ON THE EDGES OF CHARACTERISTIC IMSET POLYTOPES

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Abstract. The edges of the characteristic imset polytope, CIM \( p \), were recently shown to have strong connections to causal discovery as many algorithms could be interpreted as greedy restricted edge-walks, even though only a strict subset of the edges are known. To better understand the general edge structure of the polytope we describe the edge structure of faces with a clear combinatorial interpretation: for any undirected graph \( G \) we have the face CIM \( G \), the convex hull of the characteristic imsets of DAGs with skeleton \( G \). We give a full edge-description of CIM \( G \) when \( G \) is a tree, leading to interesting connections to other polytopes. In particular the well-studied stable set polytope can be recovered as a face of CIM \( G \) when \( G \) is a tree. Building on this connection we are also able to give a description of all edges of CIM \( G \) when \( G \) is a cycle, suggesting possible inroads for generalization. We then introduce an algorithm for learning directed trees from data, utilizing our newly discovered edges, that outperforms classical methods on simulated Gaussian data.

1. Introduction

Let \( [p] := \{1, \ldots, p\} \). For a directed acyclic graph (DAG) \( \mathcal{G} = ([p], E) \) Studený, Hemmecke and Lindner introduced the characteristic imset [23] defined as the function \( c_\mathcal{G} : \{ S \subseteq [p] : |S| \geq 2 \} \rightarrow \{0, 1\} \) where

\[
c_\mathcal{G}(S) = \begin{cases} 
1 & \text{if there exists } i \in S \text{ such that } S \setminus \{i\} \subseteq \text{pa}_\mathcal{G}(i), \\
0 & \text{otherwise.}
\end{cases}
\]

Since \( c_\mathcal{G} \) is a function from a finite set into \( \mathbb{R} \) we identify it with a vector of length \( 2^p - p - 1 \), and thus we can consider the characteristic imset polytope:

\[
\text{CIM}_p := \text{conv} (c_\mathcal{G} : \mathcal{G} = ([p], E) \text{ a DAG}).
\]

The polytope CIM \( p \) is a full-dimensional 0/1-polytope whose vertices are exactly the characteristic imsets of DAGs [22, 23]. A \textit{v-structure} is an induced subgraph of the form \( i \rightarrow j \leftarrow k \) and the \textit{skeleton} of a directed graph \( \mathcal{G} \) is the undirected graph that has the same adjacencies as \( \mathcal{G} \). A unique DAG \( \mathcal{G} \) cannot in general be recovered from the characteristic imset \( c_\mathcal{G} \). We can, however, easily recover both the skeleton and the v-structures. Vice versa, any two graphs that share the same skeleton and v-structures have the same characteristic imset [9, 23] (see Lemma 1.2 and 1.4). Two DAGs that have the same skeleton and the same v-structures are known as Markov equivalent (Theorem 1.1), and hence belong to the same Markov equivalence class (MEC). That is, each characteristic imset corresponds to a unique MEC. A graphical representation of a MEC, called the \textit{essential graph}, was given by Andersson et. al. [1]. The essential graph of a DAG \( \mathcal{G} \) is a partially directed graph that has the same skeleton as \( \mathcal{G} \) and directed edges being exactly those edges that have the same direction in all DAGs in the MEC of \( \mathcal{G} \).
The polyhedral geometry of \( \text{CIM}_p \) has been previously studied. Cussens, Haws and Studeny were able to obtain classes of facets of \( \text{CIM}_p \) [4]. These facets are however not exhaustive and, due to the high dimensionality of \( \text{CIM}_p \), a complete facet description is only available for small \( p (p \leq 4) \). In [10], lower-dimensional faces of \( \text{CIM}_p \) with a more direct combinatorial interpretation were identified. For example, given any undirected graph \( G \) we have the face
\[
\text{CIM}_G := \text{conv} (c_G; G = ([p], E) \text{ a DAG with skeleton } G).
\]
It was also shown in [10] that generalizations of reversing and adding in edges of DAGs constitute edges of \( \text{CIM}_p \). This raises the question as to whether there is a graphical explanation of other edges as well. While a complete characterization of the edges of \( \text{CIM}_p \) appears challenging, a complete characterization of those edges corresponding to edges of \( \text{CIM}_G \) for well-chosen families of \( G \) is achievable.

The focus of this paper is on \( \text{CIM}_G \) when \( G \) is a tree. First, in Section 1.2 we will consider the case when \( G \) is a star. Using some standard techniques from the theory of partially ordered sets (posets) we will see that, in this case, \( \text{CIM}_G \) is a simplex (see Lemma 1.9). As trees are locally stars we can utilize this local structure to impose more global conditions for adjacency in the edge graph of \( \text{CIM}_G \), resulting in a complete characterization of all edges of \( \text{CIM}_G \) for \( G \) a tree, both in terms of DAGs (Theorem 2.12) and in terms of essential graphs (Theorem 2.7). For completeness, we include Section 3.1, specifically Proposition 3.1, which generalizes these results to forests.

In Section 3.2 we also observe a connection between \( \text{CIM}_G \) and another well-studied polytope; namely the stable set polytope, \( \text{STAB}(G) \). For a given graph \( G, \text{STAB}(G) \) has vertices corresponding to the stable sets of \( G \). Chvatal gave a characterization of the edges of \( \text{STAB}(G) \) in terms of the stable sets [3]. Here, we present a unimodular equivalence between a certain face of the characteristic imset polytope \( \text{CIM}_G \) for \( G \) a tree and the stable set polytope of a tree (Proposition 3.10). Hence, we recover Chvatal’s results in these cases. The connection between the stable set polytope and the characteristic imset polytope also allows us to describe the edges of \( \text{CIM}_{C_p} \), where \( C_p \) is the cycle with \( p \) nodes (Theorem 3.9), suggesting that there may be a more general connection.

In Section 4, we discuss the application of these geometric observations to the problem of causal discovery. Given that we have all edges of \( \text{CIM}_G \), when \( G \) is a tree, we define a new algorithm, Algorithm 1, for learning a directed tree (also known as a polytree) from data. We prove that this algorithm is asymptotically consistent, and the same follows for another algorithm defined in [10] (Proposition 4.3). We observe that the additional search capabilities provided by our geometric observations on the edge structure of \( \text{CIM}_G \) results in improved performance over classical methods on simulated Gaussian data (Section 4.2).

1.1. Preliminaries. Let \( G = ([p], E) \) be a directed graph. We will denote with \( i \rightarrow j \in G \) if \( (i, j) \in E \), and if this is the case we say that \( i \) is a parent of \( j \) and \( j \) is a child of \( i \). The set of parents and children of \( i \) in \( G \) is denoted with \( \text{pa}_G(i) \) and \( \text{ch}_G(i) \), respectively. Analogously, if \( G = ([p], E) \) is undirected we denote \( i \sim j \in G \) if \( \{i, j\} \in E \), and say that \( i \) and \( j \) are neighbors in \( G \). The set of all neighbors of \( i \) in \( G \) is denoted by \( \text{ne}_G(i) \) and the closure of a node \( i \) is defined as \( \text{cl}_G(i) = \{i\} \cup \text{ne}_G(i) \).

The skeleton of a directed graph \( G \) is the undirected graph \( G \) with the same set of nodes, but each edge \( i \rightarrow j \in G \) is replaced with \( i \sim j \in G \). A path in an
undirected graph $G$ is a sequence of distinct vertices $P = (v_0, v_1, \ldots, v_n)$ such that $v_{i-1} - v_i \in G$ for all $i \in [n]$, and any path in which we allow $v_0 = v_1$ is called a cycle. A graph $G$ is connected if for every pair of nodes $i$ and $j$ there exists a path $P$ such that $v_0 = i$ and $v_n = j$, and $G$ is a tree if it is connected and does not contain a cycle. A path in a directed graph $G$ is a path in the skeleton, and the path is directed if $v_{i-1} \rightarrow v_i \in G$ for all $i \in [n]$. A directed path in $G$ is a directed cycle if $v_0 = v_n$, and $G$ is connected if the skeleton is connected. For a directed graph $G$ we say that $i$ and $j$ are neighbors if $i$ and $j$ are neighbors in the skeleton of $G$ and denote the corresponding set with $\text{ne}_G(i)$. If there is a directed path $i \rightarrow \cdots \rightarrow j$ in $G$ we say that $i$ is an ancestor of $j$ and that $j$ is a descendant of $i$. We denote the set of all ancestors of $i$ in $G$ with $\text{an}_G(i)$, the set of all descendants with $\text{de}_G(i)$, and the set of all non-descendants with $\text{nd}_G(i)$.

If $A$ is a subset of the nodes of $G$ we let $G|_A$ denote the induced graph on $A$; that is, $G|_A$ has the nodes $A$ and for any $i, j \in A$ we have $i \rightarrow j \in G|_A$ if and only if $i \rightarrow j \in G$. An induced subgraph of $G$ of the form $i \rightarrow j \leftarrow k$ is called a v-structure. A node $i$ is a leaf in a tree $G$ if it has a unique neighbor. A node that is not a leaf is called an interior node. The induced subgraph of $G$ on all interior nodes of $G$ is denoted $G^\circ$. If $G$ is a tree and $D$ is a subset of the vertices, then $\text{span}_G(D)$ denotes the unique minimal spanning tree of $D$.

We will also consider partially directed graphs; i.e., graphs whose edges can be either directed or undirected. Assume $P = (v_0, v_1, \ldots, v_k)$ is a path in the skeleton of a partially directed graph, then we will say that $P \rightarrow v_k$ in $G$ if we have $v_0 \rightarrow v_1 \rightarrow \cdots \rightarrow v_k$ in $G$. A path $P$ in the skeleton of a DAG $G$ from $v_0$ to $v_n$ is $d$-connecting given $C$ if for every $v_i$, $0 < i < k$ such that $v_{i-1} \rightarrow v_i \leftarrow v_{i+1}$ we have $C \cap (\text{de}_G(v_i) \cup \{v_i\}) \neq \emptyset$, and for every other $v_i$ we have $v_i \notin C$. We say that two subsets $A, B \subseteq [p]$ are $d$-connected given a third subset $C \subseteq [p]$ if there exists $i \in A$ and $j \in B$ such that there is a $d$-connecting path from $i$ to $j$ given $C$ in $G$. Otherwise, we say $A$ and $B$ are $d$-separated given $C$ in $G$.

For any DAG $G = ([p], E)$ we associate a set of random variables $X_1, \ldots, X_p$ and we say that the joint distribution $P$ of $(X_1, \ldots, X_p)$ is Markov to $G$ if $P$ entails $X_i \perp X_{\text{nd}_G(i) \setminus \text{pa}_G(i)} \mid X_{\text{pa}_G(i)}$ for all $i \in [p]$. Equivalently $P$ is Markov to $G$ if we have $X_A \perp X_B \mid X_C$ whenever $A$ and $B$ are $d$-separated given $C$ in $G$ [8]. Furthermore, $P$ is faithful to $G$ if $P$ entails exactly the CI statements encoded by $G$. It can happen that two DAGs encode the same set of CI statements. In this case, we say that the DAGs are Markov equivalent and that they belong to the same Markov equivalence class (MEC). The graphical side of Markov equivalence is well-understood with this classical result from Verma and Pearl.

**Theorem 1.1.** [26] Two DAGs are Markov equivalent if and only if they have the same skeleton and the same v-structures.

Using DAGs to model complex systems is nowadays common within many areas [5, 11, 16, 19]. Algorithms for inferring a MEC from data is a well-studied area and many algorithms for doing so have been proposed [2, 7, 18, 25, 26, 27]. Many of these algorithms are score-based; i.e., given a scoring criterion $S(\cdot, \mathbb{D})$, where $\mathbb{D}$ is a random sample from the joint distribution of $(X_1, \ldots, X_p)$, we aim to find the DAG $G$ maximizing $S(G, \mathbb{D})$. A commonly used scoring criterion is the *Bayesian information criterion* (BIC), which is defined in Section 4.

To get a unique representative for each MEC Andersson, Madigan and Perlman introduced essential graphs [1], a special family of partially directed graphs. The
essential graph of an MEC is the graph that has the same skeleton as each DAG in the MEC, and a directed edge \( i \to j \) if and only if we have \( i \to j \in G \) for all DAGs \( G \) in the MEC. Using this definition the authors gave a complete classification of the directed edges of essential graphs, namely \( i \to j \) is directed in an essential graph \( G \) if and only if it is strongly protected in \( G \) [1, Theorem 4.1].

As an alternative to working with DAGs or essential graphs, Studený described how to use vector encodings to represent CI models [22]. Studený, Lindner, and Hemmecke developed this idea in [23] and introduced the characteristic imset (as defined in the introduction), from which the skeleton and the v-structures are easily recovered.

**Lemma 1.2.** [23] Let \( G \) be a DAG with nodes \([p]\). Then for any distinct nodes \( i, j, \) and \( k \) we have

1. \( i \leftarrow j \) or \( j \to i \) in \( G \) if and only if \( c_G(\{i, j\}) = 1 \).
2. \( i \to j \leftarrow k \) is a v-structure in \( G \) if and only if \( c_G(\{i, j, k\}) = 1 \) and \( c_G(\{i, k\}) = 0 \).

Moreover, as the characteristic imset encodes the CI statements we get the following alternative characterization of Markov equivalence.

**Theorem 1.3.** [23] Two DAGs \( G \) and \( H \) are Markov equivalent if and only if \( c_G = c_H \).

As is noted in [23], any score equivalent, decomposable scoring criterion can be seen as an affine function over the characteristic imsets, motivating the definition of the characteristic imset polytope. The following is direct from Theorem 1.1 and Lemma 1.2.

**Lemma 1.4.** [9, Corollary 2.2.6] Two characteristic imsets \( c_G \) and \( c_H \) are equal if and only if \( c_G(S) = c_H(S) \) for all sets \( |S| \in \{2, 3\} \).

### 1.2. Two examples

The general question of characterizing all edges of \( \text{CIM}_p \) or \( \text{CIM}_G \) seems to be hard in general. However, in certain cases it can be done. Here we will give two such examples that will be relevant for later results. As \( \text{CIM}_p \) is a 0/1 polytope, that is every coordinate of the vertices are either 0 or 1, it makes sense to consider a change in a single coordinate.

**Definition 1.5 (Addition).** Let \( G \) and \( H \) be two DAGs on node set \([p]\). We say the pair \( \{G, H\} \) is an addition if \( c_H = c_G + e_{S^*} \) for some \( S^* \subset [p] \) with \( |S| \geq 2 \). We further say that \( \{G, H\} \) is an edge addition if \( |S^*| = 2 \) and a v-structure addition if \( |S^*| = 3 \).

One can equivalently define an addition as \( c_G \) and \( c_H \) having Hamiltonian distance 1 from one another. As \( \text{CIM}_p \) is a 0/1-polytope this also implies that convex hull \( \text{conv}(c_G, c_H) \) is an edge whenever \( \{G, H\} \) is an addition. The partition into edge- and v-structure additions becomes clearer in light of the following proposition. We see that not only are all additions either an edge or v-structure addition, but we also characterize them in terms of the underlying graphs, \( G \) and \( H \).

**Proposition 1.6.** Let \( G \) and \( H \) be DAGs on node set \([p]\), and suppose that the pair \( \{G, H\} \) is an addition such that

\[ c_H = c_G + e_{S^*}, \]
where $|S^*| \geq 2$. Then either $S^* = \{i, j\}$ for some $i, j \in [p]$, all v-structures of $\mathcal{H}$ are present in $\mathcal{G}$, and the skeletons of $\mathcal{G}$ and $\mathcal{H}$ differ by the presence of the edge $\{i, j\}$, or $S^* = \{i, j, k\}$ and $\mathcal{G}$ and $\mathcal{H}$ have the same skeleton but differ by a single v-structure $i \rightarrow k \leftarrow j$.

**Proof.** Suppose first that $|S^*| = 2$. Then $S^* = \{i, j\}$ for some $i, j \in [p]$ for which $c_G(\{i, j\}) = 0$ and $c_H(\{i, j\}) = 1$, and so the skeletons of $\mathcal{G}$ and $\mathcal{H}$ differ by the presence of the edge $\{i, j\}$. Since $c_H = c_G + e_{S^*}$, it follows that $c_H(S) = c_G(S)$ for all $S \subseteq [p]$ with $|S| = 3$. By Lemma 1.2 we have $c_H(S) = 1$ for such an $S$ if and only if $S$ is complete in $\mathcal{H}$ or if the induced subgraph $\mathcal{H}_S$ is a v-structure. Moreover, if the set $S = \{i, j, k\}$ is not complete in the skeleton of $\mathcal{H}$, then there is at most one way to orient its edges on $\{i, j, k\}$ to produce a v-structure. Thus, since $c_H(S) = c_G(S)$ for all $S \subseteq [p]$ with $|S| = 3$, it follows that $\mathcal{G}$ and $\mathcal{H}$ have the same v-structures except for possibly v-structures of the form $i \rightarrow k \leftarrow j \in \mathcal{G}$ for some $k \in [n]$.

