{\nu}(\vec{\omega}^*_H(\vec{\tau}))) \le (\vec{\Delta}^*_G(\vec{\nu}(\vec{\pi})), \vec{\Delta}^*_H(\vec{\nu}(\vec{\tau})))$.*

Proof. Let $\vec{\pi}' = \vec{\nu}(\vec{\pi})$ and $\vec{\tau}' = \vec{\nu}(\vec{\tau})$. Assume $(G, \vec{\pi}) \equiv_{\vec{\omega}^*} (H, \vec{\tau})$. We must show that $(G, \vec{\pi}', u') \equiv_{\vec{\Delta}} (H, \vec{\tau}', v')$ for all $u', v' \in V^{k+1}$ where $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$. Then, since $\vec{\pi}' \approx \vec{\tau}'$ by Lemma A.7, it follows that $(G, \vec{\pi}') \equiv_{\vec{\Delta}^*} (H, \vec{\tau}')$.

Let $u', v' \in V^{k+1}$ where $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$. By Lemma A.7, we have $(G, \vec{\pi}', u') \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}', v')$. It thus remains to show that $|\Delta^i(u') \cap \vec{\pi}'_t| = |\Delta^i(v') \cap \vec{\tau}'_t|$ for all $1 \le i \le k+1$ and all $1 \le t \le m'$ where $m' = |\vec{\pi}'| = |\vec{\tau}'|$.

Let $u = \rho(u')$ and $v = \rho(v')$. From Lemma A.7, we have $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$. Then, by assumption, $(G, \vec{\pi}, u') \equiv_{\vec{\omega}} (H, \vec{\tau}, v')$, and so, there exists a bijection $\psi : V \to V$ such that $\vec{\omega}_{\vec{\pi}}(u', w) = \vec{\omega}_{\vec{\tau}}(v', \psi(w))$ for all $w \in V$. Next, we show that $|\vec{\Delta}^{k+1}_G(u') \cap \vec{\pi}'_t| = |\vec{\Delta}^{k+1}_H(v') \cap \vec{\tau}'_t|$ for all $1 \le t \le m'$. Let $U_t = \{w \in V : \phi_k(u', w) \in \vec{\pi}'_t\}$ and $W_t = \{w \in V :$

$\phi_k(v', w) \in \vec{\tau}'_t\}$. We will show that $\psi(U_t) = W_t$ implying that $|\vec{\Delta}^{k+1}_G(u') \cap \vec{\pi}'_t| = |U_t| = |W_t| = |\vec{\Delta}^{k+1}_H(v') \cap \vec{\tau}'_t|$ as required. Now, for all $w \in U_t$, we have $[u]_{\vec{\pi}} = [v]_{\vec{\tau}}$ and $\vec{\omega}_{\vec{\pi}}(u, w) = \vec{\omega}_{\vec{\tau}}(v, \psi(w))$, which by Lemma A.7 implies that $[\phi_{k+1}(u', w)]_{\vec{\pi}'} = [\phi_{k+1}(v', \psi(w))]_{\vec{\tau}'}$, and thus, $\psi(w) \in W_t$. Thus, $\psi(U_t) \subseteq W_t$, and analogously, $\psi(W_t) \subseteq U_t$ as required. Lastly, since $\vec{\pi} \equiv_{\vec{\mathcal{S}}^*} \vec{\tau}$ and $\vec{\pi}' \equiv_{\vec{\mathcal{S}}^*} \vec{\tau}'$ by Lemma A.7, for all $\sigma \in \mathcal{S}_{k+1}$, we have $[\sigma(u)]_{\vec{\pi}'} = [\sigma(v)]_{\vec{\tau}'}$ and $(G, \vec{\pi}', \rho(\sigma(u))) \equiv_{\vec{\omega}} (H, \vec{\tau}', \rho(\sigma(v)))$. Therefore, $|\Delta^i(u) \cap \vec{\pi}'_t| = |\Delta^i(v) \cap \vec{\tau}'_t|$ for all $1 \le i \le k$ and all $1 \le t \le m$ as required.

Secondly, assume $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$. Let $\vec{\pi}'' = \vec{\nu}(\vec{\omega}^*_G(\vec{\pi}))$ and $\vec{\tau}'' = \vec{\nu}(\vec{\omega}^*_H(\vec{\tau}))$. From above, $(G, \vec{\pi}'') \equiv_{\vec{\Delta}^*} (H, \vec{\tau}'')$. By Corollary A.2, $(\vec{\omega}^*_G(\vec{\pi}), \vec{\omega}^*_H(\vec{\tau})) \le (\vec{\pi}, \vec{\tau})$, and then, from Lemma A.7, $(\vec{\pi}'', \vec{\tau}'') \le (\vec{\pi}', \vec{\tau}')$. Therefore, by Lemma A.1, $(\vec{\pi}'', \vec{\tau}'') \le (\vec{\Delta}^*_G(\vec{\pi}'), \vec{\Delta}^*_H(\vec{\tau}'))$ and $(G, \vec{\Delta}^*_G(\vec{\pi}') \equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\tau}'))$ as required. □

Combining Lemmas 2.35 and 2.37, we arrive at the following result stating the equivalence of the k-dim $\vec{\omega}$-V-C algorithm and $(k+1)$-dim $\vec{\Delta}$-V-C algorithm.

Corollary 2.38. *Let $G, H \in \mathcal{G}$. Let $k > 1$ and let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$ and $\vec{\nu}(\vec{\pi}) \approx \vec{\nu}(\vec{\tau})$. Then, we have $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$ if and only if $(G, \vec{\Delta}^*_G(\vec{\nu}(\vec{\pi}))) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\nu}(\vec{\tau})))$. Moreover, if $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$, then $(\vec{\omega}^*_G(\vec{\pi}), \vec{\omega}^*_H(\vec{\tau})) \simeq (\vec{\rho}(\vec{\Delta}^*_G(\vec{\nu}(\vec{\pi}))), \vec{\rho}(\vec{\Delta}^*_H(\vec{\nu}(\vec{\tau}))))$.*

Proof. Let $\vec{\pi}' = \vec{\nu}(\vec{\pi})$ and $\vec{\tau}' = \vec{\nu}(\vec{\tau})$. Assume $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$. From Lemma 2.37, we have $(G, \vec{\Delta}^*_G(\vec{\pi}')) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\tau}'))$. Also, from Lemma 2.37, we have $(\vec{\nu}(\vec{\omega}^*_G(\vec{\pi})), \vec{\nu}(\vec{\omega}^*_H(\vec{\tau}))) \le (\vec{\Delta}^*_G(\vec{\pi}'), \vec{\Delta}^*_H(\vec{\tau}'))$, which implies $(\vec{\omega}^*_G(\vec{\pi}), \vec{\omega}^*_H(\vec{\tau})) \le (\vec{\rho}(\vec{\Delta}^*_G(\vec{\pi}')), \vec{\rho}(\vec{\Delta}^*_H(\vec{\tau}')))$ since $\vec{\rho}(\vec{\nu}(\vec{\omega}^*_G(\vec{\pi}))) = \vec{\omega}^*_G(\vec{\pi})$ and $\vec{\rho}(\vec{\nu}(\vec{\omega}^*_H(\vec{\tau}))) = \vec{\omega}^*_H(\vec{\tau})$ from Lemma A.5 since $\vec{\omega}^*_G(\vec{\pi})$ and $\vec{\omega}^*_G(\vec{\pi})$ are $\vec{\Delta}$-stable.

Assume $(G, \vec{\Delta}^*_G(\vec{\pi}')) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\tau}'))$. Let $\vec{\pi}'' = \vec{\rho}(\vec{\pi}')$ and $\vec{\tau}'' = \vec{\rho}(\vec{\tau}')$. Then, since $\vec{\pi}' \approx \vec{\tau}'$, we have $(G, \vec{\pi}') \equiv_{\vec{\Delta}} (H, \vec{\tau}')$ by Corollary A.2, which implies that $\vec{\pi}'' \approx \vec{\tau}''$. Then, since $\vec{\pi} \approx \vec{\tau}$ and $\vec{\pi}'' \approx \vec{\tau}''$, and also, $\vec{\pi}'' \preceq \vec{\pi}$ and $\vec{\tau}'' \preceq \vec{\tau}$ from Lemma A.5, we have $(\vec{\pi}'', \vec{\tau}'') \le (\vec{\pi}, \vec{\tau})$. Now, from Lemma 2.35, we have $(G, \vec{\omega}^*_G(\vec{\pi}'')) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}''))$ and $(\vec{\rho}(\vec{\Delta}^*_G(\vec{\pi}')), \vec{\rho}(\vec{\Delta}^*_H(\vec{\tau}'))) \le (\vec{\omega}^*_G(\vec{\pi}''), \vec{\omega}^*_H(\vec{\tau}''))$, and since $(\vec{\omega}^*_G(\vec{\pi}''), \vec{\omega}^*_H(\vec{\tau}'')) \le (\vec{\pi}'', \vec{\tau}'') \le (\vec{\pi}, \vec{\tau})$ by Corollary A.2, $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$ and $(\vec{\omega}^*_G(\vec{\pi}''), \vec{\omega}^*_H(\vec{\tau}'')) \le (\vec{\omega}^*_G(\vec{\pi}), \vec{\omega}^*_H(\vec{\tau}))$ by Lemma A.1 implying $(\vec{\rho}(\vec{\Delta}^*_G(\vec{\pi}')), \vec{\rho}(\vec{\Delta}^*_H(\vec{\tau}'))) \le (\vec{\omega}^*_G(\vec{\pi}), \vec{\omega}^*_H(\vec{\tau}))$, as required. □

Specifically, we have $(G, \vec{\omega}^k_G) \equiv_{\vec{\omega}} (H, \vec{\omega}^k_H)$ if and only if $(G, \vec{\Delta}^{k+1}_G) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^{k+1}_H)$. Moreover, $(G, \vec{\omega}^k_G) \equiv_{\vec{\omega}} (H, \vec{\omega}^k_H)$ or $(G, \vec{\Delta}^{k+1}_G) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^{k+1}_H)$ implies $(\vec{\omega}^k_G, \vec{\omega}^k_H) \simeq (\vec{\rho}(\vec{\Delta}^{k+1}_G), \vec{\rho}(\vec{\Delta}^{k+1}_H))$.

3. Sherali–Adams relaxations

In this section, we give explicit descriptions of the Sherali–Adams relaxations for different graph automorphism and isomorphism polytopes.

3.1. Birkhoff polytope

In this section, we give an explicit description of the Sherali–Adams relaxations of the Birkhoff polytope. The Birkhoff polytope (for a given positive integer n) is the polytope whose integer points are all $n \times n$ permutation matrices:

$$B = \{X \in [0, 1]^{n\times n} : Xe = X^T e = e\}.$$

The Birkhoff polytope is precisely $\mathcal{T}_G$ when G is the complete graph K_n or a stable graph. It is well-known that the Birkhoff polytope is integral (its extreme points are integer), so the Sherali–Adams relaxations of the Birkhoff polytope are not interesting in themselves. However, we use the Birkhoff polytope to illustrate the Sherali–Adams approach explicitly, as this serves as the foundation for Sherali–Adams relaxations of polytopes we are interested in. We also prove some minor results that are useful later in the paper. We begin with a more explicit formulation of the Birkhoff polytope. This is given by the inequalities below:

$$\sum_{w\in V} X_{uw} - 1 = 0 \qquad \forall u \in V,$$
$$\sum_{w\in V} X_{wv} - 1 = 0 \qquad \forall v \in V,$$
$$0 \le X_{uv} \le 1 \qquad \forall u, v \in V.$$

The first step in computing the kth Sherali–Adams relaxation is to multiply each equation above with monomials $\prod_{(r,s)\in I} X_{rs}$ for all $I \subseteq V^2 = \{(u, v) : u, v \in V\}$ where $|I| \le k-1$. Moreover, we must introduce the inequalities $\prod_{(u,v)\in I} X_{uv} \prod_{(u,v)\in J\setminus I}(1 - X_{uv}) \ge 0$ for all $I \subseteq J \subseteq V^2$ where $|J| \le k$. We do so as follows:

$$\prod_{(r,s)\in I} X_{rs} \left(\sum_{w\in V} X_{uw}\right) - \prod_{(r,s)\in I} X_{rs} = 0 \qquad \forall I \subseteq V^2, |I| \le k-1, \forall u \in V,$$

$$\prod_{(r,s)\in I} X_{rs}\left(\sum_{w\in V} X_{wv}\right) - \prod_{(r,s)\in I} X_{rs} = 0 \qquad \forall I \subseteq V^2, |I| \le k-1, \forall v \in V,$$
$$\prod_{(u,v)\in I} X_{uv} \prod_{(u,v)\in J\setminus I} (1 - X_{uv}) \ge 0 \qquad \forall I \subseteq J \subseteq V^2, |J| \le k.$$

Next, we linearize the above equations to produce the kth-degree Sherali–Adams extended formulation relaxation, $\hat{B}^k$. Here, we have replaced X_{uv}^2 with X_{uv} and replaced the monomial $\prod_{(u,v)\in I} X_{uv}$ where $I \subseteq V^2$ with the variable Y_I.

$$\sum_{w\in V} Y_{I\cup\{(u,w)\}} - Y_I = 0 \qquad \forall I \subseteq V^2, |I| \le k-1, \forall u \in V, \tag{4}$$
$$\sum_{w\in V} Y_{I\cup\{(w,v)\}} - Y_I = 0 \qquad \forall I \subseteq V^2, |I| \le k-1, \forall v \in V, \tag{5}$$
$$\sum_{I\subseteq K\subseteq J} (-1)^{|K\setminus I|} Y_K \ge 0 \qquad \forall I \subseteq J \subseteq V^2, |J| \le k, \tag{6}$$
$$Y_\emptyset = 1. \tag{7}$$

Recall that the integer points in B are the set of $n \times n$ permutation matrices. The integer points in $\hat{B}^k$ are in bijection with the integer points in B. Indeed, a permutation matrix $P \in \{0, 1\}^{n\times n}$ is in one-to-one correspondence with the point $Y_I \in \hat{B}^k$ if

$$Y_I = 1 \Leftrightarrow X_{uv} = 1 \quad \forall\, (u, v) \in I, \qquad Y_I = 0 \quad \text{otherwise}.$$