Suppose now that $|S^*| = 3$. Then $S^* = \{i, j, k\}$ for some $i, j, k \in [p]$. Since $c_H = c_G + e_{S^*}$, it follows that $\mathcal{G}$ and $\mathcal{H}$ have the same skeleton and that $c_G(S^*) = 0$. Hence, we know that $S^*$ is not complete in either of $\mathcal{G}$ or $\mathcal{H}$. From this, and the fact that $c_H(S^*) = 1$, it follows that the induced subgraph $\mathcal{H}_S$ of $\mathcal{H}$ is a v-structure. Since $c_G(S) = c_H(S)$ for all $S \neq S^*$ with $|S| = 3$, a similar argument to the previous case shows that all other v-structures in $\mathcal{G}$ and $\mathcal{H}$ are the same.

Finally suppose that $|S^*| \geq 4$. That gives us $c_G(S) = c_H(S)$ for all $|S| \leq 3$ and by Lemma 1.4 we have $c_G = c_H$, a contradiction. \qed 

From this it also follows that edge additions are a special type of edge pair, and that v-structure additions are a special type of turn pair, as defined in [10]. We will also see how v-structure additions show up naturally in Section 3.2.

In the next case we instead show that restricting the skeleton, as opposed to restricting a relation between the characteristic imsets, can also lead to cases where we can describe the edges. This next example will also be useful later when we consider trees. First we will give one lemma. Given a finite set $P$, let $\mathbb{R}[P]$ denote the vector space of dimension $|P|$ where the basis vectors are indexed by the elements of $P$.

**Lemma 1.7.** Given a finite partial order $(P, \preceq)$. Define $b_p$ for any $p \in P$ as

$$b_p := \sum_{q \preceq p} e_q$$

where $e_q$ denotes the standard basis of $\mathbb{R}[P]$. Then $\{b_p\}_{p \in P}$ is a basis for $\mathbb{R}[P]$.

**Proof.** By the Möbius inversion formula $e_p = \sum_{q \preceq p} \mu_P(q, p) b_q$. Thus $b_p$ is the image of $e_p$ under an invertible linear transformation. The result follows. \qed 

Then we consider the following case:

**Proposition 1.8.** Assume $G' = ([p - 1], E')$ is a vertex disjoint union of complete graphs $K_{p_1}, \ldots, K_{p_m}$. Let $G = ([p], E)$ be the graph with $v_G(p) = [p - 1]$ and the induced graph $G_{[p - 1]} = G'$. Then $\text{CIM}_G$ is a $d$-simplex with $d = 2^{p-1} - 1 - \sum_{s \in [m]} (2^{p_s} - 1)$.

**Proof of Proposition 1.8.** We begin by counting the number of MECs. As the MEC is determined by the skeleton and v-structures, and we have fixed the skeleton,
we only need to consider sets \( \{i, j, k\} \) such that \( G_{\{i,j,k\}} = i-j-k \). From the assumptions on \( G \) all triples of this form have \( j = p, i \in K_p, \) and \( k \in K_{p'} \) where \( s \neq s' \).

Thus, the MEC of \( \mathcal{G} \) is completely determined by \( \text{pa}_G(p) \). If \( |\text{pa}_G(p)| \leq 1 \) we have no v-structures, and all such DAGs are Markov equivalent. Likewise, if \( \text{pa}_G(p) \subseteq K_p \) for some \( s \in \{m\} \). Hence, the number of MECs are counted as 1 plus the number of ways to choose \( \text{pa}_G(p) \) such that \( |\text{pa}_G(p)| \geq 2 \) and \( \text{pa}_G(p) \not\subseteq K_p \) for any \( s \in \{m\} \). Using the fact that \( \sum_{s \in \{m\}} p_s = p - 1 \), this quantity is

\[
1 + 2^{p-1} - (p - 1) - 1 - \sum_{s \in \{m\}} (2^{p_s} - p_s - 1) = 2^{p-1} - \sum_{s \in \{m\}} (2^{p_s} - 1).
\]

Next we wish to show that all \( c_\mathcal{G} \) are affinely independent. Let \( \mathcal{D} \) be a DAG such that \( \text{pa}_\mathcal{D}(p) = \emptyset \) and skeleton \( G \), then \( \mathcal{D} \) has no v-structures. Using the above, a straightforward calculation then gives us that for any DAG \( \mathcal{G} \) with skeleton \( G \) we get

\[
c_\mathcal{G} = c_\mathcal{D} + \sum_{S \in \mathcal{S}} e_S
\]

where \( \mathcal{S} = \{T \cup \{p\} : T \subseteq \text{pa}_\mathcal{G}(p), \not\exists s \in \{m\} \text{ such that } T \subseteq K_p \} \). Notice that we do not have any sets of size 2 or less in \( \mathcal{S} \). Moreover, the parents of \( p \) uniquely determine the MEC unless we are in the class containing \( \mathcal{D} \). Thus,

\[
P := \{T \cup \{p\} : |S| \geq 2, \not\exists s \in \{m\} \text{ such that } T \subseteq K_p \} \cup \{\emptyset\}
\]

can be partially ordered by inclusion and for every DAG \( \mathcal{G} \) there exists a unique \( S \in P \) such that \( c_\mathcal{G} = c_\mathcal{D} + \sum_{T \in P} e_T \). Thus we can apply Lemma 1.7 to \( \{c_\mathcal{G} - c_\mathcal{D} : \mathcal{G} \text{ a DAG with skeleton } G\} \), and the result follows.

Applying the above proposition with \( p_i = 1 \) for all \( i \) we get the following lemma:

**Lemma 1.9.** If \( G = ([p], E) \) is a star, then \( \text{CIM}_G \) is a \( 2^p - p - 1 \)-simplex.

The proof of Proposition 1.8 is possible due to the fact that the skeleton imposes a one-to-one correspondence between the MECs and the principal order ideals of a poset. In Section 3.4 we will see another example of when this method can be applied, however, it seems that this is a rather rare quality of \( G \).

All edges we have encountered thus far are, in a sense, local in the graph; i.e., all known edges only depend on vertices that are, or will become, neighbours. The question then arises whether all edges of \( \text{CIM}_p \) are local, or if there are edges \( \text{conv}(c_\mathcal{G}, c_\mathcal{H}) \) where the relation between \( \mathcal{G} \) and \( \mathcal{H} \) depends on some global structure.

2. Trees

In this section we will examine the edge structure of \( \text{CIM}_G \) when \( G \) is a tree. As we saw in Lemma 1.9, \( \text{CIM}_G \) is a simplex when \( G \) is a star. In this section we will see how this can be used to impose a local structure on essential graphs whose skeleton is a tree. With this local structure we then impose more global structures and are able to recover all edges of \( \text{CIM}_G \). Our first characterization will be in terms if essential graphs. As this characterization might be hard to deal with in practice, we will give a characterization in terms of DAGs as well (see Section 2.2).
2.1. The Essential Side of the Trees. The authors of [1] introduced the essential graph as a unique representative of an MEC. As edges of a polytope, in a sense, represent a minimal change between vertices, the question of finding edges of CIM becomes “what does a minimal change of the essential graph look like?”. To answer this question we introduce essential flips (Definition 2.5), and show that these indeed characterize the edges of CIM when G is a tree.

As previously mentioned, in [1] the authors gave a complete characterization of the directed edges of essential graphs. However, in the case of trees, the criterion simplifies significantly. In the later proofs we will frequently make use of the following proposition.

Proposition 2.1. Let G be a DAG whose skeleton is a tree. An arrow i → j is essential in G if and only if either

1. There is a node k such that i → j ← k is an induced subgraph of G, or
2. i is a descendant of a node with (at least) two parents.

Proof. Suppose first that there exists a node k such that i → j ← k is an induced subgraph of G. As this forms a v-structure, it follows that i → j is essential. Suppose next that there is an ancestor k of i such that k has two parents, say p1 and p2. Assume for the sake of contradiction that i → j is non-essential. Since i is a descendant of k, there exists a directed path from k to j in G: k → k1 → ··· → km → i → j. If i → j is non-essential then there exists an element of the Markov equivalence class of G, say H, in which i ← j. Since G has skeleton a tree and km → i → j in G is not a v-structure, then it is also not a v-structure in H. Since H must have the same skeleton as G, it must be that km ← i in H. Iterating this argument up the directed path from k to j in G, we get that H contains the directed path k ← k1 ← ··· ← km ← i ← j. However, k has two parents, p1 and p2, and, as the skeleton of G was a tree, hence G contains the v-structure p1 → k ← p2. Since the triples p1, k, k1 and p2, k, k1 do not form v-structures in G they must also not form v-structures in H. Hence, it must be that p1 ← k and p2 ← k in H, meaning that H lacks a v-structure that is in G, a contradiction.

Conversely, suppose that i → j is essential in G. Then i → j is strongly protected in the essential graph D of G. Since G a tree it follows that either (a) i → j ← k0 or (b) k0 → i → j is an induced subgraph of D for some node k0. In the case that we have (a), we are done. In the case that we have only (b), we know that k0 → i is essential in D (as it is directed in D). Hence, iterating this argument assuming that the new edge is always strongly protected as in (b), we find a directed path in D: k_m → k_{m-1} → ··· → k_0 → i → j where pa_D(k_m) = ∅ and pa_D(k_i) = {k_{i+1}} for i = 0, . . . , m − 1. In this case, k_m → k_{m-1} is not strongly protected in D, which is a contradiction.

We then have the following lemma.

Lemma 2.2. Let G be a DAG whose skeleton is a tree. If i → j is an essential arrow of G then every edge with j as an endpoint is essential in G.

Proof. If i → j is essential and k is adjacent to j then either i → j ← k is a v-structure in G or i → j → k is an induced subgraph of G. In the latter case, by Proposition 2.1, since i → j is essential, either we have a v-structure at j or i is a descendant of a node with two non-adjacent parents in G. Regardless of the case, it follows from Proposition 2.1 (2) that the arrow i → k is also essential in G. □
Proof. Suppose there is a v-structure centered at only if $G|j \in \mathcal{S}$.

Lemma 2.4. Let $\mathcal{G}$ and $\mathcal{H}$ be two essential graphs with skeleton $G = ([p], E)$ and assume $G$ is a tree. Let $N_i := \{S \subseteq [p]: i \in S \subseteq \text{ne}_G(i) \cup \{i\}, |S| \geq 3\}$. Then we define

$$\Delta(\mathcal{G}, \mathcal{H}) := \{i \in [p]: c_G|_{N_i} \neq c_H|_{N_i}\}.$$ 

Notice that $\Delta(\mathcal{G}, \mathcal{H})$ is empty if and only of $\mathcal{G}$ and $\mathcal{H}$ are Markov equivalent. The set $\Delta(\mathcal{G}, \mathcal{H})$ is natural to consider since it can equivalently be defined as all nodes $j$ such that we have a v-structure $i \rightarrow j \leftarrow k$ in $\mathcal{G}$ but not in $\mathcal{H}$, or vice versa.

Lemma 2.4. Let $\mathcal{G}$ and $\mathcal{H}$ be two essential graphs on node set $[p]$. Suppose $\mathcal{G}$ and $\mathcal{H}$ both have the same skeleton $G$ and that $G$ is a tree. Then $j \in \Delta(\mathcal{G}, \mathcal{H})$ if and only if $\mathcal{G}$ and $\mathcal{H}$ contain different sets of v-structures centered at $j$.

Proof. Suppose there is a v-structure centered at $j$ in $\mathcal{G}$ that is not in $\mathcal{H}$, say $i \rightarrow j \leftarrow k$. Then $\{k, j, i\} \in N_j$ and $c_G(\{k, j, i\}) = 1 \neq 0 = c_H(\{k, j, i\})$. Thus, $j \in \Delta$.

Conversely, suppose that $j \in \Delta$. Then there exists $S \subseteq N_j$ such that $c_G(S) \neq c_H(S)$. Without loss of generality, assume $c_G(S) = 1$ and $c_H(S) = 0$. Since $j \in S$ and $G$ is a tree, then $c_G(S) = 1$ if and only if $k \rightarrow j$ for all $i \in S \setminus \{j\}$. Thus, since $|S| \geq 3$, $\mathcal{G}$ contains a v-structure that is not in $\mathcal{H}$. \hfill $\square$

Now we have an understanding of both the essential graphs and how a change in the characteristic imset affects changes in v-structures and vice versa. With this we can present the relation of particular interest of this section.

Definition 2.5 (Essential flip). Let $\mathcal{G}$ and $\mathcal{H}$ be two non-Markov equivalent essential graphs with skeleton $G$, a tree, and denote $\Delta = \Delta(\mathcal{G}, \mathcal{H})$. Assume that both $\mathcal{G}|_{\text{span}(\Delta)}$ and $\mathcal{H}|_{\text{span}(\Delta)}$ do not contain any undirected edges. Assume moreover that each edge of $\mathcal{G}$ and $\mathcal{H}$ differ on $G|_{\text{span}(\Delta)}$. Then we say that the pair $\{\mathcal{G}, \mathcal{H}\}$ is an essential flip.

For convenience we will say that a pair of DAGs constitutes an essential flip if their essential graphs constitute an essential flip. Let us consider an example of an essential flip.

Example 2.6. In Figure 1 we give two graphs $\mathcal{G}$ and $\mathcal{H}$ such that $\{\mathcal{G}, \mathcal{H}\}$ constitutes an essential flip. Here we have $\Delta(\mathcal{G}, \mathcal{H}) = \{\delta_i\}_{i=1}^n$. We see that edges outside $G|_{\text{span}(\Delta(\mathcal{G}, \mathcal{H}))}$ can change both direction and essentiality. Moreover, the inclusion $\Delta(\mathcal{G}, \mathcal{H}) \subseteq \text{span}(\Delta(\mathcal{G}, \mathcal{H}))$ can be strict, here with $n_3 \in \text{span}(\Delta(\mathcal{G}, \mathcal{H})) \setminus \Delta(\mathcal{G}, \mathcal{H})$.

While the definition of essential flips may seem unintuitive they give us a complete characterization of edges of the CIM$_G$ polytope, whenever $G$ is a tree.

Theorem 2.7. If $G$ is a tree, then $\text{conv}(c_G, c_H)$ is an edge of CIM$_G$ if and only if the pair $\{\mathcal{G}, \mathcal{H}\}$ is an essential flip.

This is the result of Proposition 2.8 and Proposition 2.11 below, each showing one way of the equivalence.
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\[ \delta_1 \delta_2 \delta_3 \delta_4 \delta_5 \delta_6 \delta_7 \]
\[ n_1 n_2 n_7 n_8 n_1 n_2 n_7 n_8 \]
\[ \delta_1 \delta_3 \delta_5 \delta_6 \delta_7 \delta_9 \delta_11 \]
\[ n_3 n_4 n_5 n_6 n_4 n_5 n_6 n_3 \]
\[ \delta_2 \delta_4 \delta_3 \delta_6 \delta_7 \delta_6 \delta_7 \]
\[ n_9 n_10 n_10 n_9 \]
\[ \delta_7 \delta_1 \delta_2 \delta_1 \delta_2 \]
\[ n_11 n_12 n_12 n_11 \]

\[ \mathcal{G} \]
\[ \mathcal{H} \]
\[ \mathcal{D} \]

**Figure 1.** An example of an essential flip \( \{ \mathcal{G}, \mathcal{H} \} \). Here we have \( \Delta(\mathcal{G}, \mathcal{H}) = \{ \delta_i \}_{i=1}^7 \). Here we also give \( \mathcal{D} \) as an example for the proof of Proposition 2.8, it can however also be checked that both \( \{ \mathcal{G}, \mathcal{D} \} \) and \( \{ \mathcal{H}, \mathcal{D} \} \) also constitute essential flips. See Example 2.6 and Example 2.9 for more details.

**Proposition 2.8.** If \( \{ \mathcal{G}, \mathcal{H} \} \) is an essential flip where \( \mathcal{G} \) and \( \mathcal{H} \) are essential graphs with skeleton \( G \), and \( G \) is a tree, then \( \text{conv}(c_\mathcal{G}, c_\mathcal{H}) \) is an edge of \( \text{CIM}_G \).

As the following proof is rather technical we advise the reader to keep Example 2.6 and Example 2.9 in mind.