Many of the inequalities in (6) above are redundant. In fact, the only inequalities we need to keep are $Y_I \ge 0$ for all $I \subseteq V^2$. We show that the other inequality constraints $\sum_{I\subseteq K\subseteq J} (-1)^{|K\setminus I|} Y_K \ge 0$ for all $I \subseteq J \subseteq V^2$, $|J| \le k$ are implied by the constraints (4), (5) and the condition $Y_I \ge 0$, for all $I \subseteq V^2$. This is established by induction on $|J \setminus I|$. This is trivially true when $|J \setminus I| = 0$, so assume it is true for $|J \setminus I| \le l$. Let $(u, v) \in J \setminus I$, with $|J \setminus I| \le l + 1$. Then,

$$\sum_{I\subseteq K\subseteq J} (-1)^{|K\setminus I|} Y_K$$
$$= \sum_{I\subseteq K\subseteq (J\setminus\{(u,v)\})} \left((-1)^{|K\setminus I|} Y_K - (-1)^{|K\setminus I|} Y_{K\cup\{(u,v)\}}\right) \tag{8}$$
$$= \sum_{I\subseteq K\subseteq (J\setminus\{(u,v)\})} \left((-1)^{|K\setminus I|} Y_K - (-1)^{|K\setminus I|}\left(Y_K - \sum_{w\in V\setminus\{v\}} Y_{K\cup\{(u,w)\}}\right)\right) \tag{9}$$
$$= \sum_{I\subseteq K\subseteq (J\setminus\{(u,v)\})} \left(\sum_{w\in V\setminus\{v\}} (-1)^{|K\setminus I|} Y_{K\cup\{(u,w)\}}\right) \tag{10}$$
$$= \sum_{w\in V\setminus\{v\}} \left(\sum_{I\subseteq K\subseteq (J\setminus\{(u,v)\})} (-1)^{|K\setminus I|} Y_{K\cup\{(u,w)\}}\right) \tag{11}$$
$$= \sum_{w\in V\setminus\{v\}} \left(\sum_{(I\cup\{(u,w)\})\subseteq K\subseteq (J\setminus\{(u,v)\})} (-1)^{|K\setminus (I\cup\{(u,w)\})|} Y_K\right) \tag{12}$$
$$\ge 0. \tag{13}$$

To progress from (8) to (9), we used Eq. (4). To show (12) is non-negative, we have that $\sum_{\bar{I}\subseteq K\subseteq \bar{J}} (-1)^{|K\setminus \bar{I}|} Y_K \ge 0$ where $\bar{I} = I \cup \{(u, w)\}$ and $\bar{J} = J \setminus \{(u, v)\}$ for all $w \in V \setminus \{v\}$ by assumption since $|\bar{J} \setminus \bar{I}| \le l$.

Thus, we arrive at the following description of $\hat{B}^k$. There are still redundant inequalities here, but for the purpose of this paper, this description suffices.

$$\sum_{w\in V} Y_{I\cup\{(u,w)\}} - Y_I = 0 \qquad \forall I \subseteq V^2, |I| \le k-1, \forall u \in V, \tag{14}$$
$$\sum_{w\in V} Y_{I\cup\{(w,v)\}} - Y_I = 0 \qquad \forall I \subseteq V^2, |I| \le k-1, \forall v \in V, \tag{15}$$
$$Y_I \ge 0 \qquad \forall I \subseteq V^2, |I| \le k, \tag{16}$$
$$Y_\emptyset = 1. \tag{17}$$

The following sets of equations, which we will find useful later, are implied by (14) and (15):

$$\sum_{v_1,\dots,v_s\in V} Y_{\{(u_1,v_1),\dots,(u_s,v_s)\}} = 1 \quad \forall u_1,\dots,u_s \in V,\ \forall s \le k, \tag{18}$$

$$\sum_{u_1,\dots,u_s\in V} Y_{\{(u_1,v_1),\dots,(u_s,v_s)\}} = 1 \quad \forall v_1,\dots,v_s \in V,\ \forall s \le k. \tag{19}$$

This set of equations is equivalent to saying that any given sequence of vertices $u_1,\dots,u_s \in V$ must map onto to one and only one other sequence of vertices $v_1,\dots,v_s \in V$. We can prove this by induction on s. This is true for $s = 1$. So, let us assume that it is true for s and we will prove it is true for $s + 1$.

$$\sum_{v_1,\dots,v_{s+1}\in V} Y_{\{(u_1,v_1),\dots,(u_{s+1},v_{s+1})\}} = \sum_{v_1,\dots,v_s\in V} Y_{\{(u_1,v_1),\dots,(u_s,v_s)\}} = 1 \quad \forall u_1,\dots,u_{s+1} \in V,$$
$$\sum_{u_1,\dots,v_{s+1}\in V} Y_{\{(u_1,v_1),\dots,(u_{s+1},v_{s+1})\}} = \sum_{u_1,\dots,u_s\in V} Y_{\{(u_1,v_1),\dots,(u_s,v_s)\}} = 1 \quad \forall v_1,\dots,v_{s+1} \in V.$$

In the above equations, the first equality follows from Eqs. (14) and (15) and the second follows by assumption.

Another useful set of equations, which are also implied by (14) and (15) are as follows:

$$Y_{I\cup\{(u,v_1),(u,v_2)\}} = 0 \quad \forall u, v_1, v_2 \in V, v_1 \ne v_2, I \subseteq V^2, |I| \le k-2, \tag{20}$$

$$Y_{I\cup\{(u_1,v),(u_2,v)\}} = 0 \quad \forall u_1, u_2, v \in V, u_1 \ne u_2, I \subseteq V^2, |I| \le k-2. \tag{21}$$

These equations say that no bijection from V to V can map u onto v_1 and u onto v_2 if $v_1 \ne v_2$, and similarly, no bijection can map u_1 onto v and u_2 onto v if $u_1 \ne u_2$. We prove this as follows: Let $u, v \in V$ and $I \subseteq V^2$ where $|I| \le k-2$. Then, from Eq. (14), we have

$$\sum_{w\in V} Y_{I\cup\{(u,v)(u,w)\}} - Y_{I\cup\{(u,v)\}} = \sum_{w\in V\setminus\{v_1\}} Y_{I\cup\{(u,v)(u,w)\}} = 0.$$

This implies that $Y_{I\cup\{(u,v)(u,w)\}} = 0$ for all $w \in V$ where $w \ne v$. Similarly, from Eq. (15), we have

$$\sum_{w\in V} Y_{I\cup\{(u,v)(w,v)\}} - Y_{I\cup\{(u,v)\}} = \sum_{w\in V\setminus\{u\}} Y_{I\cup\{(u,v)(w,v)\}} = 0.$$

This implies that $Y_{I\cup\{(u,v)(w,v)\}} = 0$ for all $w \in V$ where $w \ne u$ as required.

In order to relate Sherali–Adams relaxations with combinatorial algorithms, we find it more convenient to use a slightly different notation than above for formulating $\hat{B}^k$. We use the following k-tuple notation.

Definition 3.1. Given k-tuples $u, v \in V^k$, we define $\langle u, v\rangle = \{(u_1, v_1), \dots, (u_k, v_k)\}$.

Using this new notation, we can replace Y_I by $Y_{\langle u,v\rangle}$ in the formulation of $\hat{B}^k$ for any $I \subseteq V^2$. The reformulation of $\hat{B}^k$ with this notation is as follows:

$$\sum_{w\in\Delta^i(v)} Y_{\langle u,w\rangle} - Y_{\langle u,v\rangle\setminus\{(u_i,v_i)\}} = 0 \qquad \forall u, v \in V^k, 1 \le i \le k, \tag{22}$$

$$\sum_{w\in\Delta^i(u)} Y_{\langle w,v\rangle} - Y_{\langle u,v\rangle\setminus\{(u_i,v_i)\}} = 0 \qquad \forall u, v \in V^k, 1 \le i \le k, \tag{23}$$

$$Y_{\langle u,v\rangle} \ge 0 \qquad \forall u, v \in V^k, \tag{24}$$

$$Y_\emptyset = 1. \tag{25}$$

There is a lot of redundancy in the above formulation of $\hat{B}^k$ since there are many ways of writing I as $\langle u, v\rangle$ for some $u, v \in V^k$, but we will find the above description very useful.

We can also reformulate (18) and (19) using tuple notation:

$$\sum_{u\in V^k} Y_{\langle u,v\rangle} = 1 \qquad \forall u \in V^k, \tag{26}$$

$$\sum_{v\in V^k} Y_{\langle u,v\rangle} = 1 \qquad \forall v \in V^k. \tag{27}$$

This set of equations enforces that any given k-tuple of vertices $u \in V^k$ must map onto to one and only one other k-tuple $v \in V^k$.

We can also reformulate (20) and (21) concisely using tuple notation as follows:

$$Y_{\langle u,v\rangle} = 0 \quad \forall u, v \in V^k, u \not\equiv_{\mathcal{C}} v. \tag{28}$$

Recall that $u \not\equiv_{\mathcal{C}} v$ means that $u_i = u_j$ and $v_i \ne v_j$ for some $1 \le i, j \le k$.

3.2. Tinhofer polytope

In this section, we give an explicit description of the Sherali–Adams relaxations of the graph isomorphism polytope $\mathcal{T}_{G,H}$ for graphs G and H. As described in the introduction, the polyhedron $\mathcal{T}_{G,H}$ is defined explicitly as follows:

$$\mathcal{T}_{G,H} = \left\{ X \in B : \sum_{w \in \delta_G(v)} X_{uw} - \sum_{w \in \delta_H(u)} X_{wv} = 0 \ \forall u, v \in V \right\}.$$

There is a nice and intuitive interpretation of the set of the constraints (in addition to $X \in B$) for the Tinhofer polytope. Let $u, v \in V$ and $X \in B \cap \{0, 1\}^{n \times n}$, and let $\psi : V \to V$ be the corresponding bijection to the permutation matrix X. Then, the expression $\sum_{w \in \delta_G(v)} X_{uw}$ equals 1 if $\psi(u) \in \delta_H(v)$ and equals 0 otherwise. Similarly, the expression $\sum_{w \in \delta_H(u)} X_{wv}$ equals 1 if $\psi^{-1}(v) \in \delta_G(u)$ and equals 0 otherwise. Thus, u is adjacent to $\psi^{-1}(v)$ in G if and only if $\psi(u)$ is adjacent to v in H, or in other words, edges must map onto edges and non-edges must map onto non-edges.

Recall that the last three sets of equations define the Birkhoff polytope, which we generated the Sherali–Adams relaxation for in the last section. We therefore determine the Sherali–Adams relaxation of the first set of equations. First, we multiply the equations with monomials $\prod_{(r,s) \in I} X_{rs}$ for all $I \subseteq V^2 = \{(u, v) : u, v \in V\}$ where $|I| \leq k - 1$.

$$\prod_{(r,s) \in I} X_{rs} \left(\sum_{w \in \delta_H(v)} X_{uw} - \sum_{w \in \delta_G(u)} X_{wv} \right) = 0 \quad \forall I \subseteq V^2, |I| \leq k - 1, \forall u, v \in V.$$

Next, we linearize the above equations.

$$\sum_{w \in \delta_H(v)} Y_{I \cup \{(u,w)\}} - \sum_{w \in \delta_G(u)} Y_{I \cup \{(w,v)\}} = 0 \quad \forall I \subseteq V^2, |I| \leq k - 1, \forall u, v \in V. \tag{29}$$

In order to relate the relaxation $\hat{\mathcal{T}}^k_{G,H}$ with the k-dim V-C algorithm, we find it more convenient to use k-tuple notation as in the previous section.

$$\sum_{w \in \delta^i_H(v)} Y_{\langle u,w \rangle} - \sum_{w \in \delta^i_G(u)} Y_{\langle w,v \rangle} = 0 \quad \forall u, v \in V^k, 1 \leq i \leq k. \tag{30}$$

Then, combining the above equations with the equations for the kth Sherali–Adams relaxation of the Birkhoff polytope gives the kth-degree Sherali–Adams extended formulation relaxation of $\mathcal{T}_{G,H}$, which we denote by $\hat{\mathcal{T}}^k_{G,H}$.

$$\hat{\mathcal{T}}^k_{G,H} = \left\{ Y \in \hat{B}^k : \sum_{w \in \delta^i_H(v)} Y_{\langle u,w \rangle} - \sum_{w \in \delta^i_G(u)} Y_{\langle w,v \rangle} = 0 \ \forall u, v \in V^k, 1 \leq i \leq k \right\}.$$

Recall the integer points in $\mathcal{T}_{G,H}$ are in bijection with isomorphisms from G to H. In an analogous manner, the integer points in $\hat{\mathcal{T}}^k_{G,H}$ are in bijection with isomorphisms from G to H as follows. A point $Y \in \hat{\mathcal{T}}^k_{G,H}$ is integer if and only if there exists an isomorphism $\psi \in ISO(G, H)$ such that for all $u, v \subseteq V^k$, we have $Y_{\langle u,v \rangle} = 1$ if $\psi(u_i) = v_i$ for all $1 \leq i \leq k$ and $Y_{\langle u,v \rangle} = 0$ otherwise.

The kth Sherali–Adams relaxations of the Tinhofer polytopes $\mathcal{T}_G$ and $\mathcal{T}_{G,H}$ are then the polytopes $\mathcal{T}^k_G \subseteq B$ and $\mathcal{T}^k_{G,H} \subseteq B$ respectively defined as the projection of $\hat{\mathcal{T}}^k_G$ and $\hat{\mathcal{T}}^k_{G,H}$ onto B respectively. Lastly, if $\mathcal{T}^k_G = \{\mathcal{I}_n\}$, then $|AUT(G)| = 1$ and if $\mathcal{T}^k_{G,H} = \emptyset$, then $ISO(G, H) = \emptyset$.

3.3. Δ-polytope

We define the semi-algebraic set $Q_{G,H} \subseteq B$ as the set of all $X \in B$ such that

$$X_{u_1v_1} X_{u_2v_2} = 0 \quad \forall \{u_1, u_2\} \in E_G, \{v_1, v_2\} \notin E_H, \tag{31}$$

$$X_{u_1v_1} X_{u_2v_2} = 0 \quad \forall \{u_1, u_2\} \notin E_G, \{v_1, v_2\} \in E_H. \tag{32}$$

Note that $Q_{G,H} \cap \{0, 1\}^{n \times n} = \mathcal{T}_{G,H} \cap \{0, 1\}^{n \times n}$, that is, the set of permutation matrices in bijection with $ISO(G, H)$. This is because Eqs. (31) and (32) enforce that edges must map onto edges and non-edges must map onto non-edges.