**Proof.** Throughout this proof we will say that an essential graph \( \mathcal{D} \) looks like \( \mathcal{G} \) (or \( \mathcal{H} \)) at \( i \) if we have \( c_\mathcal{D}|_{\mathcal{N}_i} = c_\mathcal{G}|_{\mathcal{N}_i} \) (or \( c_\mathcal{D}|_{\mathcal{N}_i} = c_\mathcal{H}|_{\mathcal{N}_i} \)). Equivalently, via Lemma 2.4, \( \mathcal{D} \) looks like \( \mathcal{G} \) at \( i \) if and only if \( \mathcal{D} \) and \( \mathcal{G} \) share the same \( v \)-structures centered at \( i \). We will find successively smaller faces of \( \text{CIM}_G \), each containing both \( c_\mathcal{G} \) and \( c_\mathcal{H} \). Each of these faces will be defined via cost functions \( W_1, \ldots, W_6 \) that successively imposes more restrictions on the essential graphs encoding for vectors in the faces. In some sense, \( W_1 \) will fix all coordinates that \( c_\mathcal{G} \) and \( c_\mathcal{H} \) share, \( W_2 \) will make sure
that around each node we will look like either $G$ or $H$, and $W_3$ will direct all paths in $G_{|\text{span}(\Delta)}$. $W_3$ will make sure that for each non-endpoint of paths, $i \in \text{span}(\Delta)$ we have that if we locally look like $G$ around $i$, we have a path $P \subseteq \text{span}(\Delta)$ with $i \in P$ that is directed as in $G$, and similarly if we look like $H$. Using $W_3$ we will make all paths be directed as in either $G$ or $H$, as opposed to some directed as in $G$ and some as in $H$, and $W_3$ will take care of the endpoints of paths in a similar fashion as $W_3$ took care of non-endpoints. Crucially, in our construction we will have score functions $g_i$ and $h_i$ that are indicator functions of the $v$-structures of $G$ and $H$, respectively, around a node $i$. These are constructed via Lemma 1.9. We will continuously use Lemma 2.2, which states that if we have an essential edge $i \leftarrow j$ in $G$, then $G_{|\text{cl}(i)}$ is fully directed. We will also say that an essential graph $D$ maximizes a cost function $W$ if $c_D$ maximizes $W^T c_D$.

We begin by defining

$$W_1(S) := \begin{cases} 1 & \text{if } c_G(S) = c_H(S) = 1, \\ -1 & \text{if } c_G(S) = c_H(S) = 0, \\ 0 & \text{otherwise.} \end{cases}$$

Then any essential graph $D$ maximizing $W_1$ must have $c_D(S) = c_G(S)$ whenever $c_G(S) = c_H(S)$. 

Restricting $\text{CIM}_G$, via projection, to $\text{span}(e_S: S \in N_i)$ is the same as considering $\text{CIM}_{G_{|\text{cl}(i)}}$, as the value of the characteristic imset $c_D(S)$ only depends on $D|S$. As $G$ is a tree, $G_{|\text{cl}(i)}$ is a star and thus, by Lemma 1.9, $\text{CIM}_{G_{|\text{cl}(i)}}$ is a simplex. Hence, for each node $i \in [p]$ there exists an affine function $w_i$ such that $w_i$ only depends on $N_i$ and maximizes on $\text{conv}(c_G|_{N_i}, c_H|_{N_i})$. Moreover, as $\text{CIM}_{G_{|\text{cl}(i)}}$ is a simplex, we can assume that $w_i^T c_g = w_i^T c_H = 1$ and $w_i^T c_D = -1$ if $c_D|_{N_i} \neq c_G|_{N_i}$ and $c_D|_{N_i} \neq c_H|_{N_i}$. Then let $W_2 = \sum_{i \in [p]} w_i$. It follows that $W_2^T c_G = W_2^T c_H = p$ and that $W_2^T c_D < p - 1$ if we do not have $c_D|_{N_i} = c_G|_{N_i}$ or $c_D|_{N_i} = c_H|_{N_i}$ for every $i \in [p]$. Note that if $N_i = \emptyset$, that is $|\text{ne}_G(i)| \leq 1$, for some $i \in [p]$ we get that $w_i$ is the constant function 1.

Similarly, for every $i \in \Delta$ we can let $g_i$ and $h_i$ be affine functions that only depend on $N_i$ and satisfy

$$h_i^T c_G = g_i^T c_G = 1, \quad g_i^T c_H = h_i^T c_G = 0,$$

and

$$g_i^T c_D = h_i^T c_D = 0, \quad c_D|_{N_i} \neq c_G|_{N_i} \quad \text{and} \quad c_D|_{N_i} \neq c_H|_{N_i}.$$ 

For every $i \in [p] \setminus \Delta$ we let $g_i$ and $h_i$ be affine functions, again only dependent on $N_i$, such that $h_i^T c_G = g_i^T c_G = 1$ and $g_i^T c_D = 0$ if $c_D|_{N_i} \neq c_G|_{N_i}$. Then $g_i$ and $h_i$ work as indicator functions for an essential graph looking like $G$ or $H$ around $i$, in terms of $v$-structures.

Let $C$ be the set of all directed paths in $G_{|\text{span}(\Delta)}$. Since $G$ and $H$ differ on every edge of $G_{|\text{span}(\Delta)}$, this is also the set of directed paths in $H_{|\text{span}(\Delta)}$. Let $C$ be partially ordered by inclusion. Later in the proof, a maximal path will refer to a maximal path in $C$ with respect to this partial order. Take $P = (v_0, v_1, \ldots, v_n)$ to be a maximal element of $C$, by symmetry we can assume that we have $v_0 \rightarrow v_1 \rightarrow \cdots \rightarrow v_n$ in $G$. Notice that by definition of essential flip we have $v_0 \leftarrow v_1 \leftarrow \cdots \leftarrow v_n$ in $H$.

We will now construct $W_3$ and show that $c_G$ and $c_H$ maximize $W_3$ under the assumption that we maximize $W_1$ and $W_2$, which both $c_G$ and $c_H$ do. Therefore, assume that $D$ is an essential graph maximizing $W_1$ and $W_2$. By construction of $W_1$
and $W_2$ this is the same as either $c_D|_{N_k} = c_G|_{N_k}$ or $c_D|_{N_k} = c_H|_{N_k}$ for all $k \in [p]$.

Since the edge $v_0 \rightarrow v_1$ is directed in $G$, by Proposition 2.1, we have three cases; 

**Case I:** there exists a v-structure $i \rightarrow v_0 \leftarrow k$ in $G$; 

**Case II:** we have a v-structure $i \rightarrow j \leftarrow k$ with $j \rightarrow \cdots \rightarrow v_0$ in $G$; 

**Case III:** we have a v-structure $v_0 \rightarrow v_1 \leftarrow k$ for some $k \in [p]$. These cases are not exclusive, however at least one must be true.

**Case I:** If $c_D|_{N_{v_0}} = c_G|_{N_{v_0}}$ we must have $c_D(\{i, v_0, k\}) = c_D(\{i, v_0, k\}) = 1$ and hence $D$ must have the v-structure $i \rightarrow v_0 \leftarrow k$ as well. If we have $v_0 \leftarrow v_1$ in $D$ we have the v-structure $i \rightarrow v_0 \leftarrow v_1$ in $D$ but not in $G$, hence $c_D|_{N_{v_0}} \neq c_G|_{N_{v_0}}$. Thus we conclude that if $c_D|_{N_{v_0}} = c_G|_{N_{v_0}}$ then $v_0 \rightarrow v_1$ in $D$.

**Case II:** If $j \in \Delta$ we then have a directed path $j \rightarrow \cdots \rightarrow v_0 \rightarrow \cdots \rightarrow v_n$ bigger than $P$ in $G|_{\text{span}(\Delta)}$, contradicting the maximally of $P$ in $C$. In the same way we get that $j' \notin \Delta$ for all $j'$ on the path between $j$ and $v_0$. Hence $c_G|_{N_i} = c_H|_{N_i} = c_P|_{N_i}$ for all $i$ between $i$ and $v_0$, including $i$ but not $v_0$ as $D$ maximized $W_1$. Thus we have an essential edge $\rightarrow v_0$ in $G$, $H$ and $D$. We can by Lemma 2.2 say that if $c_D|_{N_{v_0}} = c_G|_{N_{v_0}}$ we must have $v_0 \rightarrow v_1$ in $D$.

**Case III:** If $c_D|_{N_{v_1}} = c_G|_{N_{v_1}}$, then $D$ must have the v-structure $v_0 \rightarrow v_1 \leftarrow k$. Hence if $c_D|_{N_{v_1}} = c_G|_{N_{v_1}}$, we must have $v_0 \rightarrow v_1$ in $D$. Notice the difference in index from the previous cases, $v_1$ instead of $v_0$.

Hence no matter the case there exists a node $\alpha \in \Delta$ such that $c_D|_{N_{\alpha}} = c_G|_{N_{\alpha}}$ implies that $v_0 \rightarrow v_1 \in D$, under the assumption that $D$ maximizes both $W_1$ and $W_2$. Similarly there exists a node $\beta \in \Delta$ such that $c_D|_{N_{\beta}} = c_H|_{N_{\beta}}$ implies that $v_{n-1} \leftarrow v_n \in D$. For each maximal path $P$, we fix a pair of these nodes as $\alpha_P$ and $\beta_P$. If possible, as it is in **Case I** and **Case II** above, we choose $\alpha_P$ and $\beta_P$ as endpoints of $P$. In Example 2.9 we have given an example how these vertices are chosen.

For each maximal path in $P = v_0 \rightarrow \cdots \rightarrow v_n$ in $G|_{\text{span}(\Delta)}$ we let $w_P = -(g_{\beta_P} + h_{\alpha_P})$. Define $W_3 = \sum w_P$ where we sum over all maximal paths in $C$. By construction of $w_P$ we have $w_P^2 c_G = w_P^2 c_H = -1$. Again assuming $D$ maximizes $W_1$ and $W_2$, we want to prove that $W_3^2 c_D \leq W_3^2 c_G = W_3^2 c_H$. Then it is enough to show that $w_P^2 c_D \leq w_P^2 c_G = w_P^2 c_H$ for every $P$. If this is not the case, by construction of $w_P$, we have $g_{\beta_P}^T c_D = h_{\alpha_P}^T c_D = 0$. As $D$ maximized $W_1$ and $W_2$ we must have $c_D|_{N_{\beta_P}} = c_H|_{N_{\beta_P}}$ and $c_D|_{N_{\alpha_P}} = c_G|_{N_{\alpha_P}}$. If the length of $P$ is greater than $1$ ($n \geq 2$) we must have $v_0 \rightarrow \cdots \leftarrow v_n$ in $D$, but as neither $G$ or $H$ has a v-structure along the path $v_0 \cdots v_n$, neither can $D$, a contradiction. If $n = 1$ the edge $v_0 \rightarrow v_1$ must be directed in both directions in $D$, which cannot happen. Hence, any essential graph $D$ such that $c_D$ maximizes $W_1$ and $W_2$ has $W_3^2 c_D \leq W_3^2 c_G = W_3^2 c_H$. If $w_P^2 c_D = -2$ for some $P$, we get $W_3^2 c_D \leq W_3^2 c_G - 1 < W_3^2 c_G$. For all maximal paths $P \in C$, as neither $G$ or $H$ has a v-structure along $P$, neither can $D$. Moreover, if $w_P^2 c_D = -1$ we have we must have $g_{\beta_P}^T c_D = 0$ or $h_{\alpha_P}^T c_D = 0$, and as $D$ maximized $W_2$ we get $h_{\beta_P}^T c_D = 1$ or $g_{\alpha_P}^T c_D = 1$, respectively. Hence we get $v_0 \rightarrow v_1$ or $v_{n-1} \leftarrow v_n$ in $D$. Thus $D\mid_P$ must be a directed path, assuming $c_D$ maximizes $W_1$, $W_2$ and has $W_3^2 c_D = W_3^2 c_G$. This is what we meant when we said that $W_3$ directs all paths in $G|_{\text{span}(\Delta)}$ either as in $G$ or $H$.

We will now construct $W_4$ that will make sure that if $i$ is not an endpoint of any maximal path in $C$ and a graph $D$ looks like $G$ at $i$, then there is a maximal path $P$ containing $i$ such that $D\mid_P = G\mid_P$, and similar for $H$. This will be similar to how
$W_3$ directed all paths. For example $\delta_5$ in $D$, Figure 1, does not have this property; despite the maximal path $(\delta_3, \delta_4, \delta_5, \delta_6)$ being directed as in $H$, see Figure 1, we have $c_{D'|N_i} = c_{G'|N_i}$.

To avoid this, we consider all nodes $i \in \Delta$ such that $i$ is not the endpoint of any maximal path $P \in C$. As $i \in \Delta$ there must exist a v-structure $k \to i \leftarrow j$ in $G$ or $H$. Assume it is in $G$. Fix a maximal path $P$ with $i \in P$. Notice as $i \in P$, and $i$ has at least one v-structure in $G$, there is at least one v-structure at $i$ containing an edge of $P$ in $G$. This v-structure cannot be present if $P$ is directed as in $H$. Let $w_i' = -(h_i + g_{\beta_i})$. We claim that we cannot have $w_i'^T c_D = 0$ if $c_D$ maximizes $W_1$, $W_2$ and has $W_3^T c_D = W_3^T c_G$. Then we would have $h_i^T c_D = 0$ and $g_{\beta_i}^T c_D = 0$, or, as $c_D$ maximized $W_1$ and $W_2$, $g_{\beta_i}^T c_D = 1$ and $h_i^T c_D = 1$. By the above argument we than get $P|_D = P|_H$, as well as the v-structure in $G$, but as mentioned above this cannot happen. If there was no v-structure at $i$ in $G$, there must have been a v-structure at $i$ in $H$, and hence we let $w_i' = -(h_i + h_{\alpha_i})$ and proceed similarly. Let $W_4 = \sum w_i'$ where we sum over all $i \in \Delta$ that are not endpoints of any maximal paths in $G(\text{span}(\Delta))$. Thus we conclude that any essential graph $D$ that maximizes $W_1$, $W_2$, has $W_3^T c_D = W_3^T c_G$, and $W_4^T c_D = W_4^T c_G$. Then, by our above reasoning, for any two maximal paths $P_1, P_2 \in C$ we have $D|_{P_i}$ are directed paths and coincides with either $G|_{P_i}$ or $H|_{P_i}$. Assume $P_1 \cap P_2$ is non-empty. Then if $|P_1 \cap P_2| \geq 2$, $P_1$ and $P_2$ must share an edge, as $G$ was assumed to be a tree. Then there can only exist two ways of fully directing $P_1 \cup P_2$, which must coincide with either $G$ or $H$. If $P_1 \cap P_2 = \{i\}$ then we either have $c_D|_{N_i} = c_G|_{N_i}$ or $c_D|_{N_i} = c_H|_{N_i}$. By maximality of $P_1$ and $P_2$ we get 3 cases, either $i$ is the source of both $P_1$ and $P_2$ in $G$, $i$ is the endpoint of both $P_1$ and $P_2$ in $G$, or $i$ is a node in the middle of both $P_1$ and $P_2$. We note that if we have at least one v-structure in $c_{G}(i)$ in both $G$ and $H$, then $c_{G}(i)$ must be fully directed whenever we have $c_D|_{N_i} = c_G|_{N_i}$ or $c_D|_{N_i} = c_H|_{N_i}$. Thus we must have $D|_{P_1 \cup P_2} = G|_{P_1 \cup P_2}$ or $D|_{P_1 \cup P_2} = H|_{P_1 \cup P_2}$. In the third case we must have v-structures in both $G$ and $H$. Hence the interesting case is when $i$ is the source of both $P_1$ and $P_2$ in either $G$ or $H$. If it is the source in $G$, let $w_{P_1, P_2} = (2h_i - h_{\beta_P} - h_{\beta_{\beta_P}})$. Otherwise $i$ is the source of $P_1$ and $P_2$ in $H$, and we let $w_{P_1, P_2} = (2g_i - g_{\alpha_P} - g_{\alpha_{\alpha_P}})$. Notice that $w_{P_1, P_2}^T c_G = w_{P_1, P_2}^T c_H = 0$ regardless of which case.

Now that the summends are constructed we can show that these behave as intended, we do however advise the reader to again consider Example 2.9.

Let us begin to show that $w_{P_1, P_2}^T c_D \leq w_{P_1, P_2}^T c_G = 0$ for all appropiate $D$. If we were to have $w_{P_1, P_2}^T c_D > 0$ we must have $h_i^T c_D = 1$ (or $g_i^T c_D = 1$, but it is the same up to symmetry). That is, we have $P_1 \to i \leftarrow P_2$ in $D$. As $D$ was assumed to have $W_3^D c_D = W_3^D c_G$ we must have $(g_{\beta_P} + h_{\alpha_P})^T c_D = 1$. Since we had that $P_1$ is directed as in $H$, we cannot have $g_{\alpha_P}^T c_D = 1$. By assumption $c_D$ maximized $W_2$, hence we then must have $h_{\alpha_P}^T c_D = 1$, and by the above $g_{\beta_P}^T c_D = 0$. Again by the assumption that $c_D$ maximizes $W_2$ we get $h_{\beta_P}^T c_D = 1$. We can repeat this argument with $P_2$ and get $h_{\beta_P}^T c_D = 1$. Hence $w_{P_1, P_2}^T c_D = 0$, a contradiction. Therefore we let
$W_5 = \sum w_{P,Q}$ where we sum over all pairs of maximal paths in $C$ whose intersection is a single point. Then, by the above, we get $W_7^T c_D \leq W_7^T c_G = W_7^T c_H$, assuming that $D$ maximizes $W_1, W_2$, has $W_1^T c_D = W_1^T c_G$, and $W_2^T c_D = W_2^T c_G$. If $D$ would have two maximal paths $P_1$ and $P_2$ such that $P_1 \cap P_2 \neq \emptyset$ but $D|_{P_1} = G|_{P_1}$ and $D|_{P_2} = H|_{P_2}$, then by the above we must have that $P_1$ and $P_2$ intersect in a single point $i$ such that $i$ is the middle of a v-structure in either $G$ or $H$. We can without loss of generality assume it is a v-structure in $H$ and thus a source in $G$. Then we must have $P_1 \rightarrow i \rightarrow P_2$ in $D$. We defined $w_{P_1,P_2} = (2h_i - h_\beta_{P_1} - h_\beta_{P_2})$. As we do not have the v-structure present in $H$ at $i$ in $D$ we must have $h_\beta_i c_D = 0$, but as argued above we must have $h_\beta_i c_D = 1$. Hence, $w_{P_1,P_2} c_D < w_{P_1,P_2} c_G$.