We now describe the Sherali–Adams relaxations of $Q_{G,H}$ the first two sets of equations. The first step in computing the kth Sherali–Adams relaxation is introducing:

$$\prod_{(r,s) \in I} X_{rs} \left(X_{u_1v_1} X_{u_2v_2} \right) = 0 \quad \forall I \subseteq V^2, |I| \leq k - 1, \{u_1, u_2\} \in E_G, \{v_1, v_2\} \notin E_H,$$

$$\prod_{(r,s) \in I} X_{rs} \left(X_{u_1v_1} X_{u_2v_2} \right) = 0 \quad \forall I \subseteq V^2, |I| \leq k - 1, \{u_1, u_2\} \notin E_G, \{v_1, v_2\} \in E_H.$$

Next, we linearize the above equations.

$$Y_{I\cup\{(u_1,v_1),(u_2,v_2)\}} = 0 \quad \forall I \subseteq V^2, |I| \le k-1, \{u_1,u_2\} \in E_G, \{v_1,v_2\} \notin E_H, \tag{33}$$

$$Y_{I\cup\{(u_1,v_1),(u_2,v_2)\}} = 0 \quad \forall I \subseteq V^2, |I| \le k-1, \{u_1,u_2\} \notin E_G, \{v_1,v_2\} \in E_H. \tag{34}$$

In tuple notation, these equations are as follows:

$$Y_{\langle u,v\rangle} = 0 \quad \forall u, v \in V^{k+1}, \{u_i,u_j\} \in E_G, \{v_i,v_j\} \notin E_H \text{ for some } 0 \le i < j \le k+1,$$

$$Y_{\langle u,v\rangle} = 0 \quad \forall u, v \in V^{k+1}, \{u_i,u_j\} \notin E_G, \{v_i,v_j\} \in E_H \text{ for some } 0 \le i < j \le k+1.$$

We can write these equations more concisely as follows:

$$Y_{\langle u,v\rangle} = 0 \quad \forall u, v \in V^{k+1}, \quad (G,u) \not\equiv_{\mathcal{C}} (H,v). \tag{35}$$

Note that we are including the implied Eq. (28) in the above set of equations since $(G,u) \equiv_{\mathcal{C}} (H,v)$ implies $u \equiv_{\mathcal{C}} v$. Then, we arrive at the k-th Sherali–Adams extended formulation $\hat{\mathcal{Q}}^k_{G,H}$ as follows:

$$\hat{\mathcal{Q}}^k_{G,H} = \{Y \in \hat{B}^k : Y_{\langle u,v\rangle} = 0 \; \forall u, v \in V^k, (G,u) \not\equiv_{\mathcal{C}} (H,v)\}.$$

Note that we have omitted the variables $Y_{\langle u,v\rangle}$ from $\hat{\mathcal{Q}}^k_{G,H}$ where $|\langle u,v\rangle| = k+1$ since $Y_{\langle u,v\rangle} = 0$ and the variables $Y_{\langle u,v\rangle}$ do not appear in the Birkhoff polytope $\hat{B}^k$.

Note that trivially $(G,u) \not\equiv_{\mathcal{C}} (H,v)$ for all $u, v \in V$. Thus, $\hat{\mathcal{Q}}^1_{G,H} = \hat{B}^1$, so the first iteration is not interesting.

The kth Sherali–Adams relaxations of the Δ polytopes $\mathcal{Q}_G$ and $\mathcal{Q}_{G,H}$ are then the polytopes $\mathcal{Q}^k_G \subseteq B$ and $\mathcal{Q}^k_{G,H} \subseteq B$ respectively defined as the projection of $\hat{\mathcal{Q}}^k_G$ and $\hat{\mathcal{Q}}^k_{G,H}$ onto B respectively. Lastly, if $\mathcal{Q}^k_G = \{\mathcal{I}_n\}$, then $|AUT(G)| = 1$ and if $\mathcal{Q}^k_{G,H} = \emptyset$, then $ISO(G,H) = \emptyset$.

3.4. Comparison of polyhedra

In this section, we prove Lemma 1.3, which states that $Q^{k+1}_{G,H} \subseteq \mathcal{T}^k_{G,H} \subseteq Q^k_{G,H}$. First, we show that $\mathcal{T}^k_{G,H} \subseteq Q^k_{G,H}$, which is implied by the next lemma and corollary.

Lemma 3.2. *Let $G, H \in \mathcal{G}$, and ket $Y \in \hat{\mathcal{T}}^k_{G,H}$. Then, $Y_{\langle u,v\rangle} = 0$ for all $u, v \in V^k$ where $(G,u) \not\equiv_{\mathcal{C}} (H,v)$.*

Proof. Let $u_1, u_2, v_1 \in V$ such that $\{u_1,u_2\} \notin E_G$, and let $I \subseteq V^2$ where $|I| \le k-2$. Then, from Eq. (29), we have

$$\sum_{w\in\delta_H(v_1)} Y_{I\cup\{(u_1,v_1),(u_2,w)\}} - \sum_{w\in\delta_G(u_2)} Y_{I\cup\{(u_1,v_1),(w,v_1)\}} = \sum_{w\in\delta_H(v_1)} Y_{I\cup\{(u_1,v_1),(u_2,w)\}} = 0.$$

The first equality follows since $Y_{I\cup\{(u_1,v_1),(w,v_1)\}} = 0$ for all $w \in \delta_G(u_2)$ from Eq. (28) since $u_1 \notin \delta_G(u_2)$. Thus, it follows that $Y_{I\cup\{(u_1,v_1),(u_2,w)\}} = 0$ for all $w \in \delta_H(v_1)$.

Similarly, let $u_1, v_1, v_2 \in V$ such that $\{v_1,v_2\} \notin E_G$, and let $I \subseteq V^2$ where $|I| \le k-2$. Then, from Eq. (29), we have

$$\sum_{w\in\delta_H(v_2)} Y_{I\cup\{(u_1,v_1),(u_1,w)\}} - \sum_{w\in\delta_G(u_1)} Y_{I\cup\{(u_1,v_1),(w,v_2)\}} = -\sum_{w\in\delta_G(u_1)} Y_{I\cup\{(u_1,v_1),(w,v_2)\}} = 0.$$

The first equality follows since $Y_{I\cup(u_1,v_1)(u_1,w)} = 0$ for all $w \in \delta_H(v_2)$ from Eq. (28) since $v_1 \notin \delta_G(v_2)$. Thus, it follows that $Y_{I\cup\{(u_1,v_1),(w,v_2)\}} = 0$ for all $w \in \delta_G(u_1)$ as required. $\square$

The corollary below then follows directly from the definition of $\hat{\mathcal{Q}}^k_{G,H}$ and $\hat{\mathcal{T}}^k_{G,H}$.

Corollary 3.3. *Let $G, H \in \mathcal{G}$. We have $\hat{\mathcal{T}}^k_{G,H} \subseteq \hat{\mathcal{Q}}^k_{G,H}$, and $\mathcal{T}^k_{G,H} \subseteq \mathcal{Q}^k_{G,H}$.*

We now show that $Q^{k+1}_{G,H} \subseteq \mathcal{T}^k_{G,H}$, which is implied by the following lemma. First, let $\rho : \hat{B}^{k+1} \to \hat{B}^k$ be the projection of $\hat{B}^{k+1}$ onto $\hat{B}^k$, that is, for $Y \in \hat{B}^{k+1}$, we define $\rho(Y) \in \hat{B}^k$ where $\rho(Y)_I = Y_I$ for all $|I| \le k$.

Lemma 3.4. *Let $G, H \in \mathcal{G}$. We have $\rho(\hat{\mathcal{Q}}^{k+1}_{G,H}) \subseteq \hat{\mathcal{T}}^k_{G,H}$.*

Proof. Let $Y \in Q^{k+1}_{G,H}$. Then, for all $u, v \in V$ and $I \subseteq V^2$ where $|I| \le k-1$, we have

$$\begin{aligned}
\sum_{w\in\delta_H(v)} Y_{I\cup\{(u,w)\}} &= \sum_{w\in\delta_H(v)} \sum_{w'\in V} Y_{I\cup\{(u,w),(w'v)\}} \\
&= \sum_{w\in\delta_H(v)} \sum_{w'\in\delta_G(u)} Y_{I\cup\{(u,w),(w'v)\}} \\
&= \sum_{w\in V} \sum_{w'\in\delta_G(u)} Y_{I\cup\{(u,w),(w',v)\}} = \sum_{w'\in\delta_G(u)} Y_{I\cup\{(w'v)\}}.
\end{aligned}$$

The first and last equalities are valid for $\hat{B}^{k+1}_{G,H}$ and follow from Eqs. (14) and (15) respectively. The second equality is valid for $\hat{\mathcal{Q}}^{k+1}_{G,H}$ and follows since $Y_{I\cup\{(u,w),(w'v)\}} = 0$ for all $w \in \delta_H(v)$ and $w' \in \bar{\delta}_G(u)$ from Eq. (34), and similarly, the third equality is valid for $\hat{\mathcal{Q}}^{k+1}_{G,H}$ and follows since $Y_{I\cup\{(u,w),(w'v)\}} = 0$ for all $w \in \bar{\delta}_H(v)$ and $w' \in \delta_G(u)$ from Eq. (33). Thus, $\rho(Y) \in \hat{\mathcal{T}}^k_{G,H}$ as required. $\square$

4. Comparison of combinatorial and polyhedral approaches

In this section, we compare the combinatorial algorithm with the polyhedral approach of using Sherali–Adams relaxations.

In order to compare the combinatorial and polyhedral approaches, we introduce *partition polytopes*, which are a natural polyhedral analogue of vertex partitions. Given a partition $\pi \in \Pi^k$ and a polytope $P \subseteq \hat{B}^k$, we define the *partition polytope of* P with respect to π, written $P(\pi)$, as the following polytope:

$$P(\pi) = \{Y \in P : Y_{\langle u,v\rangle} = 0\ \forall u, v \in V^k, u \not\equiv_\pi v\}.$$

Similarly, given ordered partitions $\vec{\pi}$ and $\vec{\tau}$ and a polytope $P \subseteq \hat{B}^k$, we define the *partition polytope of* P with respect to $\vec{\pi}$ and $\vec{\tau}$, written $P(\vec{\pi}, \vec{\tau})$, as the following polytope:

$$P(\vec{\pi}, \vec{\tau}) = \{Y \in P : Y_{\langle u,v\rangle} = 0\ \forall u, v \in V^k, [u]_{\vec{\pi}} \neq [v]_{\vec{\tau}}\}.$$

We call the important partition polytopes $\hat{B}^k(\pi)$ and $\hat{B}^k(\vec{\pi}, \vec{\tau})$ as the *Birkhoff partition polytopes.* There is natural bijection between integer points in $\hat{B}^k(\pi)$ set of bijections $\psi : V \to V$ such that $\psi(\pi_i) = \pi_i$ for all $\pi_i \in \pi$, and similarly, there is a natural bijection between the integer points in $\hat{B}^k(\vec{\pi}, \vec{\tau})$ and set of bijections $\psi : V \to V$ such that $\psi(\vec{\pi}) = \vec{\tau}$.

Note that we have $\hat{B}^k(\mathcal{C}^k_G) = \hat{\mathcal{Q}}^k_G$ and if $(G, \vec{\mathcal{C}}^k_G) \equiv_{\vec{\mathcal{C}}} (H, \vec{\mathcal{C}}^k_H)$, then $\hat{B}^k(\vec{\mathcal{C}}^k_G, \vec{\mathcal{C}}^k_H) = \hat{\mathcal{Q}}^k_{G,H}$ by construction.

Using the concept of partition polytopes, we can give a precise definition of when a polytope can be considered to contain the same combinatorial information as a V-C equivalence relation.

Definition 4.1. Let $G \in \mathcal{G}$. We say that a given polyhedron $P \subseteq \hat{B}^k$ and a V-C equivalence relation α are *combinatorially equivalent* with respect to G if for all $\pi \in \Pi^k$and for all $u, v \in V^k$, we have $(G, \alpha^*_G(\pi), u) \not\equiv_\alpha (G, \alpha^*_G(\pi), v)$ if and only if $Y_{\langle u,v\rangle} = 0$ for all $Y \in P(\pi)$.

It follows immediately from the definition that if P and α are combinatorially equivalent, then $P(\pi) = P(\alpha^*_G(\pi))$. Also, as shown in the lemma below, if P is combinatorially equivalent to α, then crucially $\vec{\alpha}^*_G(\pi)$ is complete if and only if $P(\pi) = \{\hat{\mathcal{I}}^k_n\}$ or equivalently $\rho^k(P(\pi)) = \{\mathcal{I}_n\}$ where $\rho^k : \hat{B}^k \to B$ is a projective map. Here, $\hat{\mathcal{I}}^k_n$ is the extended identity matrix where for all $u, v \in V^k$, we have $\hat{\mathcal{I}}^k_{n,\langle u,v\rangle} = 1$ if $u = v$ and 0 otherwise.

Lemma 4.2. *Let $P \subseteq \hat{B}^k$ and let α be a V-C equivalence relation. If P and α are combinatorially equivalent, then for all $\pi \in \Pi^k$, we have $\alpha^*_G(\pi)$ is complete if and only if $P(\pi) = \{\hat{\mathcal{I}}^k_n\}$ or equivalently $\rho^k(P(\pi)) = \{\mathcal{I}_n\}$.*

Proof. First, let $Y \in P(\pi)$ such that $Y_{\langle u,v\rangle} = 0$ if and only if $u \neq v$ for all $u, v \in V^k$. Then, from Eq. (26), we must have $Y_{\langle u,u\rangle} = 1$ for all $u \in V^k$, and so, $Y = \hat{\mathcal{I}}^k_n$. Now, assume that $\alpha^*_G(\pi)$ is complete. We must have $P(\pi) \neq \emptyset$ since $Y_{\langle u,u\rangle} \neq 0$ for some $Y \in P(\pi)$ and $u \in V^k$ from the definition of combinatorial equivalence. Then, for all $Y \in P(\pi)$, we have $Y_{\langle u,v\rangle} = 0$ if and only if $u \neq v$ for all $u, v \in V^k$, but this implies $Y = \hat{\mathcal{I}}^k_n$ for all $Y \in P(\pi)$ from above, and thus, $P(\pi) = \{\hat{\mathcal{I}}^k_n\}$. Second, assume $|P(\pi)| > 1$. Then, there must exist a $Y \in P(\pi)$ such that $Y_{\langle u,v\rangle} \neq 0$ for some $u \neq v$ (otherwise there is only one possible $Y \in P(\pi)$ from above). Thus, $(G, \alpha^*_G(\pi), u) \equiv_\alpha (G, \alpha^*_G(\pi), v)$, and $\alpha^*_G(\pi)$ is not complete.

Lastly, we show that $P(\pi) = \{\hat{\mathcal{I}}^k_n\}$ if and only if $\rho^k(P(\pi)) = \{\mathcal{I}_n\}$. The forward implication is clear, so we prove the converse. Assume $\rho^k(P(\pi)) = \{\mathcal{I}_n\}$, and let $Y \in P(\pi)$. Then, $\rho^k(P(\pi)) = \{\mathcal{I}_n\}$ implies that for all $u, v \in V^k$ where $|\langle u, v\rangle| = 1$, we have $Y_{\langle u,v\rangle} = 1$ if $u = v$ and $Y_{\langle u,v\rangle} = 0$ otherwise. By Lemma A.15, we have $Y_{\langle u,v\rangle} = 0$ for all $u, v \in V^k$ where $|\langle u, v\rangle| \geq 2$ and $u \neq v$ since there must exist $u', v' \in V^k$ where $\langle u', v'\rangle \subseteq \langle u, v\rangle$, $u' \neq v'$, $|\langle u', v'\rangle| = 1$ and $Y_{\langle u',v'\rangle} = 0$. $\square$

We now extend the definition of combinatorial equivalence to V-C preorders.

Definition 4.3. Let $G, H \in \mathcal{G}$. We say that a given polyhedron $P \subseteq \hat{B}^k$ and a V-C preorder $\vec{\alpha}$ are *combinatorially equivalent* with respect to (G, H) if for all $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ and for all $u, v \in V^k$, we have

1. if $(G, \vec{\pi}, u) \not\equiv_{\vec{\alpha}} (H, \vec{\tau}, v)$, then $Y_{\langle u,v\rangle} = 0$ for all $Y \in P(\vec{\pi}, \vec{\tau})$; and
2. if $(G, \vec{\pi}) \equiv_{\vec{\alpha}^*} (H, \vec{\tau})$, then $P(\vec{\pi}, \vec{\tau}) \neq \emptyset$, and moreover, if $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (H, \vec{\tau}, v)$, then there exists $Y \in P(\vec{\pi}, \vec{\tau})$ such that $Y_{\langle u,v\rangle} \neq 0$.

We show below that if P and $\vec{\alpha}$ are combinatorially equivalent, then $(G, \vec{\pi}) \not\equiv_{\vec{\alpha}} (H, \vec{\pi})$ implies $P(\vec{\pi}, \vec{\tau}) = \emptyset$, and moreover, if $\vec{\pi} \approx \vec{\tau}$, then $P(\vec{\pi}, \vec{\tau}) = P(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_G(\vec{\pi}))$. Thus, it follows immediately that if $\vec{\pi} \approx \vec{\tau}$, then $P(\vec{\pi}, \vec{\tau}) = \emptyset$ if and only if $(G, \vec{\alpha}^*_G(\vec{\pi})) \not\equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_G(\vec{\pi}))$ and $(G, \vec{\alpha}^*_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}))$ implies $(G, \vec{\alpha}^*_G(\vec{\pi}), u) \not\equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}), v)$ if and only if $Y_{\langle u,v\rangle} = 0$ for all $Y \in P(\vec{\pi}, \vec{\tau})$ and $u, v \in V^k$. So, if P and $\vec{\alpha}$ are combinatorially equivalent, then the polytope and the partition contain the same combinatorial information in some sense. Also, if $\vec{\alpha}$ and P are combinatorially equivalent, then it follows that α (the induced V-C equivalence relation) and P are also combinatorially equivalent.

We now show some useful properties of combinatorial equivalence. First, we show that if P and $\vec{\alpha}$ are combinatorially equivalent, then $(G, \vec{\pi}) \not\equiv_{\vec{\alpha}} (H, \vec{\pi})$ implies $P(\vec{\pi}, \vec{\tau}) = \emptyset$.

Lemma 4.4. *Let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ such that for all $u, v \in V^k$, if $(G, \vec{\pi}, u) \not\equiv_{\vec{\alpha}} (H, \vec{\tau}, v)$, then $Y_{\langle u,v\rangle} = 0$ for all $Y \in P(\vec{\pi}, \vec{\tau})$. If $(G, \vec{\pi}) \not\equiv_{\vec{\alpha}} (H, \vec{\tau})$, then $P(\vec{\pi}, \vec{\tau}) = \emptyset$.*

Proof. Since $(G, \vec{\pi}) \not\equiv_{\vec{\alpha}} (H, \vec{\tau})$, there exists $\hat{u} \in V^k$ such that $|U| \neq |W|$ where

$$U = \{w \in V^k : (G, \vec{\pi}, w) \equiv_{\vec{\alpha}} (G, \vec{\pi}, \hat{u})\} \quad \text{and} \quad W = \{w \in V^k : (H, \vec{\tau}, w) \equiv_{\vec{\alpha}} (G, \vec{\pi}, \hat{u})\}.$$

Note that $(G, \vec{\pi}, u) \equiv_{\vec{\alpha}} (H, \vec{\tau}, v)$ for all $u \in U$ and $v \in W$. Now, from (26), for all $u \in U$, we have $\sum_{v \in V^k} Y_{\langle u,v\rangle} = 1$ implying $\sum_{v \in W} Y_{\langle u,v\rangle} = 1$ since for all $v \notin W$, we have $(G, \vec{\pi}, u) \not\equiv_{\vec{\alpha}} (H, \vec{\tau}, v)$ implying that $Y_{\langle u,v\rangle} = 0$. Similarly, from (27), for all $v \in W$, we have that $\sum_{u \in V^k} Y_{\langle u,v\rangle} = 1$ implying $\sum_{u \in U} Y_{\langle u,v\rangle} = 1$. Then,

$$|U| = \sum_{u \in U} 1 = \sum_{u \in U} \left(\sum_{v \in W} Y_{\langle u,v\rangle} \right) = \sum_{v \in W} \left(\sum_{u \in U} Y_{\langle u,v\rangle} \right) = \sum_{v \in W} 1 = |W|.$$

Thus, $|U| = |W|$, which is a contradiction. □

The next two lemmas show that if P and $\vec{\alpha}$ are combinatorially equivalent and $\vec{\pi} \approx \vec{\tau}$, then $P(\vec{\pi}, \vec{\tau}) = P(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_G(\vec{\pi}))$.

Lemma 4.5. *Let $P \subseteq \hat{B}^k$ and let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ such that for all $u, v \in V^k$, if $(G, \vec{\pi}, u) \not\equiv_{\vec{\alpha}} (H, \vec{\tau}, v)$, then $Y_{\langle u,v\rangle} = 0$ for all $Y \in P(\vec{\pi}, \vec{\tau})$. If $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$, then $P(\vec{\pi}, \vec{\tau}) = P(\vec{\alpha}_G(\vec{\pi}), \vec{\alpha}_H(\vec{\tau}))$.*

Proof. Firstly, recall that $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$ implies that $(\vec{\pi}, \vec{\tau}) \geq (\vec{\alpha}_G(\vec{\pi}), \vec{\alpha}_H(\vec{\tau}))$ meaning that $[u]_{\vec{\pi}} \neq [v]_{\vec{\tau}} \Rightarrow [u]_{\vec{\alpha}_G(\vec{\pi})} \neq [v]_{\vec{\alpha}_H(\vec{\tau})}$, and thus, $P(\vec{\pi}, \vec{\tau}) \supseteq P(\vec{\alpha}_G(\vec{\pi}), \vec{\alpha}_H(\vec{\tau}))$. Secondly, $(G, \vec{\pi}) \equiv_{\vec{\alpha}} (H, \vec{\tau})$ means that $[u]_{\vec{\alpha}_G(\vec{\pi})} \neq [v]_{\vec{\alpha}_H(\vec{\tau})} \Leftrightarrow (G, \vec{\pi}, u) \not\equiv_{\vec{\alpha}} (G, \vec{\tau}, v)$, and thus, $P(\vec{\pi}, \vec{\tau}) \subseteq P(\vec{\alpha}_G(\vec{\pi}), \vec{\alpha}_H(\vec{\tau}))$ as required. □

Lemma 4.6. *Let $P \subseteq \hat{B}^k$ and let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$ such that for all $u, v \in V^k$, if $(G, \vec{\pi}, u) \not\equiv_{\vec{\alpha}} (H, \vec{\tau}, v)$, then $Y_{\langle u,v\rangle} = 0$ for all $Y \in P(\vec{\pi}, \vec{\tau})$. We have $P(\vec{\pi}, \vec{\tau}) = P(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_H(\vec{\tau}))$.*

Proof. First, assume $(G, \vec{\alpha}^*_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}))$. Then, by Corollary A.2, we have $(G, \vec{\alpha}^r_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^r_H(\vec{\tau}))$ for all r implying that $P(\vec{\alpha}^r_G(\vec{\pi}), \vec{\alpha}^r_H(\vec{\tau})) = P(\vec{\alpha}^{r+1}_G(\vec{\pi}), \vec{\alpha}^{r+1}_H(\vec{\tau}))$ for all r by Lemma 4.5 above, and therefore, $P(\vec{\pi}, \vec{\tau}) = P(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_H(\vec{\tau}))$.

Second, assume $(G, \vec{\alpha}^*_G(\vec{\pi})) \not\equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}))$. Then, by Lemma 4.4, we have $P(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_H(\vec{\tau})) = \emptyset$. Now, there exists an r' such that $(G, \vec{\alpha}^r_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^r_H(\vec{\tau}))$ for all $r < r'$, and $(G, \vec{\alpha}^r_G(\vec{\pi})) \not\equiv_{\vec{\alpha}} (H, \vec{\alpha}^r_H(\vec{\tau}))$. Thus, from Lemma 4.5, we have $P(\vec{\pi}, \vec{\tau}) = P(\vec{\alpha}^r_G(\vec{\pi}), \vec{\alpha}^r_H(\vec{\tau}))$, but $P(\vec{\alpha}^r_G(\vec{\pi}), \vec{\alpha}^r_H(\vec{\tau})) = \emptyset$ from Lemma 4.4, and therefore, $P(\vec{\pi}, \vec{\tau}) = P(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_H(\vec{\tau}))$. □

In the remainder of this section, we will show the combinatorial equivalence of the V-C preorders and polyhedra we have seen previously.

4.1. The Δ-V-C algorithm and the Δ-polytope

In this section, we prove the result that Δ is combinatorially equivalent to $\hat{\mathcal{Q}}^k_G$, and also that $\vec{\Delta}$ is combinatorially equivalent to $\hat{\mathcal{Q}}^k_{G,H}$. Specifically, we have that Δ^k_G is complete if and only if $\hat{\mathcal{Q}}^{k+1}_G = \{\hat{\mathcal{I}}^k_n\}$ or equivalently $\mathcal{Q}^{k+1}_G = \{\mathcal{I}_n\}$, we have $(G, \vec{\Delta}^k_G) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^k_H)$ if and only if $\hat{\mathcal{Q}}^k_{G,H} \neq \emptyset$ or equivalently $\mathcal{Q}^k_{G,H} \neq \emptyset$.

We now show that $\vec{\Delta}$ and $\hat{\mathcal{Q}}^k$ satisfy the two conditions of Definition 4.3.

Lemma 4.7. *Let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$. For all $u, v \in V^k$, if $(G, \vec{\pi}, u) \not\equiv_{\vec{\Delta}} (H, \vec{\tau}, v)$, then $Y_{\langle u,v\rangle} = 0$ for all $Y \in \hat{\mathcal{Q}}^k(\vec{\pi}, \vec{\tau})$.*

Proof. First, if $(G, \vec{\pi}, u) \not\equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$, then clearly $Y_{\langle u,v\rangle} = 0$ for all $Y \in \hat{\mathcal{T}}^k_{G,H}(\vec{\pi}, \vec{\tau})$, so we assume that $(G, \vec{\pi}, u) \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$. Then, $(\vec{\pi}, u) \not\equiv_{\Delta} (\vec{\tau}, v)$ means that $|\Delta^i(u) \cap \vec{\pi}_t| \neq |\Delta^i(v) \cap \vec{\tau}_t|$ for some $1 \leq t \leq m$ and $1 \leq i \leq k$.