So far we have constructed $W_1, \ldots, W_5$ that direct all paths in $C$ either as in $G$ or $H$. With $W_5$, we made sure that if $c_D|_{N_i} = c_G|_{N_i}$ for any node $i$ that is not the endpoint of a maximal path in $C$ there exists a path $P$ with $i \in P$ such that $D|_P = G|_P$. Now we want similar guarantees for the endpoints as well. Due to our choice to have $\alpha_P$ and $\beta_P$ as endpoints whenever possible, $W_3$ does exactly that in Cases I and II. We will see this later in the proof. Thus let us consider the endpoints of maximal paths that had $\alpha_P$ or $\beta_P$ from Case III above. Assume there exists a node $i \in \Delta$ such that $i$ is the endpoint of a path $i \rightarrow P$ in $G$ (or $H$) and we do not have any v-structures in $G|_{cl(i)}$. Then we let $w''_i = -\left(g_i + h_\beta_P\right)$ and $W_6 = \sum w''_i$. Assume $D$ is an essential graph such that $c_D$ maximizes $W_1, W_2$, has $W_3^T c_D = W_3^T c_G$, $W_4^T c_D = W_4^T c_G$, and $W_5^T c_D = W_5^T c_G$. By assumption we must have $i \leftarrow P$ in $H$ and we must moreover have a v-structure in $H|_{cl(i)}$ as $i \in \Delta$. If $g_i ^T c_D = 0$ by $W_2$ we get $h_i ^T c_D = 1$. Thus the first edge of $P$ must be directed as in $H$ in $D$. Hence, we cannot have $g_i ^T c_D = 1$ as that would direct $P$ as in $G$. By $W_2$ we get $g_i ^T c_D = 0$, and thus $h_i ^T c_D = 1$. By $W_3$ we get $g_\beta_P c_D = 0$ and again by $W_2$ we get $h_\beta_P c_D = 1$. Hence $W_6^T c_D \leq W_7^T c_G = W_7^T c_H$.

Now that we have constructed $W_1, \ldots, W_6$ we are in a position to finish the proof. So far we have proved that there is a face $F$ of CIM$_G$ such that $c_D \in F$ if and only if $D$ maximizes $W_1, W_2$, has $W_3^T c_D = W_3^T c_G$, $W_4^T c_D = W_4^T c_G$, $W_5^T c_D = W_5^T c_G$, and $W_6^T c_D = W_6^T c_G$. Now we want to show $F$ only contains the vertices $c_G$ and $c_H$, that is $F = \text{conv}(c_G, c_H)$. By construction of $W_1, \ldots, W_6$ it follows that $\text{conv}(c_G, c_H) \subseteq F$.

Let $D$ be an essential graph such that $c_D \in F$; that is, $D$ maximizes $W_1, W_2$, has $W_3^T c_D = W_3^T c_G$, $W_4^T c_D = W_4^T c_G$, $W_5^T c_D = W_5^T c_G$, and $W_6^T c_D = W_6^T c_G$. Then for all $i \notin \Delta$ we have $c_D|_{N_i} = c_G|_{N_i} = c_H|_{N_i}$, as $c_D$ maximized $W_1$. For any fixed $i \in \Delta$, as $c_D$ maximized $W_2$ we have that either $c_D|_{N_i} = c_G|_{N_i}$ or $c_D|_{N_i} = c_H|_{N_i}$. By symmetry we can assume that $c_D|_{N_i} = c_G|_{N_i}$.

We want to show that there exists a maximal path $P \in C$ with $i \in P$ such that $D|_P = G|_P$. If $i$ is not the endpoint of a maximal path in $C$, we can choose $P$ to be the same path as when we constructed $w'_i$ (see the construction of $W_4$). As $c_D$ maximized $W_1, W_2$, had $W_3^T c_D = W_3^T c_G$, and $W_4^T c_D = W_4^T c_G$ we can apply the same argument as there and obtain $P$.

Otherwise $i$ is the endpoint of some maximal path $P \in C$. If we have a v-structure in $G|_{cl(i)}$, then $G|_{cl(i)}$ must be fully directed. As $c_D|_{N_i} = c_G|_{N_i}$ we get that $D|_{cl(i)}$ is fully directed, specifically the edge in $cl(i)$ belonging to $P$. Thus $P$ must be directed the same way in both $G$ and $D$. If we do not have a v-structure in $G|_{cl(i)}$ we must have a v-structure in $H|_{cl(i)}$, as $i \in \Delta$. Then we can divide this into two cases, either $P \rightarrow i$ in $G$ or $P \leftarrow i$ in $G$. In the case of $P \rightarrow i$ in $G$ we
have $P \leftarrow i$ in $\mathcal{H}$, as $P \in \mathcal{C}$ and thus $P \subseteq \text{span}(\Delta)$. Thus following our cases we must have chosen $\beta_P = i$. As $W_3^T \mathcal{C}_P = W_3^T \mathcal{C}_G$ we have $(g_i + h_{\beta_P})^T \mathcal{C}_D = 1$ and since $\mathcal{C}_D|_{\mathcal{N}_i} = c_{\mathcal{G}}|_{\mathcal{N}_i}$, we must have $h_{\beta_P}^T \mathcal{C}_D = 0$. Then we get that $g_{\alpha_P}^T \mathcal{C}_D = 1$, thus $\mathcal{D}|_P = \mathcal{G}|_P$ and hence $P$ is a valid choice. In the case of $P \leftarrow i$ in $\mathcal{G}$ we are exactly in the case where we created $w''_P$. Then we have $(g_i + h_{\beta_P})^T \mathcal{C}_D = 1$, which gives us $h_{\beta_P}^T \mathcal{C}_D = 0$, by $W_2$ we get $g_{\alpha_P}^T \mathcal{C}_D = 1$, and again by $W_2$ we get $g_{\alpha_P}^T \mathcal{C}_D = 1$. Hence $P$ must be directed as in $\mathcal{G}$ in $\mathcal{D}$.

Now the proof reduces to taking another node $j$ and showing that $\mathcal{C}_D|_{\mathcal{N}_j} = c_{\mathcal{G}}|_{\mathcal{N}_j}$. As $\mathcal{C}_D|_{\mathcal{N}_j} = c_{\mathcal{G}}|_{\mathcal{N}_j}$, for all nodes $j \notin \Delta$, as $\mathcal{D}$ maximized $W_1$ and $W_2$, we let $j \in \Delta \setminus \{i\}$. For the sake of contradiction, if $\mathcal{C}_D|_{\mathcal{N}_j} = c_{\mathcal{H}}|_{\mathcal{N}_j}$, by the above, we have two maximal paths, in $\mathcal{C}$, $P_1$ and $P_2$, containing $i$ and $j$ respectively, such that $P_1$ is directed as in $\mathcal{G}$ and $P_2$ is directed as in $\mathcal{H}$. As $\mathcal{G}$ is connected we can find maximal paths $\{Q_k\}_{k=1}^t \in \mathcal{C}$ such that $P_1 = Q_1$, $P_2 = Q_t$, and $Q_k \cap Q_{k+1} \neq \emptyset$ for all $1 \leq k \leq t - 1$. As shown above when constructing $W_5$, since $\mathcal{C}_D \in \mathcal{F}$ we must have $Q_k \cup Q_{k+1}$ is directed as in either $\mathcal{G}$ or $\mathcal{H}$. However, we have $Q_1$ directed as in $\mathcal{G}$ and $Q_k \cap Q_{k+1} \neq \emptyset$. Inductively we get that all $Q_k$ are directed as in $\mathcal{G}$, a contradiction since $Q_t = P_2$ is directed as in $\mathcal{H}$.

Thus the only characteristic imsets in $F$ are $c_{\mathcal{G}}$ and $c_{\mathcal{H}}$. Hence $\text{conv}(c_{\mathcal{G}}, c_{\mathcal{H}})$ is an edge of $\text{CIM}_G$.

**Example 2.9.** In Example 2.6 we gave an example of an essential flip $\{\mathcal{G}, \mathcal{H}\}$, see Figure 1. Following the proof of Proposition 2.8 we have three maximal paths in $\mathcal{C}$, $P_1 = (\delta_3, \delta_2, n_3, b_1)$, $P_2 = (\delta_3, \delta_1, \delta_5, \delta_6)$, and $P_3 = (\delta_3, \delta_1)$ with $\alpha_{P_1} = \delta_2$ (Case III), $\alpha_{P_2} = \delta_4$ (Case I), $\alpha_{P_3} = \delta_5$ (Case III), $\beta_{P_1} = \delta_5$ (Case I), and $\alpha_{P_3} = \beta_{P_3} = \delta_7$ (Case III and Case II, respectively). Notice that if we would not have the convention of choosing endpoints whenever possible we could have chosen $\beta_{P_2} = \delta_5$.

The essential graph $\mathcal{D}$ looks like $\mathcal{G}$ or $\mathcal{H}$ at every node, but is not Markov equivalent to either. It is straightforward to see that $\mathcal{D}$ maximizes $W_1$, $W_2$, and has $W_3^T \mathcal{C}_D = W_3^T \mathcal{C}_G$. However, as $P_2$ is directed as in $\mathcal{H}$ in $\mathcal{D}$ but $\mathcal{C}_D|_{\mathcal{N}_{b_5}} = c_{\mathcal{G}}|_{\mathcal{N}_{b_5}}$, and $\delta_5$ is only in one maximal path, $\mathcal{C}_D$ does not maximize $W_4$.

Moreover, in $\mathcal{D}$ the path $P_1$ is directed as in $\mathcal{G}$ but the path $P_2$ is directed as in $\mathcal{H}$. As the intersection between $P_1$ and $P_2$ is a single point, $\mathcal{D}$ cannot maximize $W_5$ either. Indeed, as $\delta_5$ is the source of $P_1$ and $P_2$ in $\mathcal{G}$ we defined $w_{P_1, P_2} = 2\delta_5 - h_{\delta_5} - h_{\delta_6}$. Then it follows that $w_{P_1, P_2}^T \mathcal{C}_D = -1 < 0 = w_{P_1, P_2}^T \mathcal{C}_G = w_{P_1, P_2}^T \mathcal{C}_H$.

In our construction of $W_6$ when considering $\delta_3$ we could have chosen any one path of $P_1$, $P_2$, or $P_3$. Then, following the construction of $W_6$ we have $w_{P_1}'' = -(g_{b_3} + h_{b_5})$, $w_{P_2}'' = -(g_{b_3} + h_{b_5})$, and $w_{P_3}'' = -(g_{b_3} + h_{b_5})$ as summands in $W_6$. As $\mathcal{D}$ looks like $\mathcal{G}$ at $\delta_3$, both have no $\nu$-structures, but the path $P_2$ is directed as in $\mathcal{H}$ we will have $w_{P_1, P_2}''^T \mathcal{C}_D = w_{P_1, P_2}''^T \mathcal{C}_G = -1$ and $w_{P_1, P_2}''^T \mathcal{C}_H = -2$. Notice that $w_{P_1, P_3}''^T \mathcal{C}_D = w_{P_1, P_3}''^T \mathcal{C}_G = -1$ for all maximal paths $P_1$.

Thus essential flips give rise to edges of $\text{CIM}_G$, and in fact they give us a complete characterization. To show this we will use the following well-known fact.

**Lemma 2.10.** Let $P$ be a polytope and let $v$ be a vertex of $P$. If there exists non-zero vectors $u_1$ and $u_2$ such that $v + u_1$, $v + u_2$, and $v + u_1 + u_2$ are all vertices of $P$, then $\text{conv}(v, v + u_1, v + u_2)$ is not an edge of $P$.

Then the converse of Proposition 2.8 follows as well.
Proposition 2.11. If $G$ and $H$ are essential graphs such that \{G, H\} is not an essential flip, then conv(c_G, c_H) is not an edge of CIM_G, where $G$ is a tree.

Proof. Recall that $\Delta(G, H) = \{i \in [p]: c_G|_{N_i} \neq c_H|_{N_i}\}$. Since \{G, H\} is not an essential flip, by symmetry there either exists an undirected edge in $i \rightarrow j \in G|_{span(\Delta)}$ or we have an edge $i \rightarrow j \in H|_{span(\Delta)}$.

Case I, $i \rightarrow j \in G|_{span(\Delta)}$: Take any DAG $H'$ in the Markov equivalence class of $H$. By symmetry we can assume that $i \rightarrow j \in H'$. Since $i \rightarrow j$ was undirected in $G$, there exists a DAG $G'$ Markov equivalent to $G$ with $i \rightarrow j \in G'$. Let $C_1$ be the nodes in the connected component in $G' \setminus \{i \rightarrow j\}$ containing $i$ and $C_2$ be the complement of $C_1$. Let $D_1$ be the DAG such that $D_1|_{C_1} = H'|_{C_1}$, $D_1|_{C_2} = G'|_{C_2}$, and $i \rightarrow j \in D_1$. Let $D_2$ be the DAG such that $D_2|_{C_1} = G'|_{C_1}$, $D_2|_{C_2} = H'|_{C_2}$, and $i \rightarrow j \in D_2$. Letting $u_1 = c_{D_1} - c_H$ and $u_2 = c_{D_2} - c_{H'}$, we claim that $c_G = c_{H'} + u_1 + u_2$, or, equivalently, $c_{G'} = c_{H'} + u_1 + u_2$. By Lemma 1.4 it is enough to show that $c_G(S) = c_{D_1}(S) + c_{D_2}(S) - c_{H'}(S)$ holds for all sets $S$ of size 2 and 3. Since all $G$, $D_1$, $D_2$, and $H$ all share the same skeleton the equality is true for all sets of size 2.

Then, for any set $S = \{s_1, s_2, s_3\}$, if we do not have that $G|_{S} \simeq P_3$, we have $c_G(S) = c_{D_1}(S) = c_{D_2}(S) = c_{H'}(S) = 0$ and thus the equality holds. If $S \subseteq C_1$ or $S \subseteq C_2$ then either $c_{D_1}(S) = c_{H'}(S)$ and $c_{D_2}(S) = c_{H'}(S)$, or $c_{D_1}(S) = c_{H'}(S)$ and $c_{D_2}(S) = c_{H'}(S)$, respectively. This follows from the construction of $D_1$ and $D_2$. The final case is when $\{i, j\} \subseteq S$, which follows similarly as $G'$, $D_1$, $D_2$, and $H'$ all have the same direction of $i \rightarrow j$, again by construction.

All that is left to check in Lemma 2.10 is that $u_1$ and $u_2$ are non-zero. Equivalently we can say that $D_1$ is not Markov equivalent to either $G$ or $H$. As $i \rightarrow j \in span_G(\Delta)$ and $G$ was a tree we must have $\Delta \cap C_1 \neq \emptyset$ and $\Delta \cap C_2 \neq \emptyset$. Thus there exists nodes $\alpha \in \Delta \cap C_1$ and $\beta \in \Delta \cap C_2$ such that $c_1|_{S_\alpha} = c_H|_{S_\alpha} \neq c_H|_{S_\alpha}$ and $c_{D_1}|_{S_\beta} = c_H|_{S_\alpha} \neq c_H|_{S_\beta}$. Hence $u_1 \neq 0$ and similarly for $u_2$.

Case II, $i \rightarrow j \in G|_{span(\Delta)}$: In this case we can take any two DAGs $G'$ Markov equivalent to $G$ and $H'$ Markov equivalent to $H$. Notice that $i \rightarrow j \in G'$ and $i \rightarrow j \in H'$. Then we can repeat the exact same construction as in Case I.

A remarkable fact about these polytopes is that every non-edge is of the form of Lemma 2.10. This is something rather unusual even for 0/1-polytopes and fails already in dimension 3. The question if this is true for all CIM_G polytopes is open.