First, we derive some valid equations for $\hat{\mathcal{Q}}^k_{G,H}(\vec{\pi}, \vec{\tau})$. Now, for all $1 \leq s, t \leq m$, $1 \leq i \leq k$ and $u \in \vec{\pi}_s$, we have the following valid equation derived immediately from Eqs. (22) and (23):

$$\begin{aligned}
&\sum_{v\in\vec{\tau}_t}\left(\sum_{w\in\Delta^i(v)} Y_{\langle u,w\rangle} - \sum_{w\in\Delta^i(u)} Y_{\langle w,v\rangle}\right) = 0\\
&\Rightarrow \sum_{v\in\vec{\tau}_t}\sum_{w\in\Delta^i(v)\cap\vec{\tau}_s} Y_{\langle u,w\rangle} - \sum_{v\in\vec{\tau}_t}\sum_{w\in\Delta^i(u)\cap\vec{\pi}_t} Y_{\langle w,v\rangle} = 0\\
&\Rightarrow \sum_{w\in\vec{\tau}_s}\sum_{v\in\Delta^i(w)\cap\vec{\tau}_t} Y_{\langle u,w\rangle} - \sum_{w\in\Delta^i(u)\cap\vec{\pi}_t}\sum_{v\in\vec{\tau}_t} Y_{\langle w,v\rangle} = 0\\
&\Rightarrow \sum_{w\in\vec{\tau}_s} |\Delta^i(w)\cap\vec{\tau}_t| Y_{\langle u,w\rangle} - \sum_{w\in\Delta^i(u)\cap\vec{\pi}_t} 1 = 0\\
&\Rightarrow \sum_{w\in\vec{\tau}_s} |\Delta^i(w)\cap\vec{\tau}_t| Y_{\langle u,w\rangle} - |\Delta^i(u)\cap\vec{\pi}_t| = 0\\
&\Rightarrow \sum_{w\in\vec{\tau}_s} |\Delta^i(w)\cap\vec{\tau}_t| Y_{\langle u,w\rangle} - |\Delta^i(u)\cap\vec{\pi}_t| \sum_{w\in\vec{\tau}_s} Y_{\langle u,w\rangle} = 0\\
&\Rightarrow \sum_{w\in\vec{\tau}_s} \left(|\Delta^i(w)\cap\vec{\tau}_t| - |\Delta^i(u)\cap\vec{\pi}_t|\right) Y_{\langle u,w\rangle} = 0. \qquad (36)
\end{aligned}$$

Similarly, swapping the role of $\vec{\pi}$ and $\vec{\tau}$, for all $1 \le s, t \le m$, $1 \le i \le k$ and $v \in \vec{\tau}_s$, we have the following valid equation:

$$\begin{aligned}
&\sum_{u\in\vec{\pi}_t}\left(\sum_{w\in\Delta^i(v)} Y_{\langle u,w\rangle} - \sum_{w\in\Delta^i(u)} Y_{\langle w,v\rangle}\right) = 0\\
&\Rightarrow \sum_{w\in\vec{\pi}_s} \left(|\Delta^i(w)\cap\vec{\pi}_t| - |\Delta^i(v)\cap\vec{\tau}_t|\right) Y_{\langle w,v\rangle} = 0. \qquad (37)
\end{aligned}$$

Using the above Eqs. (36) and (37) and the inequalities that $Y_{\langle u,v\rangle} \ge 0$ for all $u, v \in V^k$, we can conclude that $Y_{\langle u,v\rangle} = 0$ for all $u \in \vec{\pi}_s$ and $v \in \vec{\tau}_s$ where $|\Delta^i(u)\cap\vec{\pi}_t| \ne |\Delta^i(v)\cap\vec{\tau}_t|$ for some $1 \le t \le m$ and $1 \le i \le k$. This requires some further argument as follows.

We will proceed by induction. Let $M \in \mathbb{N}^n$. Assume that $Y_{\langle u,v\rangle} = 0$ for all $u, v \in V^k$ such that $|\Delta^i(u)\cap\vec{\pi}_t| \ne |\Delta^i(v)\cap\vec{\tau}_t|$ and $|\Delta^i(u)\cap\vec{\pi}_t|, |\Delta^i(v)\cap\vec{\tau}_t| \le M$. This is true for $M = 0$, so let us assume it is true for M, and we show it is true $M+1$.

Let $1 \le s \le m$, $u \in \vec{\pi}_s$ and $v \in \vec{\tau}_s$ such that $|\Delta^i(u)\cap\vec{\pi}_t| \ne |\Delta^i(v)\cap\vec{\tau}_t|$ and $|\Delta^i(u)\cap\vec{\pi}_t|, |\Delta^i(v)\cap\vec{\tau}_t| \le M+1$. First, assume that $|\Delta^i(u)\cap\vec{\pi}_t| < |\Delta^i(v)\cap\vec{\tau}_t|$. Then, by Eq. (36), we have

$$\sum_{w\in\vec{\tau}_s} \left(|\Delta^i(w)\cap\vec{\tau}_t| - |\Delta^i(u)\cap\vec{\pi}_t|\right) Y_{\langle u,w\rangle} = 0.$$

Now, by assumption, $Y_{\langle u,w\rangle} = 0$ for all $w \in \vec{\tau}_s$ where $|\Delta^i(w)\cap\vec{\tau}_t| < |\Delta^i(u)\cap\vec{\pi}_t|$; thus, after eliminating those variables, the equation above becomes a sum of non-negative variables with non-negative coefficients implying that each variable with a positive coefficient is 0, and in particular, $Y_{\langle u,v\rangle} = 0$. Second, assume that $|\Delta^i(v)\cap\vec{\tau}_t| < |\Delta^i(u)\cap\vec{\pi}_t|$. Then, similarly, using Eq. (37), we have $Y_{\langle u,v\rangle} = 0$. $\square$

Next, we show that using the partitions $\vec{\pi}$ and $\vec{\tau}$ where $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$, then we can construct a feasible solution $Y \in \hat{\mathcal{Q}}^k_{G,H}(\vec{\pi}, \vec{\tau})$ such that $Y_{\langle u,v\rangle} > 0$ if and only if $(G, \vec{\pi}, u) \equiv_{\vec{\Delta}} (H, \vec{\tau}, v)$.

Lemma 4.8. *Let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$. Then, $\hat{\mathcal{Q}}^k_{G,H}(\vec{\pi}, \vec{\tau}) \ne \emptyset$, and more specifically, $Y \in \hat{\mathcal{Q}}^k_{G,H}(\vec{\pi}, \vec{\tau})$ where $Y_\emptyset = 1$ and for all $u, v \in V^k$, $Y_{\langle u,v\rangle} = |\vec{\pi}_s|^{-1} = |\vec{\tau}_s|^{-1}$ if $[u]_{\vec{\pi}} = [v]_{\vec{\tau}} = s$ and $Y_{\langle u,v\rangle} = 0$ otherwise.*

Proof. First, we need to show that Y is well-defined meaning that for all $u \in \vec{\pi}_s$, $v \in \vec{\tau}_t$, $u' \in \vec{\pi}_{s'}$, $v' \in \vec{\tau}_{t'}$ where $\langle u, v\rangle = \langle u', v'\rangle$, if $s = t$, then $s' = t'$ and $|\vec{\pi}_s| = |\vec{\pi}_{s'}| = |\vec{\tau}_t| = |\vec{\tau}_{t'}|$, otherwise if $s \ne t$, then $s' \ne t'$. See Corollary A.14 for a proof of this.

Clearly, by definition, Y satisfies the constraints (35), (24) and (25), so we must show that Y satisfies Eqs. (22) and (23). Consider the two k-tuples $u \in \vec{\pi}_s$ and $v \in \vec{\tau}_t$. Then,

$$\sum_{w\in\Delta^i(v)} Y_{\langle u,w\rangle} = \sum_{w\in\Delta^i(v)\cap\vec{\tau}_s} Y_{\langle u,w\rangle} = \sum_{w\in\Delta^i(v)\cap\vec{\tau}_s} |\vec{\tau}_s|^{-1} = |\Delta^i(v)\cap\vec{\tau}_s||\vec{\tau}_s|^{-1}$$

and

$$\sum_{w\in\Delta^i(u)} Y_{\langle w,v\rangle} = \sum_{w\in\Delta^i(u)\cap\vec{\pi}_t} Y_{\langle w,v\rangle} = \sum_{w\in\Delta^i(u)\cap\vec{\pi}_t} |\vec{\pi}_t|^{-1} = |\Delta^i(u)\cap\vec{\pi}_t||\vec{\pi}_t|^{-1}.$$

Let $u' = \phi_i(u, u_j) = (u_1, \ldots, u_{i-1}, u_j, u_{i+1}, \ldots, u_k)$ and let $v' = \phi_i(v, v_j) = (v_1, \ldots, v_{i-1}, v_j, v_{i+1}, \ldots, v_k)$, and let $1 \le s', t' \le m$ where $u' \in \vec{\pi}_{s'}$ and $v' \in \vec{\tau}_{t'}$. Then, $Y_{\langle u,v\rangle \setminus \{(u_i,v_i)\}} = Y_{\langle u',v'\rangle}$, and $Y_{\langle u',v'\rangle} = |\vec{\tau}_{t'}|^{-1} = |\vec{\pi}_{s'}|^{-1}$ if $s' = t'$ and $Y_{\langle u',v'\rangle} = 0$ otherwise. Thus, in order to show that Eqs. (22) and (23) are satisfied, we must show that, if $s' = t'$, then $|\Delta^i(u) \cap \vec{\pi}_t||\vec{\pi}_t|^{-1} = |\vec{\pi}_{s'}|^{-1}$ and $|\Delta^i(v) \cap \vec{\tau}_s||\vec{\tau}_s|^{-1} = |\vec{\tau}_{s'}|^{-1}$, and if $s' \ne t'$, then $|\Delta^i(u) \cap \vec{\pi}_t| = 0$ and $|\Delta^i(v) \cap \vec{\tau}_s| = 0$.

First, assume that $s' = t'$. By Lemma A.11, we have $|\vec{\pi}_s| = |\Delta^i(u) \cap \vec{\pi}_s||\vec{\pi}_{s'}|$ and $|\vec{\pi}_t| = |\Delta^i(u) \cap \vec{\pi}_t||\vec{\pi}_{t'}|$ as required.

Next, assume $s' \ne t'$. First, let $w \in \Delta^i(v)$. Then, $|\Delta^i(u) \cap \vec{\pi}_{s'}| = |\{u'\}| = 1$, but $|\Delta^i(w) \cap \vec{\tau}_{s'}| = 0$ since $\vec{\tau}_{s'}$ must have the same combinatorial type as $\vec{\pi}_{s'}$ meaning that $u_{i-1} = u_i$ for all $u \in \vec{\tau}_{s'}$ and the only tuple in $\Delta^i(w) = \Delta^i(v)$ of that type is v', but $v' \in \vec{\tau}_{t'}$. So, $[u]_{\vec{\pi}} \ne [w]_{\vec{\tau}}$, and thus, $|\Delta^i(v) \cap \vec{\pi}_t| = 0$. Similarly, let $w' \in \Delta^i(u)$. Then, $|\Delta^i(v) \cap \vec{\tau}_{t'}| = |\{v'\}| = 1$, but $|\Delta^i(w') \cap \vec{\pi}_{s'}| = 0$, and therefore, $[w']_{\vec{\pi}} \ne [v]_{\vec{\tau}}$, and thus, $|\Delta^i(u) \cap \vec{\tau}_s| = 0$ as required. $\square$

4.2. The δ-V-C algorithm and the Tinhofer polytope

In this section, we prove Theorem 1.1 by showing that δ is combinatorially equivalent to $\hat{\mathcal{T}}^k_G$, and also, $\vec{\delta}$ is combinatorially equivalent to $\hat{\mathcal{T}}^k_{G,H}$. Specifically, we have that δ^k_G is complete if and only if $\hat{\mathcal{T}}^{k+1}_G = \{\hat{\mathcal{I}}^k_n\}$ or equivalently $\mathcal{T}^{k+1}_G = \{\mathcal{I}_n\}$, we have $(G, \vec{\delta}^k_G) \equiv_{\vec{\delta}} (H, \vec{\delta}^k_H)$ if and only if $\hat{\mathcal{T}}^k_{G,H} \ne \emptyset$ or equivalently $\mathcal{T}^k_{G,H} \ne \emptyset$ as required for Theorem 1.1. We now show that $\vec{\delta}$ and $\hat{\mathcal{T}}^k_{G,H}$ satisfy the two conditions of Definition 4.3.

Lemma 4.9. *Let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$. For all $u, v \in V^k$, if $(G, \vec{\pi}, u) \not\equiv_{\vec{\delta}} (H, \vec{\tau}, v)$, then $Y_{\langle u,v\rangle} = 0$ for all $Y \in \hat{\mathcal{T}}^k_{G,H}(\vec{\pi}, \vec{\tau})$.*

Proof. The proof of this lemma is analogous to the proof of Lemma 4.9. First, if $(G, \vec{\pi}, u) \not\equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$, then clearly $Y_{\langle u,v\rangle} = 0$ for all $Y \in \hat{\mathcal{T}}^k_{G,H}(\vec{\pi}, \vec{\tau})$, so we assume that $(G, \vec{\pi}, u) \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}, v)$. Then, $(G, \vec{\pi}, u) \not\equiv_{\delta} (H, \vec{\tau}, v)$ means that $|\delta^i_G(u) \cap \vec{\pi}_t| \ne |\delta^i_H(v) \cap \vec{\tau}_t|$ or $|\bar{\delta}^i_G(u) \cap \vec{\pi}_t| \ne |\bar{\delta}^i_H(v) \cap \vec{\tau}_t|$ for some $1 \le t \le m$ and $1 \le i \le k$.

First, we derive some valid equations for $P(\vec{\pi}, \vec{\tau})$. Now, for all $1 \le s, t \le m$, $1 \le i \le k$ and $u \in \vec{\pi}_s$, we have the following valid equation:

$$\begin{aligned}
&\sum_{v \in \vec{\tau}_t} \left(\sum_{w \in \delta^i_H(v)} Y_{\langle u,w\rangle} - \sum_{w \in \delta^i_G(u)} Y_{\langle w,v\rangle} \right) = 0 \\
&\Rightarrow \sum_{v \in \vec{\tau}_t} \sum_{w \in \delta^i_H(v) \cap \vec{\tau}_s} Y_{\langle u,w\rangle} - \sum_{v \in \vec{\tau}_t} \sum_{w \in \delta^i_G(u) \cap \vec{\pi}_t} Y_{\langle w,v\rangle} = 0 \\
&\Rightarrow \sum_{w \in \vec{\tau}_s} \sum_{v \in \delta^i_H(w) \cap \vec{\tau}_t} Y_{\langle u,w\rangle} - \sum_{w \in \delta^i_G(u) \cap \vec{\pi}_t} \sum_{v \in \vec{\tau}_t} Y_{\langle w,v\rangle} = 0 \\
&\Rightarrow \sum_{w \in \vec{\tau}_s} |\delta^i_H(w) \cap \vec{\tau}_t| Y_{\langle u,w\rangle} - \sum_{w \in \delta^i_G(u) \cap \vec{\pi}_t} 1 = 0 \\
&\Rightarrow \sum_{w \in \vec{\tau}_s} |\delta^i_H(w) \cap \vec{\tau}_t| Y_{\langle u,w\rangle} - |\delta^i_G(u) \cap \vec{\pi}_t| = 0 \\
&\Rightarrow \sum_{w \in \vec{\tau}_s} |\delta^i_H(w) \cap \vec{\tau}_t| Y_{\langle u,w\rangle} - |\delta^i_G(u) \cap \vec{\pi}_t| \sum_{w \in \vec{\tau}_s} Y_{\langle u,w\rangle} = 0 \\
&\Rightarrow \sum_{w \in \vec{\tau}_s} \left(|\delta^i_H(w) \cap \vec{\tau}_t| - |\delta^i_G(u) \cap \vec{\pi}_t| \right) Y_{\langle u,w\rangle} = 0.
\end{aligned} \tag{38}$$

Similarly, swapping the role of G and H, and $\vec{\pi}$ and $\vec{\tau}$, we have the following valid equation for all $1 \le s, t \le m$, $1 \le i \le k$ and $v \in \vec{\tau}_s$:

$$\begin{aligned}
&\sum_{u \in \vec{\pi}_t} \left(\sum_{w \in \delta^i_H(v)} Y_{\langle u,w\rangle} - \sum_{w \in \delta^i_G(u)} Y_{\langle w,v\rangle} \right) = 0 \\
&\Rightarrow \sum_{w \in \vec{\pi}_s} \left(|\delta^i_G(w) \cap \vec{\pi}_t| - |\delta^i_H(v) \cap \vec{\tau}_t| \right) Y_{\langle w,v\rangle} = 0.
\end{aligned} \tag{39}$$

Using the above Eqs. (38) and (39) and the inequalities that $Y_{\langle u,v\rangle} \ge 0$ for all $u, v \in V^k$, we can conclude that $Y_{\langle u,v\rangle} = 0$ for all $u \in \vec{\pi}_s$ and $v \in \vec{\tau}_s$ where $|\delta^i_G(u) \cap \vec{\pi}_t| \ne |\delta^i_H(v) \cap \vec{\tau}_t|$ for some $1 \le t \le m$ and $1 \le i \le k$. This requires an argument by induction that is analogous to the argument in the proof of Lemma 4.7 by replacing Δ with δ_G.

Next, we prove that $Y_{\langle u,v\rangle} = 0$ for all $u \in \vec{\pi}_s$ and $v \in \vec{\tau}_s$ where $|\bar{\delta}^i_G(u) \cap \vec{\pi}_t| \ne |\bar{\delta}^i_H(v) \cap \tau_t|$ for some $1 \le t \le m$ and $1 \le i \le k$. First, using Eqs. (30), (26) and (27), we have

$$\sum_{w\in\delta^i_H(v)} Y_{\langle u,w\rangle} - \sum_{w\in\delta^i_G(u)} Y_{\langle w,v\rangle} = 0 \Rightarrow \sum_{w\in\bar{\delta}^i_H(v)} Y_{\langle u,w\rangle} - \sum_{w\in\bar{\delta}^i_G(u)} Y_{\langle w,v\rangle} = 0.$$

Thus, we can proceed as per the δ case replacing δ with $\bar{\delta}$ as required. □

Lemma 4.10. *Let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $(G, \vec{\pi}) \equiv_{\vec{\delta}^*} (H, \vec{\tau})$. Then, $\hat{\mathcal{T}}^k_{G,H}(\vec{\pi}, \vec{\tau}) \neq \emptyset$, and more specifically, $Y \in \hat{\mathcal{T}}^k_{G,H}(\vec{\pi}, \vec{\tau})$ where $Y_\emptyset = 1$ and for all $u, v \in V^k$, $Y_{\langle u,v\rangle} = |\vec{\pi}_s|^{-1} = |\vec{\tau}_s|^{-1}$ if $[u]_{\vec{\pi}} = [v]_{\vec{\tau}} = s$ and $Y_{\langle u,v\rangle} = 0$ otherwise.*

Proof. First, we have $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$. Thus, from Lemma 4.8, we have the Y is well-defined and $Y \in \hat{\mathcal{Q}}^k_{G,H}(\vec{\pi}, \vec{\tau})$. Thus, it remains to show that Y satisfies (30).

Now, for all $1 \le s, t \le m$, for all $1 \le r \le k$ and for all $u \in V^w_s$, $v \in \vec{\tau}_t$, we have

$$\sum_{w\in\delta^i_H(v)\cap\vec{\tau}_s} Y_{\langle u,w\rangle} - \sum_{w\in\delta^i_G(u)\cap\vec{\pi}_t} Y_{\langle w,v\rangle} = \sum_{w\in\delta^i_H(v)\cap\vec{\tau}_s} |\vec{\tau}_s|^{-1} - \sum_{w\in\delta^i_G(u)\cap\vec{\pi}_t} |\vec{\pi}_t|^{-1}$$
$$= |\delta^i_H(v)\cap\vec{\tau}_s||\vec{\tau}_s|^{-1} - |\delta^i_G(u)\cap\vec{\pi}_t||\vec{\pi}_t|^{-1}.$$

Next, we prove that the last expression is 0. First, note that for all $1 \le s, t \le m$, for all $1 \le r \le k$ and for all $u \in \vec{\pi}_s$ and $v \in \vec{\pi}_t$, we must have

$$\begin{aligned}
\sum_{u\in\vec{\pi}_s} |\delta^i_G(u)\cap\vec{\pi}_t| &= \sum_{u\in\vec{\pi}_t} |\delta^i_G(u)\cap\vec{\pi}_s| \\
\Rightarrow |\vec{\pi}_s||\delta^i_G(u)\cap\vec{\pi}_t| &= |\vec{\pi}_t||\delta^i_H(v)\cap\vec{\pi}_s| \\
\Rightarrow |\vec{\tau}_s||\delta^i_G(u)\cap\vec{\pi}_t| &= |\vec{\pi}_t||\delta^i_H(v)\cap\vec{\tau}_s| \\
\Rightarrow |\delta^i_G(u)\cap\vec{\pi}_t||\vec{\pi}_t|^{-1} &= |\delta^i_H(v)\cap\vec{\tau}_s||\vec{\tau}_s|^{-1}
\end{aligned}$$

as required. □

4.3. The ω-V-C algorithm and the Δ-polytope

In this section, we prove Theorem 1.2. We have seen that Δ and $\vec{\Delta}$ are combinatorially equivalent to $\hat{\mathcal{Q}}^k_G$ and $\hat{\mathcal{Q}}^k_{G,H}$ respectively. Moreover, we have seen that the k-dim ω and $\vec{\omega}$ are essentially equivalent to $(k+1)$-dim Δ and $\vec{\Delta}$ respectively. Combining these facts, the equivalence relation ω and the polyhedron $\hat{\mathcal{Q}}^{k+1}_G$ (actually its projection onto $\hat{B}^k$) are combinatorially equivalent in the following sense.

Corollary 4.11. *Let $G \in \mathcal{G}$ and $k > 1$. Let $\pi \in \Pi^k$. We have $\omega^*_G(\pi)$ is complete if and only if $\hat{\mathcal{Q}}^{k+1}_G(\nu(\pi)) = \{\hat{\mathcal{I}}^{k+1}_n\}$. Moreover, for all $u, v \in V^k$, we have $(G, \omega^*_G(\pi), u) \not\equiv_\omega (G, \omega^*_G(\pi), v)$ if and only if $Y_{\langle u,v\rangle} = 0$ for all $Y \in \hat{\mathcal{Q}}^{k+1}_G(\nu(\pi))$.*

Proof. Let $\pi' = \nu(\pi)$, and let $u' = u'$ and $v' = v'$. Firstly, from Corollary 2.19, we have that $\omega^*_G(\pi)$ is complete if and only if $\Delta^*_G(\pi')$ is complete, and thus, $\omega^*_G(\pi)$ is complete if and only if $\hat{\mathcal{Q}}^{k+1}_G(\pi') = \{\hat{\mathcal{I}}^{k+1}_n\}$ since Δ is combinatorially equivalent to $\hat{\mathcal{Q}}^{k+1}$. Secondly, we have $(G, \omega^*_G(\pi), u) \not\equiv_\omega (G, \omega^*_G(\pi), v)$ if and only if $(\Delta^*_G(\pi'), u') \not\equiv_\Delta (\Delta^*_G(\pi'), v')$ since $\omega^*_G(\pi) = \rho(\Delta^*_G(\pi'))$ from Corollary 2.19. Also, $(G, \Delta^*_G(\pi'), u') \not\equiv_\Delta (G, \Delta^*_G(\pi'), v')$ if and only if $Y_{\langle u',v'\rangle} = 0$ for all $Y \in \hat{\mathcal{Q}}^{k+1}_G(\pi')$ since Δ and $\hat{\mathcal{Q}}^{k+1}_G$ are combinatorially equivalent. The result follows then since $\langle u, v\rangle = \langle u', v'\rangle$. □

Specifically, we have that ω^k_G is complete if and only if $\hat{\mathcal{Q}}^{k+1}_G = \{\hat{\mathcal{I}}^{k+1}_n\}$ or equivalently $\mathcal{Q}^{k+1}_G = \{\mathcal{I}_n\}$ as required in Theorem 1.2. Similarly, $\vec{\omega}$ is combinatorially equivalent to $\hat{\mathcal{Q}}^{k+1}_{G,H}$ (actually its projection onto $\hat{B}^k$) in the following sense.

Corollary 4.12. *Let $G, H \in \mathcal{G}$ and let $k > 1$. Let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$ and $\vec{\nu}(\vec{\pi}) \approx \vec{\nu}(\vec{\tau})$. Then, $\hat{\mathcal{Q}}^k_{G,H}(\vec{\nu}(\vec{\pi}), \vec{\nu}(\vec{\tau})) \neq \emptyset$ if and only if $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$. Also, if $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$, then for all $u, v \in V^k$, we have $(G, \vec{\omega}^*_G(\vec{\pi}), u) \not\equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}), v)$ if and only if $Y_{\langle u,v\rangle} = 0$ for all $Y \in \hat{\mathcal{Q}}^k_{G,H}(\vec{\nu}(\vec{\pi}), \vec{\nu}(\vec{\tau}))$.*

Proof. Let $\vec{\pi}' = \vec{\nu}(\vec{\pi})$ and $\vec{\tau}' = \vec{\nu}(\vec{\tau})$, and let $u' = \nu(u)$ and $v' = \nu(v)$. Firstly, from Corollary 2.38, $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$ if and only if $(G, \vec{\Delta}^*_G(\vec{\pi}')) \equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\tau}'))$, and thus, since Δ is combinatorial equivalent to $\hat{\mathcal{Q}}^k_{G,H}$, we have $(G, \vec{\omega}^*_G(\vec{\pi})) \equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}))$ if and only if $\hat{\mathcal{Q}}^k_{G,H}(\vec{\pi}', \vec{\tau}') \neq \emptyset$. Secondly, we have $(G, \vec{\omega}^*_G(\vec{\pi}), u) \not\equiv_{\vec{\omega}} (H, \vec{\omega}^*_H(\vec{\tau}), v)$ if and only if $(G, \vec{\Delta}^*_G(\vec{\pi}'), u') \not\equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\tau}'), v')$ since $(\vec{\omega}^*_G(\vec{\pi}), \vec{\omega}^*_H(\vec{\tau})) \simeq (\rho(\vec{\Delta}^*_G(\vec{\pi}')), \rho(\vec{\Delta}^*_H(\vec{\tau}')))$ from Corollary 2.38. Then, since Δ is combinatorial equivalent to $\hat{\mathcal{Q}}^k_{G,H}$, we have that $(G, \vec{\Delta}^*_G(\vec{\pi}'), u') \not\equiv_{\vec{\Delta}} (H, \vec{\Delta}^*_H(\vec{\tau}'), v')$ if and only if $Y_{\langle u',v'\rangle} = 0$ for all $Y \in \hat{\mathcal{Q}}^k_{G,H}(\vec{\pi}', \vec{\tau}')$. The result follows since $\langle u, v\rangle = \langle u', v'\rangle$. □

Specifically, we have $(G, \vec{\omega}^k_G) \equiv_{\vec{\omega}} (H, \vec{\omega}^k_H)$ if and only if $\hat{\mathcal{Q}}^{k+1}_{G,H} \neq \emptyset$ or equivalently $\mathcal{Q}^{k+1}_{G,H} \neq \emptyset$ as required for Theorem 1.2.

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Appendix

In this appendix, we prove technical results that are necessary to prove the main results of the paper that we have put in this appendix to improve the readability of the paper.

First, we present two useful results for preorders.

Lemma A.1. *Let $G, H \in \mathcal{G}$ and let $\vec{\pi}, \vec{\tau}, \vec{\pi}', \vec{\tau}' \in \vec{\Pi}^k$ where $(G, \vec{\pi}') \equiv_{\vec{\alpha}^*} (H, \vec{\tau}')$ and $(\vec{\pi}', \vec{\tau}') \leq (\vec{\pi}, \vec{\tau})$. Then for all $r \geq 0$, we have $(\vec{\pi}', \vec{\tau}') \leq (\vec{\alpha}^r_G(\vec{\pi}), \vec{\alpha}^r_H(\vec{\tau}))$ and $(G, \vec{\alpha}^r_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^r_H(\vec{\tau}))$. Also, $(G, \vec{\alpha}^*_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}))$.*

Proof. We show by induction that for all $r \geq 0$, we have $(\vec{\pi}', \vec{\tau}') \leq (\vec{\alpha}^r_G(\vec{\pi}), \vec{\alpha}^r_H(\vec{\tau}))$ thus implying that $(G, \vec{\alpha}^r_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^r_H(\vec{\tau}))$ by Lemma 2.23 as required. It is true for $r = 0$. Assume it is true for some r. Then, $(\vec{\pi}', \vec{\tau}') \leq (\vec{\alpha}^r_G(\vec{\pi}), \vec{\alpha}^r_H(\vec{\tau}))$ implies that $(\vec{\pi}', \vec{\tau}') \leq (\vec{\alpha}^{r+1}_G(\vec{\pi}), \vec{\alpha}^{r+1}_H(\vec{\tau}))$ by Lemma 2.23 part (2) and since $\vec{\alpha}_G(\vec{\pi}') = \vec{\pi}'$ and $\vec{\alpha}_H(\vec{\tau}') = \vec{\tau}'$. $\square$

Corollary A.2. *Let $G, H \in \mathcal{G}$ and let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $\vec{\pi} \approx \vec{\tau}$ and $(G, \vec{\alpha}^*_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^*_H(\vec{\tau}))$. Then for all r, we have $(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_H(\vec{\tau})) \leq (\vec{\alpha}^r_G(\vec{\pi}), \vec{\alpha}^r_H(\vec{\tau}))$ and $(G, \vec{\alpha}^r_G(\vec{\pi})) \equiv_{\vec{\alpha}} (H, \vec{\alpha}^r_H(\vec{\tau}))$.*

Proof. Since $\vec{\alpha}^*_G(\vec{\pi}) \preceq \vec{\pi}, \vec{\alpha}^*_H(\vec{\tau}) \preceq \vec{\tau}, \vec{\alpha}^*_G(\vec{\pi}) \approx \vec{\alpha}^*_H(\vec{\tau})$ and $\vec{\pi} \approx \vec{\tau}$, we have $(\vec{\alpha}^*_G(\vec{\pi}), \vec{\alpha}^*_H(\vec{\tau})) \leq (\vec{\pi}, \vec{\tau})$. The result follows immediately by applying Lemma A.1. $\square$

The next result is used to compare preorders.