2.2. The Directed Side of the Trees. In the previous subsection we gave a description of the edges of CIM_G in terms of essential graphs. However, we are interested in describing transformations of a DAG $G$ that produce a DAG $H$ such that the essential graphs of $G$ and $H$ constitute an essential flip. By definition of essential flips, the difference between two essential graphs $G$ and $H$ is a connected subtree. Thus the difference between two DAGs that constitute an essential flip can only change v-structures in one unique subtree, and all other differences cannot change the essential graph. Thus if two DAGs constitute an essential flip we can assume they differ on a subtree $T$. The following theorem gives a characterization in terms of every internal node $i$ of $T$. Note that we have a symmetry between $G$ and $H$ given by e.g. $T \cap pa_G(i) = T \cap ch_H(i)$ and $pa_G(i) \setminus T = pa_H(i) \setminus T$.

Theorem 2.12. Suppose that $G$ and $H$ are DAGs with the same skeleton $G$ that is a tree. Assume the edges that differ between $G$ and $H$ form a subtree $T$ of $G$. 

Suppose further that \( \Delta(G, \mathcal{H}) \neq \emptyset \). Then the essential graphs of \( \mathcal{H} \) and \( \mathcal{G} \) form an essential flip if and only if each internal node \( i \) of \( T \) satisfy the conditions given below. We use notation \( \{\epsilon_i\} = T \cap ch_2(i) \) and \( \{p_i\} = T \cap pa_2(i) \), when these sets are singletons.

| \( T \cap pa_2(i) \) | \( T \cap ch_2(i) \) | Local criteria for \( \mathcal{G} \) and \( \mathcal{H} \) to form essential flip |
|--------------------|-----------------|---------------------------------|
| \( I \) \( \geq 2 \) | \( \geq 2 \) | |
| \( II \) \( \geq 2 \) | \( 0 \) | |
| \( III \) \( 0 \) | \( \geq 2 \) | |
| \( IV \) \( \geq 2 \) | \( 1 \) | if \( \exists \) v-structure at \( \epsilon_i \) in \( \mathcal{G} \), then \( \epsilon_i \) has essential parent in \( \mathcal{H} \) |
| \( V \) \( 1 \) | \( \geq 2 \) | if \( \exists \) v-structure at \( p_i \) in \( \mathcal{H} \), then \( p_i \) has essential parent in \( \mathcal{G} \) |
| \( VI \) \( 1 \) | \( 1 \) | if there are nodes of \( \Delta \) in both connected components of \( T \setminus \{i\} \) then \( |pa_2(i) \setminus T| \geq 1 \) or \( \epsilon_i \) has essential parent in \( \mathcal{H} \) and \( p_i \) has essential parent in \( \mathcal{G} \) |

**Proof.** Note that all vertices of \( T \) will be of exactly one of the types I-VI or a leaf of \( T \). We will make extensive use of Lemma 2.4 in this proof. In particular, it implies that \( \Delta \) is a subset of the vertices of \( T \), as vertices in \( T \) are the only spots in which \( \mathcal{G} \) and \( \mathcal{H} \) could differ in the presence of v-structures.

By Definition 2.5 of essential flip we must prove the condition that every edge on a path between two nodes in \( \Delta \) is essential in both DAGs. We start by proving that this is true for all edges of the form \( i \leftarrow j \), where \( i \) is of type I-V. If \( |T \cap pa_2(i)| \geq 2 \), then there is a v-structure at \( i \) in \( \mathcal{G} \) not in \( \mathcal{H} \) so \( i \in \Delta \) and by Lemma 2.2, it follows that all edges incident to \( i \) in \( \mathcal{G} \) are essential. Symmetrically, if \( |T \cap ch_2(i)| \geq 2 \) then \( i \in \Delta \) and all edges incident to \( i \) are essential in \( \mathcal{H} \). This implies that vertices of type I-V are always in \( \Delta \). It also implies that all edges incident to a node of type I are essential in both \( \mathcal{G} \) and \( \mathcal{H} \), and hence that case is settled.

Let \( i \leftarrow j \) be any edge in \( T \) and assume by symmetry it is directed \( i \leftarrow j \) in \( \mathcal{G} \) and assume first that \( i \) is of type II or IV and hence essential in \( \mathcal{G} \). We now go through all possibilities for \( j \). Note that \( j \) cannot be of type II since \( i \in ch_2(j) \). If \( j \) is of type III or \( V \), then \( i \rightarrow j \) is essential also in \( \mathcal{H} \) by the previous paragraph. If instead \( j \) is a leaf in \( T \) then \( j \in \Delta \) if and only if \( i \rightarrow j \) is part of a v-structure in \( \mathcal{H} \).

But then \( i \rightarrow j \) is essential in \( \mathcal{H} \) so the condition in Definition 2.5 is true for the edge \( i \leftarrow j \) in either case. The remaining possibility is that \( T \cap ch_2(j) = \{i\} \), that is \( j \) is of type IV or VI, with \( \epsilon_j = i \). If the first local criterion of type IV is true, that is \( |pa_2(j) \setminus T| \geq 1 \) then \( i \rightarrow j \) is part of a v-structure at \( j \) in \( \mathcal{H} \) and hence essential. If \( j \) is of type IV and \( |pa_2(j) \setminus T| = 0 \), the second local criterion for type IV gives that \( i \) has an essential parent in \( \mathcal{H} \) and thus \( i \rightarrow j \) is an essential edge. If \( j \) is of type VI, and there is a node of \( \Delta \) in both connected components of \( T \setminus \{j\} \) then the same reasoning as for type IV is valid. If there is no node of \( \Delta \) in the other part of \( T \setminus \{j\} \), then \( i \rightarrow j \) does not need to be essential.

Note that \( i \) cannot be of type III, since \( i \leftarrow j \). Assume now \( i \) is of type \( V \), then we know that \( i \) has at least two parents in \( \mathcal{H} \) and thus all edges incident to \( i \) in \( \mathcal{H} \), including \( i \rightarrow j \), are essential in \( \mathcal{H} \). By the local criteria in type \( V \), we have either
a parent of \( i \) outside \( T \) making \( i \leftarrow j \) essential in \( G \) or if there exist a v-structure at \( j = p_i \) in \( H \) there is an essential parent of \( j \) in \( G \), which again makes \( i \leftarrow j \) essential in \( G \). We will again go through all possibilities for \( j \). If \( j \) is a leaf in \( T \) then \( j \) is in \( \Delta \) if and only if there is a v-structure at \( j \) in \( H \) and thus \( i \leftarrow j \) is essential in \( G \) as desired. If \( j \) is of type I or IV, then every edge incident with \( j \) is essential in \( G \) including \( i \leftarrow j \). Note that \( j \) has a child in \( G \) and cannot be of type II. If \( j \) is of type III or V, then \( \text{ch}_G(j) = \text{pa}_H(j) \) has at least two elements and thus \( i \rightarrow j \) is part of a v-structure at \( j \) in \( H \) and by the local criterion for type V at \( i \) we thus have an essential parent of \( j \) in \( G \) which implies \( i \leftarrow j \) is essential in \( G \). The last possibility is that \( j \) is of type VI. If \( |\text{pa}_G(j) \setminus T| \geq 1 \) then there is a v-structure at \( j \) in \( G \) and thus \( i \leftarrow j \) is essential in \( G \). If \( |\text{pa}_G(j) \setminus T| = 0 \) then \( j \notin \Delta \) and \( i \leftarrow j \) need to be essential only if there are nodes of \( \Delta \) on both sides of \( T \setminus \{j\} \), in which case the last local criterion for type VI is a reformulation of the conditions in Proposition 2.1.

Finally, assume \( i \) is of type VI. If \( |\text{pa}_G(i) \setminus T| \geq 1 \) then there is a v-structure at \( i \) in both DAGs and all edges incident to \( i \) are essential. If \( |\text{pa}_G(i) \setminus T| = 0 \) then \( i \notin \Delta \). The edge \( i \leftarrow j \) needs to be essential only if there are nodes of \( \Delta \) on both sides of \( T \setminus \{i\} \), in which case the conditions for type VI is a reformulation of the conditions in Proposition 2.1. We have thus proved that the local criteria are sufficient.

For necessity consider first a vertex \( i \) of type IV that does not fulfill the local criteria. That is, \( |\text{pa}_G(i) \setminus T| = 0 \), and there is a v-structure at \( c_i \) in \( G \) but no essential parent of \( c_i \) in \( H \). The v-structure at \( c_i \) implies that \( c_i \in \Delta \) and \( |T \cap \text{pa}_G(i)| \geq 2 \) means \( i \in \Delta \). But since \( \text{pa}_H(i) = \{c_i\} \) and \( c_i \) has no essential parent the edge \( i \leftarrow c_i \) is not essential in \( H \). Thus \( G \) and \( H \) do not form an essential flip. Type V is symmetric to type IV with the roles of \( G \) and \( H \) interchanged.

The remaining case is if \( i \) is of type VI and does not fulfill the local criteria. That is, first that there are nodes of \( \Delta \) in both connected components of \( T \setminus \{i\} \) which means that the two edges incident to \( i \) in \( T \) must both be essential for \( G \) and \( H \) to form an essential flip. And secondly that \( |\text{pa}_G(i) \setminus T| = 0 \), and there is no essential parent of \( c_i \) in \( H \) or no essential parent of \( p_i \) in \( G \). By symmetry we can assume the former and then as in type IV conclude that the edge \( i \leftarrow c_i \) is not essential in \( H \). Thus also the local criteria for type VI are necessary.

3. Examples

We will now consider a few examples of how Theorem 2.7 can be applied. We will begin by extending the results on trees to forests via an observation about disjoint graphs. Then we will show two examples of essential flips that appear naturally when considering paths and cycles. The observations made for these examples lead to a connection between the characteristic imset polytope and the stable set polytope.

We have previously mentioned the turn pairs defined in [10] which strictly generalize edge reversals for arbitrary skeletons \( G \). However, for trees these concepts coincide, as we will show in Section 3.3. We end this section with another example of when Lemma 1.7 can be applied.

3.1. Forests. Apart from this subsection we have and will only consider skeletons \( G \) that are connected, so as to make the results more compact. However, for completeness, we will show how to generalize the results to disjoint graphs. The relevant result is the following:
Proposition 3.1. Let $G = G_1 \cup G_2$ be a disjoint union of $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$. Then $\text{CIM}_G$ is affinely equivalent to $\text{CIM}_{G_1} \times \text{CIM}_{G_2}$.

Proof. Assume we have a DAG $\mathcal{G}$ with skeleton $G$. If $c_\mathcal{G}(S) = 1$, for some set $S \subseteq [p]$ then $G|_S$ is connected. Indeed, since $c_\mathcal{G}(S) = 1$ we have a node $i$ such that $k \to i$ for all $k \in S \setminus \{i\}$, and thus we have $k - i \in G$ for all $k \in S \setminus \{i\}$. Hence for any set $S \subseteq [p]$ we have three cases, $S \subseteq V_1, S \subseteq V_2$, or none of the above. In the third case we immediately get $c_\mathcal{G}(S) = 0$ for any DAG $\mathcal{G}$ with skeleton $G$. It follows that, up to a permutation of indices, $\text{CIM}_G = \text{CIM}_{G_1} \times \text{CIM}_{G_2} \times \mathbb{0}$. Here $\mathbb{0}$ denotes the 0-vector of appropriate length corresponding to the third case above. The result follows. $\square$

Furthermore, it is well-known that if $P$ and $Q$ are two polytopes then any face of $P \times Q$ has the form $F_P \times F_Q$ where $F_P$ and $F_Q$ are faces of $P$ and $Q$ respectively. Hence, if we can characterize all faces of $\text{CIM}_G$ where $G$ is connected, we will also characterize all faces of $\text{CIM}_G$ when $G$ is not necessarily connected. This is especially true in the case of edges as $\dim(F_P \times F_Q) = \dim(F_P) + \dim(F_Q)$, for any non-empty faces $F_P$ and $F_Q$. Thus any edge of $P \times Q$ is of the form $e_P \times v_Q$ or $v_P \times e_Q$, where $e_P$ and $e_Q$ are edges of $P$ and $Q$, and $v_P$ and $v_Q$ are vertices of $P$ and $Q$, respectively. Thus an edge-walk along $P \times Q$ can be done via two simultaneous edge-walks on $P$ and $Q$. The following proposition is direct consequence of Theorem 2.7 and Proposition 3.1.

Proposition 3.2. Let $G$ be a forest and let $\mathcal{G}$ and $\mathcal{H}$ be essential graphs with skeleton $G$. Then $\text{conv}(c_\mathcal{G}, c_\mathcal{H})$ is an edge of $\text{CIM}_G$ if and only if there is a unique subtree $T$ of $G$ such that $\{\mathcal{G}|_T, \mathcal{H}|_T\}$ is an essential flip and $\mathcal{G}|_{G \setminus T} = \mathcal{H}|_{G \setminus T}$.

3.2. Splits, Shifts, and a Connection to Stable Set Polytopes. In Section 2 we considered the edges of $\text{CIM}_G$ polytopes directly. The methods used were specialized towards trees and lack a straightforward generalization. In the following section we will show a connection between another well studied polytope and $\text{CIM}_G$, where $G$ is either $I_p$ or $C_p$. This will allow us to characterize the edges of the path and the cycle. To motivate this, we first mention two examples of essential flips. The idea is that we shift and add $v$-structures along a path in $G$.

Definition 3.3 (Shift). Let $\mathcal{G}$ and $\mathcal{H}$ be two DAGs on node set $[p]$. We say the pair $\{\mathcal{G}, \mathcal{H}\}$ is a shift if there exists a path $\pi = \langle i_0, i_1, \ldots, i_{2m+1} \rangle$ in $\mathcal{G}$ and $\mathcal{H}$ such that

$$c_\mathcal{H} - \sum_{S \in S\pi, \text{odd}} e_S = c_\mathcal{G} - \sum_{S \in S\pi, \text{even}} e_S,$$

where

$$S\pi, \text{odd} := \{\{i_{j-1}, i_j, i_{j+1}\} : j = 1, 3, \ldots, 2m - 1\}$$

and

$$S\pi, \text{even} := \{\{i_{j-1}, i_j, i_{j+1}\} : j = 2, 4, \ldots, 2m\}.$$

Definition 3.4 (Split). Let $\mathcal{G}$ and $\mathcal{H}$ be two DAGs on node set $[p]$. We say the pair $\{\mathcal{G}, \mathcal{H}\}$ is a split if there exists a path $\pi = \langle i_0, i_1, \ldots, i_{2m} \rangle$ such that

$$c_\mathcal{H} - \sum_{S \in S\pi, \text{odd}} e_S = c_\mathcal{G} - \sum_{S \in S\pi, \text{even}} e_S,$$

where

$$S\pi, \text{odd} := \{\{i_{j-1}, i_j, i_{j+1}\} : j = 1, 3, \ldots, 2m - 1\}$$
and
\[ S_{\pi, \text{even}} := \{i_{j-1}, i_j, i_{j+1} \} : j = 2, 4, \ldots, 2m - 2 \].

Both shifts and splits correspond to edges of CIM\(_G\) when G is a tree.

**Proposition 3.5.** Let G and H be two DAGs with the same skeleton G, and suppose that G is a tree. If \( \{G, H\} \) is a shift or a split then \( \text{conv}(c_G, c_H) \) is an edge of CIM\(_G\).

**Proof.** It suffices to show that both shifts and splits constitute essential flips as then the result follows from Theorem 2.7. We first show this for shifts.

By definition of shift we have that \( \Delta(G, H) = \{i_1, \ldots, i_{2m}\} \). Then all we need to show is that \( G|_{\text{span}(\Delta)} \) and \( H|_{\text{span}(\Delta)} \) is fully directed, that is every edge \( i_k - i_{k+1}, \) for \( 1 \leq k \leq 2m - 1 \) is directed in G and H. If \( k \) is even we have \( c_G(\{i_{k-1}, i_k, i_{k+1}\}) = 1 \) and \( c_H(\{i_k, i_{k+1}, i_{k+2}\}) = 1 \), thus \( i_k - i_{k+1} \) is part of a v-structure in both G and H and thus directed. If \( k \) is odd, we have \( c_G(\{i_k, i_{k+1}, i_{k+2}\}) = 1 \) and \( c_H(\{i_{k-1}, i_k, i_{k+1}\}) = 1 \), and by the same reasoning \( i_k - i_{k+1} \) is directed. In both cases \( i_k - i_{k+1} \) is part of a v-structure, and hence directed, but in different directions. Thus shifts are essential flips.

It follows from the definition of splits that \( \Delta(G, H) = \{i_1, i_2, \ldots, 2m - 1\} \), then a split constitutes an essential flip if we can show that every edge \( i_k - i_{k+1}, \) for \( 1 \leq k \leq 2m - 2 \), is directed in both G and H. Then we can divide into cases depending on whether \( k \) is even or odd and proceed exactly as in the case of shifts.