Lemma A.3. *Let $G, H \in \mathcal{G}$. Let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ such that $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$, and let $u, v \in V^k$ such that $(\vec{\pi}, u) \equiv_{\vec{\Delta}} (\vec{\tau}, v)$. Then, we have $[\phi_i(u, u_j)]_{\vec{\pi}} = [\phi_i(v, v_j)]_{\vec{\tau}}$ for all $1 \leq i, j \leq k$.*

Proof. We prove the contrapositive. Let $u' = \phi_i(u, u_j) \in \vec{\pi}_{s'}$ and $v' = \phi_i(v, v_j)$ such that $[\phi_i(u, u_j)]_{\vec{\pi}} \neq [\phi_i(v, v_j)]_{\vec{\tau}}$. Then, $|\Delta^i(u) \cap \vec{\pi}_{s'}| = |\{u'\}| = 1$ since $\vec{\pi}_{s'}$ only contains tuples of the same combinatorial type as u' meaning that $w_i = w_j$ for all $w \in \vec{\pi}_{s'}$. But, $|\Delta^i(v) \cap \vec{\tau}_{s'}| = 0$ since the only tuple in $\Delta^i(v)$ with the same combinatorial type as u' is v' and $v' \notin \vec{\tau}_{s'}$ by assumption. Thus, $(\vec{\pi}, u) \not\equiv_{\vec{\Delta}} (\vec{\tau}, v)$. $\square$

Corollary A.4. *Let $G \in \mathcal{G}$. Let $\pi \in \Pi^k$ where $\Delta_G(\pi) = \pi$, and let $u, v \in V^k$ such that $(\pi, u) \equiv_{\Delta} (\pi, v)$. Then, we have $\phi_i(u, u_j) \equiv_{\pi} \phi_i(v, v_j)$ for all $1 \leq i, j \leq k$.*

The following lemma shows useful results involving the composition of the $\vec{\nu}$ and $\vec{\rho}$ map.

Lemma A.5. *Let $G \in \mathcal{G}$. Let $\vec{\pi} \in \vec{\Pi}^k$. Then, $\vec{\rho}(\vec{\nu}(\vec{\pi})) \preceq \vec{\pi}$. If $\vec{\Delta}_G(\vec{\pi}) = \vec{\pi}$, then $\vec{\rho}(\vec{\nu}(\vec{\pi})) = \vec{\pi}$.*

Proof. Let $u, v \in V^k$, and let $u' = \nu(u)$ and $v' = \nu(v)$. Let $\vec{\pi}' = \vec{\nu}(\vec{\pi})$ and $\vec{\pi}'' = \vec{\rho}(\vec{\pi}')$. First, $u \gneqq_{\vec{\pi}} v$ implies $u' \gneqq_{\vec{\pi}'} v'$ by definition of $\vec{\nu}$. Then, $u \gneqq_{\vec{\pi}''} v$ by definition of $\vec{\rho}$. Hence, $u \gneqq_{\vec{\pi}} v$ implies $u \gneqq_{\vec{\pi}''} v$. The contrapositive is thus $u \leqq_{\vec{\pi}''} v$ implies $u \leqq_{\vec{\pi}} v$, and thus, $\vec{\rho}(\vec{\nu}(\vec{\pi})) \preceq \vec{\pi}$.

Second, assume $\vec{\Delta}_G(\vec{\pi}) = \vec{\pi}$. By definition of $\vec{\rho}$, we have $u \leqq_{\vec{\pi}''} v$ if and only if $u' \leqq_{\vec{\pi}'} v'$. Then, by definition of $\vec{\nu}$, we have $u' \leqq_{\vec{\pi}'} v'$ if and only if $u \lneqq_{\vec{\pi}} v$ or $u \equiv_{\vec{\pi}} v$ and $\vec{\omega}_{\vec{\pi}}(u, u_k) \leq_{lex} \vec{\omega}_{\vec{\pi}}(v, v_k)$. But, if $u \equiv_{\vec{\pi}} v$, then $(G, \vec{\pi}, u) \equiv_{\vec{\Delta}} (H, \vec{\tau}, v)$, and thus, $\phi_i(u, u_k) \equiv_{\vec{\pi}} \phi_i(v, v_k)$ for all $1 \leq i \leq k$ from Lemma A.3. So, $u' \leqq_{\vec{\pi}'} v'$ if and only if $u \leqq_{\vec{\pi}} v$. Thus, $u \leqq_{\vec{\pi}''} v$ if and only if $u \leqq_{\vec{\pi}} v$, and $\vec{\pi}'' = \vec{\pi}$ as required. $\square$

Corollary A.6. *Let $G \in \mathcal{G}$. Let $\pi \in \Pi^k$. Then, $\rho(\nu(\pi)) \leq \pi$. If $\Delta_G(\pi) = \pi$, then $\rho(\nu(\pi)) = \pi$.*

The following lemma shows some useful results involving the $\vec{\nu}$ map.

Lemma A.7. *Let $k > 1$. Let $G, H \in \mathcal{G}$. Let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $(G, \vec{\pi}) \equiv_{\vec{\omega}} (H, \vec{\tau})$. Then, $\vec{\nu}(\vec{\pi}) \approx \vec{\nu}(\vec{\tau})$, and for all $u, v \in V^{k+1}$, we have $[u]_{\vec{\nu}(\vec{\pi})} = [v]_{\vec{\nu}(\vec{\tau})}$ if and only if $[\rho(u)]_{\vec{\pi}} = [\rho(v)]_{\vec{\tau}}$ and $\vec{\omega}_{\vec{\pi}}(\rho(u), u_{k+1}) = \vec{\omega}_{\vec{\tau}}(\rho(v), v_{k+1})$. Also, for all $\vec{\pi}'', \vec{\tau}'' \in \vec{\Pi}^k$ where $(\vec{\pi}, \vec{\tau}) \leq (\vec{\pi}'', \vec{\tau}'')$, we have $(\vec{\nu}(\vec{\pi}), \vec{\nu}(\vec{\tau})) \leq (\vec{\nu}(\vec{\pi}''), \vec{\nu}(\vec{\tau}''))$. Furthermore, we have $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$ implies $\vec{\nu}(\vec{\pi}) \equiv_{\vec{\mathcal{S}}^*} \vec{\nu}(\vec{\tau})$ and $(G, \vec{\nu}(\vec{\pi})) \equiv_{\vec{\mathcal{C}}^*} (H, \vec{\nu}(\vec{\tau}))$.*

Proof. Let $\vec{\pi}' = \vec{\nu}(\vec{\pi})$ and $\vec{\tau}' = \vec{\nu}(\vec{\tau})$. Since $(G, \vec{\pi}) \equiv_{\vec{\omega}} (H, \vec{\tau})$, there exists a tuple bijection $\gamma' : V^k \to V^k$ such that $(G, \vec{\pi}', u') \equiv_{\vec{\omega}} (H, \vec{\tau}', \gamma'(u'))$ for all $u' \in V^k$. Then, for all $u' \in V^k$, since $(G, \vec{\pi}', u') \equiv_{\vec{\omega}} (H, \vec{\tau}', \gamma(u'))$, there must exist a bijection $\psi : V \to V$ such that $\vec{\omega}_{\vec{\pi}'}(u', w) = \vec{\omega}_{\vec{\tau}'}(\gamma'(u'), \psi(w))$ for all $w \in V$. We now define the bijection $\gamma : V^{k+1} \to V^{k+1}$ where for all $u \in V^{k+1}$, we have $\gamma(u) = (\gamma(u')_1, \dots, \gamma(u')_k, \psi(u_{k+1}))$ where $u' = \rho(u)$. Thus, for all $u \in V^{k+1}$, we have $[\rho(u)]_{\vec{\pi}} = [\rho(\gamma(u))]_{\vec{\tau}}$ and $\vec{\omega}_{\vec{\pi}}(\rho(u), u_{k+1}) = \vec{\omega}_{\vec{\tau}}(\rho(\gamma(u)), \gamma(u)_{k+1})$. Then, by construction of $\vec{\nu}$, for all $u, u'' \in V^{k+1}$, we have $u \leqq_{\vec{\pi}'} u''$ if and only if $\gamma(u) \leqq_{\vec{\tau}'} \gamma(u'')$ and thus $[u]_{\vec{\pi}'} = [\gamma(u)]_{\vec{\tau}'}$; therefore, $\vec{\pi}' \approx \vec{\tau}'$ and $[u]_{\vec{\pi}'} = [v]_{\vec{\tau}'}$ if and only if $[\rho(u)]_{\vec{\pi}} = [\rho(v)]_{\vec{\tau}}$ and $\vec{\omega}_{\vec{\pi}}(\rho(u), u_{k+1}) = \vec{\omega}_{\vec{\tau}}(\rho(v), v_{k+1})$.

Let $\vec{\pi}'', \vec{\tau}'' \in \vec{\Pi}^k$ such that $(\vec{\pi}, \vec{\tau}) \le (\vec{\pi}'', \vec{\tau}'')$. Let $u, v \in V^{k+1}$ such that $[u]_{\vec{\pi}'} = [v]_{\vec{\tau}'}$. From above, we have $[\rho(u)]_{\vec{\pi}} = [\rho(v)]_{\vec{\tau}}$ and $\vec{\omega}_{\vec{\pi}}(\rho(u), u_{k+1}) = \vec{\omega}_{\vec{\tau}}(\rho(v), v_{k+1})$ implying $[\rho(u)]_{\vec{\pi}''} = [\rho(v)]_{\vec{\tau}''}$ and $\vec{\omega}_{\vec{\pi}''}(\rho(u), u_{k+1}) = \vec{\omega}_{\vec{\tau}''}(\rho(v), v_{k+1})$ since $(\vec{\pi}, \vec{\tau}) \le (\vec{\pi}'', \vec{\tau}'')$, and thus, since $(G, \vec{\pi}'') \equiv_{\vec{\omega}} (H, \vec{\tau}'')$ from Lemma 2.23, we have $[u]_{\vec{\nu}(\vec{\pi}'')} = [v]_{\vec{\nu}(\vec{\tau}'')}$ from above implying $(\vec{\pi}', \vec{\tau}') \le (\vec{\nu}(\vec{\pi}''), \vec{\nu}(\vec{\tau}''))$ as required.

Assume $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$, and so, $\vec{\pi} \equiv_{\vec{\mathcal{S}}^*} \vec{\tau}$. Let $u', v' \in V^{k+1}$ and let $u = \rho(u')$ and $v = \rho(v')$. Then, it follows by construction that $[u]_{\vec{\pi}} = [v]_{\vec{\tau}}$ and $[\phi_i(u, u'_{k+1})]_{\vec{\pi}} = [\phi_i(v, v'_{k+1})]_{\vec{\tau}}$ for all $1 \le i \le k$ if and only if $[\rho(\sigma(u'))]_{\vec{\pi}} = [\rho(\sigma(v'))]_{\vec{\tau}}$ and $[\phi_i(\rho(\sigma(u')), \sigma(u')_{k+1})]_{\vec{\pi}} = [\phi_i(\rho(\sigma(v')), \sigma(v')_{k+1})]_{\vec{\tau}}$ for all $\sigma \in \mathcal{S}_{k+1}$. Thus, $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$ if and only if $[\sigma(u')]_{\vec{\pi}'} = [\sigma(v')]_{\vec{\tau}'}$ and for all $\sigma \in \mathcal{S}_{k+1}$. Thus, $\vec{\pi}' \equiv_{\vec{\mathcal{S}}^*} \vec{\tau}'$ since $\vec{\pi}' \approx \vec{\tau}'$.

Assume $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$, and so, $(G, \vec{\pi}) \equiv_{\vec{\mathcal{C}}^*} (H, \vec{\tau})$. Let $u', v' \in V^{k+1}$ where $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$ and let $u = \rho(u')$ and $v = \rho(v')$. We must show that $(G, \vec{\pi}', u') \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}', v')$, and it follows that $(G, \vec{\pi}') \equiv_{\vec{\mathcal{C}}^*} (H, \vec{\tau}')$ since $\vec{\pi}' \equiv_{\vec{\mathcal{S}}^*} \vec{\tau}'$ and $\vec{\pi}' \approx \vec{\tau}'$. From above, we have $[u]_{\vec{\pi}} = [v]_{\vec{\tau}}$ and $\vec{\omega}_{\vec{\pi}}(u, u'_{k+1}) = \vec{\omega}_{\vec{\tau}}(v, v'_{k+1})$, and so by assumption, $(G, u) \equiv_{\vec{\mathcal{C}}} (H, v)$ and $(G, \phi_i(u, u'_{k+1})) \equiv_{\vec{\mathcal{C}}} (H, \phi_i(v, v'_{k+1}))$, which implies that $(G, u') \equiv_{\vec{\mathcal{C}}} (H, v')$, and thus, $(G, \vec{\pi}', u') \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}', v')$ as required. □

Corollary A.8. *Let $k > 1$ and let $G \in \mathcal{G}$, and let $\pi \in \Pi^k$. For all $\tau \in \Pi^k$ where $\pi \le \tau$, we have $\nu(\pi) \le \nu(\tau)$. Also, $\omega_G(\pi) = \pi$ implies $\mathcal{S}(\nu(\pi)) = \nu(\pi)$ and $\mathcal{C}_G(\nu(\pi)) = \nu(\pi)$.*

The following lemma shows some useful results involving the $\vec{\rho}$ map.