While the above proposition only applies to CIM\(_G\) when G is a tree, we believe that shifts and splits can be generalized to edges of CIM\(_G\) for more arbitrary G. Doing this could be a first step toward extending essential flips to non-trees, and possibly characterizing more edges of CIM\(_G\), regardless of G.

As mentioned, the methods we have used thus far are closely linked to the tree structure of the skeleto, and it is unclear whether they generalize to arbitrary skeletons. To this end we will now consider a relation to another well-studied polytope. Let \( G = ( [p], E) \) be an undirected graph. A set of nodes \( S \subseteq [p] \) is called **stable** (or **independent**) if no nodes of S are joined by an edge. Given a set \( S \subseteq [p] \), its incidence vector \( \chi_S \in \{0, 1\}^p \) is defined by

\[ \chi_S(u) = \begin{cases} 1 & \text{if } u \in S, \\ 0 & \text{if } u \notin S. \end{cases} \]

The **stable set polytope** of G is the convex hull
\[ \text{STAB}(G) := \text{conv}(\chi_S : S \text{ is a stable set in } G) \subseteq \mathbb{R}^p. \]

**Proposition 3.6.** For the path \( I_p \) on \( p \geq 2 \) nodes we have CIM\(_{I_p}\) = STAB\((I_{p-2})\), and for the cycle \( C_p \) on \( p \geq 4 \) nodes,
\[ \text{CIM}_{C_p} = \text{conv}(\chi_S : S \text{ is a non-empty stable set in } G). \]

**Proof.** Since \( I_p \) is the path on \( p \) nodes with edges \( \{i, i+1\} \) for all \( i \in [p-1] \) then for every pair of characteristic imsets \( c_G, c_H \) where G and H are DAGs with skeleton \( I_p \), we have that \( c_G(S) = c_H(S) \) for all \( S \subseteq [p] \), with \( |S| \geq 2 \) and \( S \neq \{i-1, i, i+1\} \) for any \( i \in \{2, \ldots, p-1\} \). Hence, CIM\(_{I_p}\) is affinely equivalent to its projection into \( \mathbb{R}^{p-2} \), where we associate the standard basis vector \( e_i \) with the standard basis vector \( e_{i-1,i+1} \) in \( \mathbb{R}^{2p-1} \). We let \( \rho(c_G) \) denote the image of \( c_G \) under this
projection. The natural bijection between MECs with skeleton $I_p$ and stable sets of $I_{p-2}$ described in [13, Theorem 2.1] then implies that
\[ \{ \rho(c_\mathcal{G}) \in \mathbb{R}^{p-2} : \mathcal{G} \text{ is a DAG with skeleton } I_p \} = \{ \chi_S \in \mathbb{R}^{p-2} : S \text{ a stable set in } I_{p-2} \}. \]

Similarly, since $C_p$ is the cycle on $p$ nodes with edges $\{i, i + 1\}$ for $i \in [p - 1]$ and $\{1, p\}$, and $p \geq 4$, then for every pair of imsets $c_\mathcal{G}$ and $c_\mathcal{H}$ where $\mathcal{G}$ and $\mathcal{H}$ are DAGs with skeleton $C_p$, we have that $c_\mathcal{G}(S) = c_\mathcal{H}(S)$ for all $S \subseteq [p]$ with $|S| \geq 2$ and $S \neq \{i - 1, i, i + 1\}$ for every $i \in [p]$ (where we treat addition modulo $p$). Hence similar to the case of $I_p$, the characteristic imset polytope $\text{CIM}_p$ is affinely equivalent to its projection into $\mathbb{R}^p$, where we map the standard basis vector $e_{i-1, i, i+1}$ in $\mathbb{R}^{2p-p-1}$ to the standard basis vector $e_i$ in $\mathbb{R}^p$, for all $i \in [p]$. Again, applying the bijection in [13, Theorem 2.1] between MECs with skeleton $C_p$ and stable sets in $C_p$ implies that
\[ \{ \rho(c_\mathcal{G}) \in \mathbb{R}^p : c_\mathcal{G} \in \text{CIM}_C \} = \{ \chi_S \in \mathbb{R}^p : S \text{ a non-empty stable set in } C_p \}, \]
which completes the proof. \hfill \qed

Since $\text{CIM}_{I_p}$ and $\text{CIM}_{C_p}$ are, almost, affinely equivalent to stable set polytopes, we can apply a result of Chvátal [3] to give a complete characterization of the edges of $\text{CIM}_{I_p}$ and $\text{CIM}_{C_p}$ in terms of splits, shifts, and $v$-structure additions.

**Theorem 3.7.** [3, Theorem 6.2] Let $G = ([p], E)$ be an undirected graph, let $a, b \in \mathbb{R}^p$ be two vertices of $\text{STAB}(G)$, and let $A$ and $B$ be their corresponding stable sets. Then $\text{conv}(a, b)$ is an edge of $\text{STAB}(G)$ if and only if the subgraph of $G$ induced by $A \setminus B \cup B \setminus A$ is connected.

Hence, to show the desired characterization of the edges of $\text{CIM}_{I_p}$ and $\text{CIM}_{C_p}$, it suffices to characterize the pairs of stable sets in $I_p$ and $C_p$, respectively, for which the subgraph of $I_p$ (or $C_p$) induced by the symmetric difference $A \setminus B \cup B \setminus A$ is connected (i.e., a path or the full cycle).

**Lemma 3.8.** Let $A$ and $B$ be stable sets in $I_p$ (or $C_p$). Then $\text{conv}(\chi_A, \chi_B)$ is an edge of $\text{STAB}(I_p)$ (or $\text{STAB}(C_p)$) if and only if
\begin{itemize}
  \item[(1)] $A \setminus B = \{i, i + 2, \ldots, i + 2j\}$ for some $i$ and $j$, and
  \item[(2)] $B \setminus A = \{i + 1, i + 3, \ldots, i + 2j - 1\}$ or $B \setminus A = \{i + 1, i + 3, \ldots, i + 2j + 1\}$.
\end{itemize}

**Proof.** The proof for $C_p$ works the same as for $I_p$ by taking addition modulo $p$, so we only state it for $I_p$. Suppose that $A$ and $B$ are two stable sets in $I_p$ such that $A \setminus B$ and $B \setminus A$ satisfy conditions (1) and (2). Then $A \setminus B \cup B \setminus A = \{i, i + 1, i + 2, \ldots, i + 2j + 1\}$ for some $i$ and $j$, and hence the induced subgraph on this set is connected. It follows from Theorem 3.7 that $\text{conv}(\chi_A, \chi_B)$ is an edge of $\text{STAB}(I_p)$.

Conversely, if $A$ and $B$ are stable sets of $I_p$ such that $\text{conv}(\chi_A, \chi_B)$ is an edge of $\text{STAB}(I_p)$, then by Theorem 3.7, we know that the subgraph of $I_p$ induced by $A \setminus B \cup B \setminus A$ is connected, and hence must be a subpath of $I_p$, say $\{i, i + 1, \ldots, i + t\}$. Since $A$ and $B$ are stable, then two neighbors on this path cannot belong to the same set $A$ or $B$. It follows that $A \setminus B$ and $B \setminus A$ must satisfy conditions (1) and (2), completing the proof. \hfill \qed

As a consequence of Lemma 3.8, we can characterize all edges of $\text{CIM}_{I_p}$ and $\text{CIM}_{C_p}$. 
**Theorem 3.9.** Let $c_G$ and $c_H$ be two characteristic imsets for DAGs both having skeleton the path $I_p$ (or the cycle $C_p$). Then $\text{conv}(c_G, c_H)$ is an edge of $\text{CIM}_{I_p}$, for $p \geq 2$ if and only if $\{G, H\}$ is a v-structure addition, shift, or split. Moreover $\text{conv}(c_G, c_H)$ is an edge of $\text{CIM}_{I_p}$ if and only if $\{G, H\}$ is a v-structure addition, shift, split, or both $G$ and $H$ contain exactly one v-structure.

**Proof.** By Proposition 3.6, we know that $\text{CIM}_{I_p} = \text{STAB}(I_{p-2}) \subseteq \mathbb{R}^{p-2}$, for $p \geq 2$, and $\text{CIM}_{C_p} = \{S \in \mathbb{R}^p : S$ a non-empty stable set in $C_p\} \subseteq \mathbb{R}^p$, for $p \geq 4$, where we have identified the standard basis vector $e_{i-1,i,i+1} \in \mathbb{R}^{2p-1}$ with the standard basis vector $e_{i-1,i,i+1} \in \mathbb{R}^{p-2}$ and $e_{i-1,i,i+1} \in \mathbb{R}^p$, respectively. Here, we again consider addition modulo $p$ in the case of the cycle $C_p$. Since the hyperplane $\sum_{i=1}^p x_i = 1$ is facet-defining for $\text{CIM}_{C_p} \subseteq \mathbb{R}^p$, the edges of $\text{CIM}_{C_p}$ are precisely the edges of $\text{STAB}(C_p)$ and the standard $p-1$-simplex in $\mathbb{R}^p$, minus those between the origin and the standard basis vectors in $\mathbb{R}^p$. As the same proof works for both the cycle and the path, apart from the previous sentence, in the following we state it only for the path $I_p$.

By Lemma 3.8, we get that for two stable sets $A$ and $B$ in $I_p$, $\text{conv}(\chi_A, \chi_B)$ is an edge of $\text{STAB}(I_{p-2})$ if and only

1. $A \setminus B = \{i, i + 2, \ldots, i + 2j\}$ for some $i$ and $j$, and
2. $B \setminus A = \{i + 1, i + 3, \ldots, i + 2j + 1\}$

As $A \setminus B \setminus A = \{i, i + 1, \ldots, i + m\}$, where $m = 2j$ or $m = 2j + 1$ accordingly, it follows that $\text{conv}(\chi_A, \chi_B)$ is an edge of $\text{STAB}(I_{p-2})$ if and only if $\pi = \langle i, i + 1, i + 2, i + 3, \ldots, i + m \rangle$ is a path in $I_{p-2}$, and

$$\chi_A - \sum_{k \in A \setminus B} e_k = \chi_B - \sum_{k \in B \setminus A} e_k.$$

Following the correspondence between vertices of $\text{CIM}_{I_p}$ and vertices of $\text{STAB}(I_{p-2})$ established above, $\text{conv}(c_G, c_H)$ is an edge of $\text{CIM}_{I_p}$ if and only if $\pi = \langle i, i + 1, i + 2, i + 3, \ldots, i + m + 2 \rangle$ is a path in $I_p$ and

$$c_G - \sum_{\{k-1,k,k+1\} \cap \{i+\ell=k\leq i+m+1\}} c_{\{k-1,k,k+1\}} = c_H - \sum_{\{k-1,k,k+1\} \cap \{i+\ell=k\leq i+m+1, \ell \geq 2\} \setminus \{i+\ell=k\leq i+m+1\}} c_{\{k-1,k,k+1\}}. $$

When $m = 0$, then $\{G, H\}$ is a v-structure addition, when $m > 0$ and odd $\{G, H\}$ is a shift, and when $m > 0$ and even $\{G, H\}$ is a split. Hence, $\text{conv}(c_G, c_H)$ is an edge of $\text{CIM}_{I_p}$ if and only if $\{G, H\}$ is a shift, split, or v-structure addition. \hfill \Box

We remark that $I^*_p = I_{p-2}$, hence Proposition 3.6 says that $\text{STAB}(I^*_p) = \text{CIM}_{I_p}$. More generally, the stable set polytope of a tree can always be realized as a face of $\text{CIM}_G$ for an appropriately chosen graph $G$.

**Proposition 3.10.** Let $G$ be a tree. Then $\text{STAB}(G^2)$ is unimodularly equivalent to a face of $\text{CIM}_G$.

**Proof.** Let $i$ be an internal node of $G$ and let $G_i$ be a DAG with skeleton $G$, $\text{pa}_G(i)$, and no other v-structures. Take $H$ to be a DAG without any v-structure. Such DAGs exists since $G$ is a tree. Similar to the proof of Proposition 2.8, there exists affine functions $w_i$ that only depend on $N_i$ such that $w_i^T c_G = w_i^T c_H = 0$ and $w_i^T c_D = -1$ if $c_D|_{N_i} \neq c_G|_{N_i}$ and $c_D|_{N_i} \neq c_H|_{N_i}$. Notice that since $i$ was taken to be an internal node we have $c_G_i \neq c_H_i$. Then we let $W = \sum w_i$ where we sum over
all internal nodes of $G$. For convenience we also let $s_i$ be affine functions similar to $w_i$ but $s_i^T c_G = 1$ and $s_i^T c_D = 0$ for all $D$ such that $c_D|_{N_i} \neq c_{G_i}|_{N_i}$. Then we can define $S(D) = \{i \in G^o : s_i^T c_D = 1\}$.

Assume $D$ maximizes $W^T c_D$, then we claim that $S(D)$ is a stable set in $D$. It is clear that $W^T c_D \leq 0$ as each $w_i$ only assumes non-positive values and as $W^T c_H = 0$ it follows that we must have $W^T c_D = 0$. Thus by the definition of $W$ we must have $w_i^T c_D = 0$ for every internal node $i$. As every internal node has degree at least 2, we must have at least one $v$-structure at every $i \in S(D)$. Then by Lemma 2.2 we must have that $D|_{\lambda_G(i)}$ is full directed and as $s_i^T c_D = 1$ we must have that every node in $\lambda_G(i)$ is an essential parent of $i$ in $D$. Then if we would have two neighboring nodes $i, j \in S(D)$ then they would each be a parent of each other, which cannot happen. Hence $S(D)$ is indeed a stable set in $G^o$.

Conversely, given a stable set $T$ in $G$, we want to construct a DAG $D$ with $S(D) = T$. For each $i \in T$ we let $p_a_D = \lambda_G(i)$. This is possible since $T$ is a stable set. Then we can direct every part in $G[p]\setminus T$ without $v$-structures. This is possible as $G[p]\setminus T$ is a forest. Left to check is that $D$ indeed maximizes $W$, which follows since $w_i^T c_D = 0$.

Hence $S$ is a bijection between essential graphs $D$ maximizing $W$ and stable sets of $G^o$. Let $F$ denote the face of $\text{CIM}_G$ maximizing $W$. Then it is direct that

$$\chi_{S(D)} = (\chi_{S(D)}(1), \ldots, \chi_{S(D)}(m))^T = (s_1^T c_D, \ldots, s_m^T c_D)^T$$

for any essential graph $D \in F$, where $m$ is the number of internal nodes of $G$. Thus we have a bijective map between the vertices of $F$ and the vertices of $\text{STAB}(G^o)$ given by $\rho: c_D \mapsto (s_1^T c_D, \ldots, s_m^T c_D)^T$. As $\rho$ is affine in each coordinate we can extend it to an affine map from the affine subspace containing $F$ to the subspace containing $\text{STAB}(G^o)$. What is left to show is that this affine map is invertible. It can however be checked that

$$\chi_T \mapsto c_H + \sum_{i \in G^o} \chi_T(i)c_{G_i}|_{N_i}$$

is the inverse of $\rho$, and it is also affine. Hence we have a bijective affine correspondence between $F$ and $\text{STAB}(G^o)$. The map $\rho$ is also unimodular since the lattice of the affine subspace of $F$ is spanned by $\{c_{G_i}|_{N_i}\}_{i \in G^o} = \{c_{G_i} - c_H\}_{i \in G^o}$. \hfill $\square$

In the case of $I_p$ and $C_p$ it can be checked that all essential graphs maximize the cost function $W$, as constructed in the proof above. This is due to the fact that every internal vertex has degree exactly two, and thus $|N_i| = 1$. Hence the face of $\text{CIM}_{I_p}$ isomorphic to $\text{STAB}(I_p^o)$ is the polytope itself. This isomorphism fails for the cycle, as the empty set (which is stable) is not mapped to a characteristic imset of any DAG. This is also why Proposition 3.6 required non-empty stable sets for the cycle.

### 3.3. The Graphical Side of Turn Pairs

It was shown in [10] that turn pairs strictly generalize reversing an edge of a DAG. However, for trees, this is not true. That is, the converse of [10, Proposition 3.2] holds when the underlying skeleton $G$ is a tree. Let us first recall the definition of a turn pair.

**Definition 3.11** (Turn pair). [10] Let $G$ and $H$ be two DAGs on node set $[p]$ and with skeleton $G$. Suppose there exist $i, j, S_i \subseteq [p]\setminus\{i, j\}$ and $S_j \subseteq [p]\setminus\{i, j\}$ such that
Then we say that \( \{G, H\} \) is a turn pair with respect to \((i, j, S_i, S_j)\) if
\[
c_H = c_G + \sum_{S \in S^+} e_S - \sum_{S \in S^-} e_S
\]
where \( S^+ := \{T \cup \{i, j\} : T \subseteq S_i, T \not\subseteq ne_G(j)\} \) and \( S^- := \{T \cup \{i, j\} : T \subseteq S_j, T \not\subseteq ne_G(i)\} \).

Then we get the following graphical characterization.

**Proposition 3.12.** Assume \( \{G, H\} \) is a turn pair where \( G \) and \( H \) both have skeleton \( G \), a tree. Then there exists a DAG \( D \) and nodes \( i' \) and \( j' \) such that

1. \( G \) and \( D \) are Markov equivalent,
2. \( i' \rightarrow j' \in D \),
3. \( D_{i' \rightarrow j'} \) is a DAG, and
4. \( H \) and \( D_{i' \rightarrow j'} \) are Markov equivalent,

**Proof.** Notice that condition (3) is immediate as \( G \) is a tree. By definition of turn pair \( \{G, H\} \) is with respect to some \((i, j, S_i, S_j)\) such that either \( S_i \neq \emptyset \) or \( S_j \neq \emptyset \). Hence we can, by symmetry, assume that \(|S_i| \geq |S_j|\) and that \(|S_i| \geq 1\). Then we have three cases, \(|S_i| = 1\) and \(|S_j| = 0\), \(|S_i| = 1\) and \(|S_j| = 1\), and \(|S_i| \geq 2\).

**Case I.** \(|S_i| = 1\) and \(|S_j| = 0\): It follows by definition of turn pair that \(|S^+| = 1\) and thus \( \{G, H\} \) is an addition with respect to \( \{i, j\} \cup S_i \).

Since \( G \) and \( H \) have the same skeleton it follows by Proposition 1.6 that they differ by a single v-structure. That is, the induced graph of \( H \) on \( \{i, j\} \cup S_i \) is a v-structure, \( \alpha \rightarrow \beta \leftarrow \gamma \). As \( c_G(\{i, j\} \cup S_i) = 0 \) we have that \( \alpha \leftarrow \beta \in G \) or \( \beta \rightarrow \gamma \in G \). We can assume by symmetry that \( \beta \rightarrow \gamma \in G \). Assume we have a node \( s \in pa_G(\gamma) \setminus \{\beta\} \). Since \( G \) is a tree it follows that \( s \neq \alpha \). Then \( c_G(\{s, \beta, \gamma\}) = 1 \) and, as \( \{s, \beta, \alpha\} \neq \{i, j\} \cup S_i \), we get \( c_H(\{s, \beta, \gamma\}) = 1 \). Again since \( G \) is a tree we get that \( \beta \rightarrow \gamma \leftarrow s \in H \), a contradiction. Thus \( pa_G(\gamma) = \{\beta\} \).

Assume we have a node \( s \in pa_H(\beta) \setminus \{\alpha, \gamma\} \). Then we have \( s \rightarrow \beta \leftarrow \gamma \in H \) and thus \( c_H(\{s, \beta, \gamma\}) = 1 \). However, as \( \{s, \beta, \gamma\} \neq \{i, j\} \cup S_i \) we get \( s \rightarrow \beta \leftarrow \gamma \in G \), a contradiction. Thus \( pa_H(\beta) = \{\alpha, \gamma\} \).

Now let us construct \( D \). Let \( G' \) denote the graph identical to \( G \) with the exception that it does not contain the edge \( \beta \rightarrow \gamma \). Let \( G'_{\beta} \) be the connected part of \( G' \) containing \( \beta \) and let \( G_{\gamma} \) be the rest of \( G' \). Define \( D \) as the orientation of \( G \) where we direct \( G_{\beta} \) as in \( H \), direct \( G_{\gamma} \), according to \( G \) and direct \( \beta \rightarrow \gamma \) as in \( \beta \rightarrow \gamma \).

First we want to show that \( D \) is Markov equivalent to \( G \). As \( G \) and \( H \) only differ by a single v-structure and \( D \) is everywhere directed as in either \( G \) or in \( H \) the only place where \( D \) can differ by a v-structure from \( G \) is around \( \beta \). However, since \( pa_D(\beta) = pa_H(\beta) \setminus \{\gamma\} = \{\alpha\} \) neither has any v-structures around \( \beta \). Thus, they must be Markov equivalent.

It follows that \( D_{\beta \rightarrow \gamma} \) will have the v-structure \( \alpha \rightarrow \beta \leftarrow \gamma \) but no other v-structures are created or destroyed when we reverse \( \beta \rightarrow \gamma \), as \( pa_D(\beta) = \{\alpha\} \). Hence \( D_{\beta \rightarrow \gamma} \) is Markov equivalent to \( H \). In conclusion, we can choose \( D \) with \( i' = \beta \) and \( j' = \gamma \).
Case II, \( S_i = \{\alpha_i\} \) and \( S_j = \{\alpha_j\} \): Since \( G \) is a tree we must have the v-structure \( \alpha_i \rightarrow i \leftarrow j \) in \( \mathcal{H} \) and the v-structure \( i \rightarrow j \leftarrow \alpha_j \) in \( G \). Then we can define \( G_i \) and \( G_j \) similar to how we defined \( G_3 \) and \( G_7 \) in Case I above. The rest is completely analogous and we get \( i' = i \) and \( j' = j \).

Case III, \( |S_i| \geq 2 \): As \( c_G(S_i \cup \{i\}) = 1 \) we have at least one v-structure \( \alpha \rightarrow i \leftarrow \gamma \) for some \( \alpha, \gamma \in S_i \) in \( G \). Thus we must have \( \beta \rightarrow i \) in \( G \) for all \( \beta \in S_i \). The same is true for \( \mathcal{H} \). Then we have \( c_G(S_i \cup \{i, j\}) = 0 \) as we cannot have \( S_i \subseteq \text{neg}_G(j) \) as \( G \) is a tree. Hence \( i \rightarrow j \) is essential in \( G \), and similar reasoning gives us \( i \leftarrow j \) is essential in \( \mathcal{H} \). Then we can choose \( D = G \). From a reasoning similar to Case I we get that \( pa_G(j) = S_j \), and that \( G_{i\leftarrow j} \) is Markov equivalent to \( \mathcal{H} \) is straightforward. Thus we get \( i' = i \) and \( j' = j \) in this case as well. \( \square \)

Thus turn pairs exactly correspond to reversing an edge in some element of the MEC.

3.4. Almost Complete Graphs. When we proved Proposition 1.8 we utilized the fact that \( G \) induced a partial order on the MECs with skeleton \( G \). Here we present another case where this happens as well.

**Proposition 3.13.** Let \( G = ([p], E) \) be the complete graph missing only the edge \( 1 \rightarrow 2 \), that is \( K_p \setminus \{1, 2\} \). Then \( \text{CIM}_G \) is a simplex of dimension \( 2^p - 2 - 1 \).

**Proof.** By the structure of \( G \) the only possible v-structures are of the form \( 1 \rightarrow i \leftarrow 2 \) for some \( 2 < i \leq p \). We wish to show that for any subset \( S \subseteq \{3, \ldots, p\} \) we have a DAG \( D_S \) such that \( 1 \rightarrow i \leftarrow 2 \in D_S \) for all \( i \in S \) but for no \( i \in \{3, \ldots, p\} \setminus S \). As every MEC is characterized by the v-structures we will then have a representative from each MEC.

As for the construction of \( D_S \), for every \( i \in S \) we direct the edges \( 1 \rightarrow i \leftarrow 2 \) as \( 1 \rightarrow i \leftarrow 2 \) and for every \( i \in \{3, \ldots, p\} \setminus S \) we direct the edges \( 1 \leftarrow i \rightarrow 2 \) as \( 1 \leftarrow i \rightarrow 2 \). Notice that we have thus far not created any cycles. Hence, the currently directed edges induce a partial order on \([p]\). Extending this order to a total order and directing the remaining edges of \( D_S \) according to this order gives us a DAG. Notice that no new v-structures can have been created in this last step, because all possible triples that could have been v-structures were already directed. Then we can calculate the characteristic imset of \( D_S \) as

\[
c_{D_S} = c_D + \sum_{T \in S} e_T \]

where \( S = \{U \cup \{1, 2\} : U \subseteq \{3, \ldots, p\}, U \cap S \neq \emptyset\} \). Equivalently we have \( 1 - e_{\{1, 2\}} - c_{D_S} = \sum_{T \in S'} e_T \) where \( S' = \{U \cup \{1, 2\} : U \subseteq [p] \setminus S\} \) where \( 1 \) is the constant 1-vector. By Lemma 1.7 the right-hand-side constitutes a basis and since translations preserve this property the result follows. \( \square \)

We have now seen several cases where posets can be of use in describing the geometry of the CIM\(_G\) polytope. Whether there is a more general connection or not is left to future work.

4. Applications

A fundamental problem in modern data science and artificial intelligence is the problem of causal inference [12], in which one is interested in estimating the cause-effect relations between jointly distributed random variables. This task is typically
broken into two well-studied subproblems: (1) the task of inferring the strength and nature of the causal effect of one variable on another, and (2) the task of estimating which variables have direct causal effects on another. The latter of the two problems is referred to as the problem of causal discovery. In its most basic form, we assume that we have a random sample $D$ drawn from the joint distribution $P$ of the random variables $(X_1, \ldots, X_p)$, and we would like to infer a DAG $G = ([p], E)$ in which the arrows $i \rightarrow j$ correspond to the direct cause-effect relations in the system; i.e., $G$ contains the arrow $i \rightarrow j$ if and only if $i$ is a direct cause of $j$. As the data $D$ is drawn from a probability distribution, and correlation does not imply causation, one must impose some assumption that associates the data-generating distribution $P$ to the underlying (unknown) causal structure $G$ we wish to infer. We say a distribution $P$ over $(X_1, \ldots, X_p)$ is Markov to a DAG $G = ([p], E)$ if there is a linear extension (topological ordering) $\pi = \pi_1 \cdots \pi_p$ of $G$ such that for all $i \in [p]$, $P$ entails the CI relation

$$X_{\pi_i} \perp \perp X_{\{\pi_1, \ldots, \pi_{i-1}\} \setminus \text{pa}_G(\pi_i)} \big| X_{\text{pa}_G(\pi_i)}.$$  

The above relations capture rudimentary causal information encoded in the distribution $P$; namely, that each variable (event) is independent of all preceding variables (events) given its direct causes. Given a DAG $G$, its associated DAG model is the collection of distributions

$$\mathcal{M}(G) = \{P : P \text{ is Markov to } G\}.$$  

Since $\mathcal{M}(G) = \mathcal{M}(H)$ if and only if $G$ and $H$ are Markov equivalent [8, 12], then, given only the data $D$, the best we can hope for is to recover $G$ up to Markov equivalence. Hence, the basic problem of causal discovery is to learn the essential graph of the causal system of the data-generating distribution based on the random sample $D$.

Proposed causal discovery algorithms typically come in one of three forms: constraint-based algorithms, such as the PC-algorithm [20, 24], that recover an essential graph via statistical tests for conditional independence, (greedy) score-based algorithms, such as the Greedy Equivalence Search (GES) [2], that assign a score to each DAG (or essential graph) based on the data and then search for the optimal scoring DAG, and hybrid algorithms, such as the Max-Min Hill Climbing Algorithm (MMHC) [25], that use a mixture of CI-testing and optimization. Most classic causal discovery algorithms rely solely on the combinatorics of DAGs. However, recent advancements have introduced discrete-geometric methods with promising results. These include the hybrid algorithm GreedySP [18] and score-based linear optimization approaches that aim to solve the LP associated to the polytope CIM$_p$ [23]. Most recently, [10] introduced a hybrid algorithm, skeletal Greedy CIM, that first estimates the skeleton $G$ of the essential graph using CI-tests and then uses the edges of CIM$_G$ identified in [10] to search over the polytope for the optimal essential graph.

Skeletal greedy CIM performed quite well on simulated data, despite using CI-tests (which are prone to error propagation) to learn the skeleton $G$ and only the subset of the edges of CIM$_G$ corresponding to turn pairs (see Definition 3.11). In the case that the unknown causal system is a directed tree (often called a polytree), the results of Theorem 2.7 can be used to overcome the latter of these two limiting factors. The CI-tests can similarly be avoided by taking advantage of the fact that we wish to learn only a polytree. In place of CI-tests, we can instead learn the
skeleton $T = ([p], E)$ of the polytree by learning a minimum weight spanning tree (MWST) of a complete graph $K_p$ where the weight assigned to each edge $i - j$ is the negation of the mutual information of $X_i$ and $X_j$:

$$I(X_i; X_j) = \int \int f(x_i, x_j) \log \left( \frac{f(x_i, x_j)}{f(x_i) f(x_j)} \right) dx_i dx_j.$$ 

Given the inferred skeleton $\hat{T}$, via the edge characterization of CIM$_T$ for $T$ presented in Theorem 2.7, we can estimate the causal structure $G$ by performing an edge walk along CIM$_{\hat{T}}$, where at each step we walk to the neighbor of the current essential graph that optimally increases the Bayesian Information Criterion (BIC) score of the model:

$$\text{BIC}(G, \mathcal{D}) = \log f(\mathcal{D}|\hat{\theta}, G^h) - \frac{d}{2} \log(|\mathcal{D}|).$$

Here, $\hat{\theta}$ is the maximum likelihood estimate for the model parameters, $d$ denotes the number of free parameters, and $G^h$ denotes the hypothesis that $\mathcal{D}$ is a random sample from a distribution entailing the CI statements encoded by the given DAG $G$. Since BIC($G, \mathcal{D}$) is known to be an (affine) linear function over CIM$_p$ [23], the algorithm terminates once no neighboring vertex of the current characteristic imset increases in BIC. We call this algorithm for learning polytrees, presented in Algorithm 1, the Essential Flip Tree Search (EFT).

**Algorithm 1** Essential Flip Tree Search (EFT)

**Input:** a random sample $\mathcal{D}$ from $(X_1, \ldots, X_p)$.

**Output:** $G = ([p], E)$ a polytree

1: $K_p \leftarrow$ a weighted complete graph on $[p]$ where $i - j$ is assigned the weight $-I(X_i; X_j)$.
2: $G = ([p], E) \leftarrow$ a minimum weight spanning tree of $K_p$
3: $G = ([p], A) \leftarrow$ a random polytree with skeleton $G$
4: $H \leftarrow G$
5: $M \leftarrow$ all subtrees of $G$
6: while TRUE do
7: $G_{\pi} \leftarrow G$ with edges in $s \in M$ reversed if $\{G_{\pi}, G\}$ constitutes an essential flip.
8: $G_M \leftarrow \{G_{\pi} : s \in M\}$
9: $H \leftarrow \text{argmax}_{D \in G_M} \text{BIC}(G_{\pi}, \mathcal{D})$
10: if BIC($G, \mathcal{D}$) $\geq$ BIC($H, \mathcal{D}$) then
11: break
12: end if
13: $G \leftarrow H$
14: end while
15: return $G$

An implementation of EFT is available at [15]. In the remainder of this section, we consider the aspects of causal discovery algorithms arising from our discrete-geometric understanding of CIM$_p$ and its faces. In subsection 4.1, we consider the asymptotic consistency of causal discovery algorithms that perform edge walks along faces of the CIM$_p$, including the hybrid algorithms EFT and skeletal Greedy CIM, as well as the purely score-based algorithm Greedy CIM presented in [10].
In subsection 4.2, we analyze the performance of EFT on simulated and real data, comparing it with classic approaches for learning polytrees such as the hybrid algorithm of Rebane and Pearl [14], which we will call the RP-algorithm. We observe that EFT outperforms such classic polytree learning algorithms, and can even outperform general causal discovery algorithms such as GES and GreedySP on real data.

4.1. A Sufficient Criterion for Consistency. It was shown in [2] that GES is asymptotically consistent when the data used to identify a BIC-optimal MEC is drawn from a distribution faithful to a DAG in the MEC; that is, GES will return the correct MEC as the sample-size goes to infinity. In short, we say that GES is consistent under the faithfulness assumption. To show that GES is consistent under faithfulness Chickering [2] defined the notion of local consistency, which informally says that adding in missing edges that should be present and removing the existing edges that should be missing increases the score. Here we will show a new version of consistency for reversing edges similar to that of local consistency (Proposition 4.2).

With this we get consistency of skeletal greedy CIM, as defined in [10], and EFT (i.e., Algorithm 1). These results will all assume consistency of the scoring criterion.

**Definition 4.1** (Consistent scoring Criterion). Let $\mathcal{D}$ be a random sample of size $m$ from some distribution $\mathbb{P}$. A scoring criterion $S$ is **consistent** if in the limit as $m$ grows large, the following two properties hold:

1. If $\mathcal{M}(\mathcal{H})$ contains $\mathbb{P}$ and $\mathcal{M}(\mathcal{G})$ does not contain $\mathbb{P}$ then $S(\mathcal{H}, \mathcal{D}) > S(\mathcal{G}, \mathcal{D})$.
2. If $\mathcal{H}$ and $\mathcal{G}$ both contain $\mathbb{P}$ and $\mathcal{G}$ contains fewer parameters than $\mathcal{H}$ then $S(\mathcal{G}, \mathcal{D}) > S(\mathcal{H}, \mathcal{D})$.