Lemma A.9. *Let $k > 1$. Let $G, H \in \mathcal{G}$. Let $\vec{\pi}, \vec{\tau} \in \vec{\Pi}^k$ where $(G, \vec{\pi}) \equiv_{\vec{\Delta}} (H, \vec{\tau})$. Then, $\vec{\rho}(\vec{\pi}) \approx \vec{\rho}(\vec{\tau})$ and for all $u', v' \in V^{k-1}$, we have $[u']_{\vec{\rho}(\vec{\pi})} = [v']_{\vec{\rho}(\vec{\tau})}$ if and only if $[\nu(u')]_{\vec{\pi}} = [\nu(v')]_{\vec{\tau}}$. Moreover, for all $u, v \in V^k$, we have $(G, \vec{\pi}, u) \equiv_{\vec{\Delta}} (H, \vec{\tau}, v)$ implies $[\rho(u)]_{\vec{\rho}(\vec{\pi})} = [\rho(v)]_{\vec{\rho}(\vec{\tau})}$. Also, for all $\vec{\pi}'', \vec{\tau}'' \in \vec{\Pi}^k$ where $(\vec{\pi}, \vec{\tau}) \le (\vec{\pi}'', \vec{\tau}'')$, we have $(\vec{\rho}(\vec{\pi}), \vec{\rho}(\vec{\tau})) \le (\vec{\rho}(\vec{\pi}''), \vec{\rho}(\vec{\tau}''))$. Furthermore, $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$ implies $\vec{\rho}(\vec{\pi}) \equiv_{\vec{\mathcal{S}}^*} \vec{\rho}(\vec{\tau})$ and $(G, \vec{\rho}(\vec{\pi})) \equiv_{\vec{\mathcal{C}}^*} (H, \vec{\rho}(\vec{\tau}))$.*

Proof. Let $\vec{\pi}' = \vec{\rho}(\vec{\pi})$ and $\vec{\tau}' = \vec{\rho}(\vec{\tau})$. Since $(G, \vec{\pi}) \equiv_{\vec{\Delta}} (H, \vec{\tau})$, there exists a tuple bijection $\gamma : V^k \to V^k$ such that $(G, \vec{\pi}, u) \equiv_{\vec{\Delta}} (H, \vec{\tau}, \gamma(u))$ for all $u \in V^k$. Now, we define the bijection $\gamma' : V^{k-1} \to V^{k-1}$ where for all $u' \in V^{k-1}$, we have $\gamma'(u') = \rho(\gamma(\nu(u')))$. Since $(G, \vec{\pi}, u) \equiv_{\vec{\Delta}} (H, \vec{\tau}, \gamma(u))$ and thus $(G, \vec{\pi}, u) \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}, \gamma(u))$, we have $\nu(\rho(u)) = u$ if and only if $\nu(\rho(\gamma(u))) = \gamma(u)$. Thus, for all $u' \in V^{k-1}$, we have $[\nu(u')]_{\vec{\pi}} = [\nu(\gamma'(u'))]_{\vec{\tau}}$ since $\nu(\rho(\nu(u'))) = \nu(u')$ and thus $\nu(\gamma'(u')) = \nu(\rho(\gamma(\nu(u')))) = \gamma(\nu(u'))$. Then, by construction of $\vec{\rho}$, for all $u', u'' \in V^{k-1}$, we have $u' \leqq_{\vec{\pi}'} u''$ if and only if $\gamma(u') \leqq_{\vec{\tau}'} \gamma(u'')$ and thus $[u']_{\vec{\pi}'} = [\gamma(u')]_{\vec{\tau}'}$; therefore, $\vec{\pi}' \approx \vec{\tau}'$ and $[u']_{\vec{\rho}(\vec{\pi})} = [v']_{\vec{\rho}(\vec{\tau})}$ if and only if $[\nu(u')]_{\vec{\pi}} = [\nu(v')]_{\vec{\tau}}$ for all $u', v' \in V^{k-1}$.

Let $u, v \in V^k$ such that $(G, \vec{\pi}, u) \equiv_{\vec{\Delta}} (H, \vec{\tau}, v)$. Then, by Lemma A.3, we have $[\phi_k(u, u_{k-1})]_{\vec{\pi}} = [\phi_k(v, v_{k-1})]_{\vec{\tau}}$ implying that $[\rho(u)]_{\vec{\pi}'} = [\rho(v)]_{\vec{\tau}'}$ from above since $\nu(\rho(u)) = \phi_k(u, u_{k-1})$ and $\nu(\rho(v)) = \phi_k(v, v_{k-1})$ as required.

Let $\vec{\pi}'', \vec{\tau}'' \in \vec{\Pi}^k$ such that $(\vec{\pi}, \vec{\tau}) \le (\vec{\pi}'', \vec{\tau}'')$. Let $u, v \in V^{k-1}$ such that $[u]_{\vec{\rho}(\vec{\pi})} = [v]_{\vec{\rho}(\vec{\tau})}$. From above, we have $[\nu(u)]_{\vec{\pi}} = [\nu(v)]_{\vec{\tau}}$ implying $[\nu(u)]_{\vec{\pi}''} = [\nu(v)]_{\vec{\tau}''}$ since $(\vec{\pi}, \vec{\tau}) \le (\vec{\pi}'', \vec{\tau}'')$, and thus, from above, $[u]_{\vec{\rho}(\vec{\pi}'')} = [v]_{\vec{\rho}(\vec{\tau}'')}$ implying $(\vec{\rho}(\vec{\pi}), \vec{\rho}(\vec{\tau})) \le (\vec{\rho}(\vec{\pi}''), \vec{\rho}(\vec{\tau}''))$ as required.

Assume $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$, and so, $\vec{\pi} \equiv_{\vec{\mathcal{S}}^*} \vec{\tau}$. Let $u', v' \in V^{k-1}$ where $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$ and let $u = \nu(u')$ and $v = \nu(v')$. Let $\sigma' \in \mathcal{S}_{k-1}$. We must show that $[\sigma'(u')]_{\vec{\pi}'} = [\sigma'(v')]_{\vec{\tau}'}$. Since $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$, we have $[u]_{\vec{\pi}} = [v]_{\vec{\tau}}$. Let $\sigma \in \mathcal{S}_k$ such that $\rho(\sigma(u)) = \sigma'(u')$ and $\rho(\sigma(v)) = \sigma'(v')$, which clearly exists. Then, $[\sigma(u)]_{\vec{\pi}} = [\sigma(v)]_{\vec{\tau}}$ by assumption. Thus, $[\sigma'(u')]_{\vec{\pi}'} = [\sigma'(v')]_{\vec{\tau}'}$ from above. Thus, $\vec{\pi}' \equiv_{\vec{\mathcal{S}}^*} \vec{\tau}'$ since $\vec{\pi}' \approx \vec{\tau}'$.

Assume $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$, and so, $(G, \vec{\pi}) \equiv_{\vec{\mathcal{C}}^*} (H, \vec{\tau})$. Let $u', v' \in V^{k-1}$ where $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$, and let $u = \nu(u')$ and $v = \nu(v')$. We must show that $(G, \vec{\pi}', u') \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}', v')$ and it follows that $(G, \vec{\pi}') \equiv_{\vec{\mathcal{C}}^*} (H, \vec{\tau}')$ since $\vec{\pi}' \equiv_{\vec{\mathcal{S}}^*} \vec{\tau}'$ and $\vec{\pi}' \approx \vec{\tau}'$. First, $[u']_{\vec{\pi}'} = [v']_{\vec{\tau}'}$ implies $[u]_{\vec{\pi}} = [v]_{\vec{\tau}}$ from above, and thus, $(G, u) \equiv_{\vec{\mathcal{C}}} (H, v)$ by assumption, which implies that $(G, u') \equiv_{\vec{\mathcal{C}}} (H, v')$. Thus, $(G, \vec{\pi}', u') \equiv_{\vec{\mathcal{C}}} (H, \vec{\tau}', v')$ as required. □

Corollary A.10. *Let $k > 1$ and let $G \in \mathcal{G}$, and let $\pi \in \Pi^k$. For all $u, v \in V^k$, we have $(G, \pi, u) \equiv_{\Delta} (G, \pi, v)$ implies $\rho(u) \equiv_{\rho(\pi)} \rho(v)$. For all $\tau \in \vec{\Pi}^k$ where $\pi \le \tau$, we have $\rho(\pi) \le \rho(\tau)$. Also, $\Delta_G(\pi) = \pi$ implies $\mathcal{C}_G(\rho(\pi)) = \rho(\pi)$ and $\mathcal{S}(\rho(\pi)) = \rho(\pi)$.*

The rest of the results below are used to compare combinatorial and polyhedral approaches.

Lemma A.11. *Let $\pi = \{\pi_1, \dots, \pi_m\} \in \Pi^k$ where $\Delta_G(\pi) = \pi$. Let $u \in \pi_s$ and $u' \in \pi_{s'}$ where $u' = \phi_i(u, u_j)$ for some $1 \le i, j \le k$ where $j \ne i$. Then, we have $\phi_{i,j}(\pi_s) = \{\phi_i(v, v_j) : v \in \pi_s\} = \pi_{s'}$ and $|\pi_s| = |\Delta^i(u) \cap \pi_s||\pi_{s'}|$.*

Proof. First, we show that $\phi_{i,j}(\pi_s) \subseteq \pi_{s'}$. Let $v \in \pi_s$, and let $v' = \phi_i(v, v_j)$. From Corollary A.4, we have $v' \equiv_{\pi} u'$, and thus, $v' \in \pi_{s'}$. So, $\phi_{i,j}(\pi_s) \subseteq \pi_{s'}$.

Next, we show that $\phi_{i,j}(\pi_s) \supseteq \pi_{s'}$. Let $v' \in \pi_{s'}$. Assume that for all $v \in V^k$ where $v' = \phi_i(v, v_j)$, we have $v \notin \pi_s$. Then, $|\Delta^i(v') \cap \pi_s| = 0$. But, $|\Delta^i(u') \cap \pi_s| > 0$ since $u \in \Delta^i(u') \cap \pi_s$. Thus, $u' \not\equiv_{\pi} v'$, a contradiction. Hence, there exists $v \in \pi_s$ such that $v' = \phi_i(v, v_j)$, and thus, $\phi_{i,j}(\pi_s) \supseteq \pi_{s'}$. Therefore, $\phi_{i,j}(\pi_s) = \pi_{s'}$.

Now, since $\phi_{i,j}(\pi_s) = \pi_{s'}$, we have $\bigcup_{v' \in \pi_{s'}} \Delta^i(v') \cap \pi_s = \pi_s$, and for all $w, w' \in \pi_{s'}$, we have $\Delta^i(w) \cap \Delta^i(w') = \emptyset$ by construction, and $|\Delta^i(w) \cap \pi_s| = |\Delta^i(w') \cap \pi_s|$ since $\Delta_G(\pi) = \pi$. Thus, $|\pi_s| = |\Delta^i(u') \cap \pi_s||\pi_{s'}| = |\Delta^i(u) \cap \pi_{s'}||\pi_{s'}|$ as required. □

Definition A.12. Let $u \in V^k$. We define $\langle u \rangle = \{u_1, \ldots, u_k\}$.

Lemma A.13. *Let $\pi = \{\pi_1, \ldots, \pi_m\} \in \Pi^k$ where $\Delta_G(\pi) = \pi$, and let $u \in \pi_s$, $v \in \pi_t$. If $\langle u \rangle = \langle v \rangle$, then $|\pi_s| = |\pi_t|$.*

Proof. Assume $\langle u \rangle = \langle v \rangle$, but $u \neq v$. Since $\mathcal{S}(\pi) = \pi$, we may assume that $\langle u \rangle = \{u_1, \ldots, u_r\}$ and $\langle v \rangle = \{v_1, \ldots, v_r\}$ where $u_i = v_i$ for all $1 \leq i \leq r$ where $r \geq |\langle u \rangle| = |\langle v \rangle|$. Now, there exists $r < i \leq k$ such that $u_i \neq v_i$. Since $\langle u \rangle = \langle v \rangle$, we must have $u_i = u_j = v_j$ for some $1 \leq j \leq r$. Let $u' = \phi_i(u, u_j) \in \pi_{s'}$, so u' differs from v in one less component than u, and $\langle u \rangle = \langle u' \rangle$. By Lemma A.11, we have $|\pi_s| = |\pi_{s'}|$. Repeating this process until we arrive at v proves the result. □

Corollary A.14. *Let $G, H \in \mathcal{G}$. Let $\vec{\pi} = (\vec{\pi}_1, \ldots, \vec{\pi}_m)$, $\vec{\tau} = (\vec{\tau}_1, \ldots, \vec{\tau}_m) \in \vec{\Pi}^k$ where $(G, \vec{\pi}) \equiv_{\vec{\Delta}^*} (H, \vec{\tau})$, and let $u \in \vec{\pi}_s$, $v \in \vec{\tau}_s$ and $u' \in \vec{\pi}_t$, $v' \in \vec{\tau}_t$. If $\langle u, v \rangle = \langle u', v' \rangle$, then $|\vec{\pi}_s| = |\vec{\pi}_t| = |\vec{\tau}_s| = |\vec{\tau}_t|$.*

Proof. The fact $\langle u, v \rangle = \langle u', v' \rangle$ implies $\langle u \rangle = \langle u' \rangle$, so applying Lemma A.13, the result follows. □

Lemma A.15. *Let $P \subseteq \hat{B}^k$, and let $Y \in P$. Let $I \subseteq V^2$. If $Y_I = 0$, then $Y_{I'} = 0$ for all $I' \supseteq I$.*

Proof. We show by induction that $Y_{I'} = 0$ for all $I' \supseteq I$ where $|I' \setminus I| \leq r$ for all r. It is trivially true for $r = 0$, so assume true for r. Let $I' \supseteq I$ where $|I' \setminus I| = r + 1$. Then, there exists $I'' \supseteq I$ where $|I'' \setminus I| = r$ and $I' = I'' \cup \{u, v\}$ for some $u, v \in V$. By assumption $Y_{I''} = 0$. Then, Eq. (14) imply that $Y_{I'} = 0$ as required. □

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