We also say that a scoring criterion $S(\cdot, \mathcal{D})$ is **score equivalent** if $S(\mathcal{G}, \mathcal{D}) = S(\mathcal{H}, \mathcal{D})$ whenever $\mathcal{G}$ and $\mathcal{H}$ are Markov equivalent. In [6] the author showed that BIC is a consistent and score equivalent scoring criterion for a large class of models which include DAG models. Moreover, in [2, 23] the authors remark that BIC is decomposable, a condition making it a suitable scoring criterion for skeletal greedy CIM and Greedy CIM. Hence, the following proposition is indeed applies to BIC.

**Proposition 4.2.** Let $\mathcal{G}$ be a DAG with $i \rightarrow j \in \mathcal{G}$, $\mathbb{P}$ a (positive) distribution faithful to $\mathcal{H}$, $\mathcal{D}$ a random sample from $\mathbb{P}$, $S(\cdot, \mathcal{D})$ a score equivalent, decomposable and consistent scoring criterion, and assume that $i$ and $j$ are neighbours in $\mathcal{H}$. Assume that $\mathcal{G}_{i \rightarrow j}$ is a DAG not Markov equivalent to $\mathcal{G}$. Then if $\mathcal{H}$ has all v-structures $k \rightarrow i \leftarrow j$ for $k \in \text{pa}_\mathcal{G}(i) \setminus \text{pa}_\mathcal{G}(j)$ and none of the v-structures $i \rightarrow j \leftarrow k$ for $k \in \text{pa}_\mathcal{G}(j) \setminus (\text{pa}_\mathcal{G}(i) \cup \{i\})$ we have $S(\mathcal{G}, \mathcal{D}) < S(\mathcal{G}_{i \rightarrow j}, \mathcal{D})$.

**Proof.** The proof is similar in nature as the proof of local consistency, see [2, Lemma 7]. Since $S(\cdot, \mathcal{D})$ is decomposable the difference in score solely depends on the structure of $G'_{\{\text{pa}(i) \cup \text{pa}(j) \cup \{i,j\}\}}$. More specifically, $\{G, G_{i \rightarrow j}\}$ is a turn pair, with $S_i = \text{pa}_\mathcal{G}(i)$ and $S_j = \text{pa}_\mathcal{G}(j) \setminus \{i\}$, and thus by the equality in Definition 3.11, the difference in score only depends on the edges between $j$ and vertices in $\text{pa}_\mathcal{G}(i)$, and edges between $i$ and vertices in $\text{pa}_\mathcal{G}(j)$. Hence we can assume that we have an edge between every pair of vertices that is not of the described form in $\mathcal{G}$. Let $\mathcal{H}$ be a DAG with all edges of $\mathcal{H}$ and for each pair of nodes $\alpha, \beta$, such that we do not have $\alpha = i$ and $\beta \in \text{pa}_\mathcal{G}(j)$ or $\alpha = j$ and $\beta \in \text{pa}_\mathcal{G}(i)$, or vice versa, we add in the edge $\alpha \rightarrow \beta$ with an acyclic orientation. This is possible as $\mathcal{H}$ is a DAG. Notice that as $\mathbb{P}$ is faithful to $\mathcal{H}$ it must be Markov to $\hat{\mathcal{H}}$, as $\hat{\mathcal{H}}$ imposes less restrictions on $\mathbb{P}$. The
only v-structures possible in $\tilde{\mathcal{H}}$ are of the form $k \rightarrow i \leftarrow j$ for $k \in \text{pa}_G(i) \setminus \text{pa}_G(j)$ or $i \rightarrow j \leftarrow k$ for $k \in \text{pa}_G(j) \setminus (\text{pa}_G(i) \cup \{i\})$. Hence, by assumption, $G_{i \leftrightarrow j}$ must be Markov equivalent to $\tilde{\mathcal{H}}$ as, also by assumption, both have exactly the same v-structures. Therefore, $P$ is Markov to $G_{i \leftrightarrow j}$. The result then follows from the consistency of $S(\cdot, \mathbb{D})$ if we can show that $P$ is not Markov to $\mathcal{G}$.

We begin with the case that $\text{pa}_G(i) \setminus \text{pa}_G(j) \neq \emptyset$. Let $k \in \text{pa}_G(i) \setminus \text{pa}_G(j)$ and note that $\mathcal{G}$ encodes $X_k \perp X_j \mid X_{\text{an}_G(j) \setminus \{k\}}$. We wish to show that this statement is not encoded by $\tilde{\mathcal{H}}$ and hence is not true in $P$. However, by assumption we have $i \in \text{an}_G(j) \setminus \{k\}$ and $k \rightarrow i \leftarrow j$ is a v-structure in $\tilde{\mathcal{H}}$. Then $X_k \perp X_j \mid X_{\text{an}_G(j) \setminus \{k\}}$ cannot be encoded by $\tilde{\mathcal{H}}$. In the language of [8], $k \rightarrow i \leftarrow j$ is a d-connecting path given $\text{an}_G(j) \setminus \{k\}$ as $i \in \text{an}_G(j) \setminus \{k\}$. Thus $P$ does not entail these conditional independence statements and hence $P$ is not Markov to $\mathcal{G}$.

If $\text{pa}_G(i) \setminus \text{pa}_G(j) = \emptyset$ we must have $\text{pa}_G(j) \setminus \text{pa}_G(i) \neq \emptyset$ as $\mathcal{G}$ and $G_{i \leftrightarrow j}$ are assumed to be Markov equivalent. Let $k \in \text{pa}_G(j) \setminus \text{pa}_G(i)$ and note that we have $i \leftarrow j \leftarrow k$ in $\mathcal{H}$. As we have $i \rightarrow j \leftarrow k$ in $G$, any distribution Markov to $\mathcal{G}$ entails $X_k \perp X_i \mid X_{\text{an}_G(i) \cup \text{an}_G(k)}$. However, as $j \notin \text{an}_G(i) \cup \text{an}_G(k)$ we can repeat the previous argument with the path $i \leftarrow j \leftarrow k$. Hence, the result follows.

What Proposition 4.2 says is that turning an edge such that we only add in wanted v-structures or remove unwanted v-structures increases BIC. Thus to show that Skeletal Greedy CIM is consistent it is enough to show that we can always find an edge $i \rightarrow j$ with this property.

**Proposition 4.3.** Skeletal Greedy CIM is consistent under faithfulness given an oracle-based test for conditional independence.

**Proof.** By faithfulness there exists a DAG $\mathcal{H}$ to which our distribution is faithful. In [20] they show that, given an oracle-based test for conditional independence, the skeleton algorithm will find the skeleton of $\mathcal{H}$, say $\mathcal{G}$. Assume we are currently at the characteristic imset of a DAG $\mathcal{G}$.

Take any topological order on $[p]$ determined by $\mathcal{H}$. Let $i$ be the smallest node in this order such that $\mathcal{H}_{\text{cl}(i)} \neq \mathcal{G}_{\text{cl}(i)}$, notice that $\text{ch}_H(i) \subseteq \text{ch}_G(i)$, else we have $i' \in \text{ch}_H(i) \setminus \text{ch}_G(i)$ giving us $\mathcal{H}_{\text{cl}(i')} \neq \mathcal{G}_{\text{cl}(i')}$, contradicting that $i$ is minimal with respect to the topological sorting. Since $\mathcal{H}$ and $\mathcal{G}$ share the same skeleton we get $\text{pa}_H(i) \supseteq \text{pa}_G(i)$. Let $j$ be the smallest node in $\text{ch}_G(i) \setminus \text{ch}_H(i)$. By our choice of $j$ we have that $G_{i \leftrightarrow j}$ is a DAG. If $\mathcal{G}$ and $G_{i \leftrightarrow j}$ are Markov equivalent we could instead have chosen $G_{i \leftrightarrow j}$ as our representative of the MEC, and thus this is a non-case. Any new v-structures must of the form $k \rightarrow i \leftarrow j$ for $k \in \text{pa}_G(i)$, but as $\text{pa}_H(i) \supseteq \text{pa}_G(i)$ this v-structure is present in $\mathcal{H}$ as well, and any destroyed v-structures must have been of the form $i \rightarrow j \leftarrow k$. However, since $i$ was smaller than $j$ in the topological sorting none of these v-structures can be present in $\mathcal{H}$. By Proposition 4.2 this increases the score. Hence we can always turn an edge to increase score, unless we are in the MEC of $\mathcal{H}$. Thus, Skeletal Greedy CIM will always find the optimum.

A first observation about the above proposition is that the proof directly extends to any algorithm that utilizes a fixed set of moves extending the turning phase of GES over the space of DAGs with a fixed skeleton. This is because the above proof shows that any such set of moves will always contain at least one move that improves the score, unless we are in the Markov equivalence class of optimal DAGs.
Indeed, we similarly get consistency of EFT when our underlying data-generating distribution is faithful to a tree.

**Proposition 4.4.** The EFT algorithm is consistent under faithfulness when the distribution is faithful to a DAG with skeleton $G$ where $G$ is a tree.

**Proof.** As was shown in [14] the MWSP of $K_p$, where the weights are the negation of the mutual information will, in the limit of infinite data, correctly recover $G$. Following the proof of Proposition 4.3 we can always find an edge $i \to j$ so that we can apply Proposition 4.2. That is, if we are currently at a DAG $G$ that is not the optimum, there is a Markov equivalent graph $G'$ with an edge $i \to j$ such that reversing this edge increases the score. Hence it is enough to show that $\{G, G_{i \leftrightarrow j}\}$ is an essential flip whenever $G$ and $G_{i \leftrightarrow j}$ are not Markov equivalent. However this follows directly from Theorem 2.12. □

In [27] it was shown that a version of GES, called GIES, based on a mixture of observational and interventional data is not consistent under the faithfulness assumption. The above result suggests that this is specifically a feature arising when data from multiple experiments is being used as opposed to a feature of the turning phase of GES. With these results we further the belief that the hardship of DAG discovery, in the case of purely observational data, is finding the skeleton of the graph.

We have now looked at how a decomposable, score equivalent and consistent scoring criterion behaves, with respect to CIM$_G$ for arbitrary $G$. It then makes sense to also consider, as we did before, CIM$_G$ when $G$ is a tree. Let $S(-,D)$ be a decomposable score equivalent consistent scoring criterion, and let $G$ be a tree. Recall that we defined $N_i = \{S \subseteq [p] : i \in S \subseteq ne_G(i) \cup \{i\}, |S| \geq 3\}$. In [23, Lemma 1] the authors show that for every score equivalent decomposable scoring criterion $S(-,D)$ there is a vector $S_D$ such that $S(G,D) = C + \sum_{i \in [p]} S_D|_{N_i}$ for some (affine) linear function $S_G$ that is constant over CIM$_G$. Note that for this decomposition we use that $G$ is a tree and thus the sets $N_i$ are mutually disjoint. Then maximizing $S_D$ over CIM$_G$, when $G$ is a tree, is the same as maximizing each $S_D|_{N_i}$ independently.

**Proposition 4.5.** Let $P$ be a (positive) distribution faithful to a DAG $G$ with skeleton $G$ a tree, and let $D$ be a random sample from $P$. Let $S(-,D)$ be a score equivalent, consistent and decomposable scoring criterion that maximizes at $c_G$. Then $c_G$ simultaneously maximizes $S_D|_{N_i}$ for all $i \in [p]$; that is, $S_D^T|_{N_i} c_G = \max_{v \in \text{CIM}_G} \{S_D^T|_{N_i} v\}$.

**Proof.** For simplicity, for all $i \in [p]$, let $s_i = S_D|_{N_i}$. Let $\{H_i\}$ be DAGs such that $s_i^T c_{H_i} = \max_{v \in \text{CIM}_G} \{s_i^T v\}$ for each $i \in [p]$. It is enough to show that $c_{H_i}|_{N_i} = c_G|_{N_i}$ for any given $i$. As $s_i$ is non-zero only for entries in $N_i$ we can assume that $H_i$ has all edges outside of $H_i|_{\text{cl}(i)}$ directed away from $j$, since the values of $S_D(S)$ for $S \not\subseteq \text{cl}(i)$ do not affect $s_i^T c_{H_i}$. Hence $H_i$ has no v-structures other than (possibly) the ones centered at $i$. Assume we have a v-structure at $j \rightarrow i \leftarrow k$ in $H_i$ not present in $G$. Then we must have either $j \leftarrow i$ or $i \rightarrow k$ in $G$, by symmetry assume $j \leftarrow i$. Then changing the direction of $j \rightarrow i$ in $H_i$ can only remove v-structures not present in $G$, so by Proposition 4.2 this increases the score of $S_D^T c_{H_i}$. By our decomposition above $S_D^T c_{H_i} = S_D^T c_{H_i} + \sum_{v \in [p]} s_v^T c_{H_i}$. Then, as no other v-structures were created,
we only change the summand $s^T \epsilon_{\mathcal{H}_i}$, contradicting the definition of $\mathcal{H}_i$. Hence $\mathcal{H}_i$ has no v-structures at $i$ not present in $\mathcal{G}$.

Assume we have v-structure at $\mathcal{G}$ not present in $\mathcal{H}_i$. Then we can make the same argument, utilizing the fact that all v-structures at $i$ in $\mathcal{H}_i$ are present in $\mathcal{G}$, as before this time adding in v-structures. Hence $\mathcal{H}_i$ and $\mathcal{G}$ must have the exact same v-structures at $i$, and the result follows. □

The above claim asserts that we could (simultaneously) find the structure of $\text{cl}(i)$ for all $i$ and then glue each part together. A priori this point of attack could lead to issues, for example if the maximum in $\text{cl}(i)$ would have $i \to j$, but when maximizing in $\text{cl}(j)$ we would have $i \leftarrow j$. The above proposition, then states that this will not happen in the limit of large data drawn from a distribution faithful to a DAG.

4.2. Experimental Results. We now analyze the empirical performance of the EFT algorithm (Algorithm 1) for learning polytrees on simulated and real data. The EFT algorithm can be viewed as operating in two phases: in the first phase the skeleton of the polytree is estimated. In the second phase, a BIC-optimal orientation of the estimated skeleton is identified. For the first phase, since classic CI-test approaches cannot be guaranteed to return a skeleton that is a tree, we use the approach of Rebane and Pearl [14], where we assign a weight to each edge $i \to j$ of a complete graph: the negative mutual information $-I(X_i; X_j)$. We then identify a minimum weight spanning forest (MWSF) of this weighted complete graph. (In the implementation available at [15], this step is done via Kruskal’s algorithm in the networkX package in Python. Other algorithms for learning a MWSF are available as well via this package and can be called in the EFT implementation at [15].)

In the second phase, edges of the estimated skeleton are oriented to recover an essential graph. Instead of the CI-tests used by the RP-algorithm (which can be prone to error propagation), EFT uses the characterization of the edges of CIM$_T$ in Theorem 2.7 to search for a BIC-optimal polytree on the estimated skeleton.

4.2.1. Simulations. We compared these two methods by analyzing their performance on randomly generated linear structural equation models with Gaussian noise whose underlying DAG is a polytree on 10 nodes. To generate these models, we uniformly at random generated a Prüfer code (i.e., a sequence of length 8 with entries in [10] that uniquely corresponds to an undirected tree on nodes [10]) to produce the skeleton $T$ of the polytree. The edges of the skeleton were then oriented independently and uniformly at random to yield a polytree $\mathcal{T}$, and each edge $i \to j$ of $\mathcal{T}$ was assigned a weight $\lambda_{ij}$ drawn from the uniform distribution over $[-1,0) \cup (0,1]$. We then sampled from a multivariate Gaussian distribution over the random variables $(X_1,\ldots,X_p)$ where

$$X_i := \sum_{k \in \text{pa}(i)} \lambda_{ki}X_k + \varepsilon_i,$$

where $\varepsilon_1,\ldots,\varepsilon_p$ are mutually independent standard normal random variables. For each $n \in \{15,20,250,500,1000,10000\}$, we generated 100 such models and drew a random sample of size $n$. The RP-algorithm, EFT, and GreedySP were then tasked with recovering the data-generating polytree $\mathcal{T}$ based on each sample. The constraint-based tests of the RP-algorithm and GreedySP were performed with a cut-off threshold of $\alpha = 0.05$, and the depth and run parameters of GreedySP were
chosen to be $d = 4, r = 5$; the default values in the causaldag python package [21] implementation of GreedySP. Although not specifically designed to learn polytrees, GreedySP was included to give a benchmark of the performance of the polytree-specific hybrid algorithms, EFT and RP, against a general hybrid causal discovery algorithm. The accuracy of each estimated DAG (computed as the fraction of off-diagonal entries in the adjacency matrix of the estimated essential graph that agree with the adjacency matrix of the essential graph of $T$) was recorded. The results are presented in Figure 2. We see that EFT outperforms both algorithms over all sample sizes greater than 50, and does increasingly better for larger sample sizes (reflecting the asymptotic consistency results observed in subsection 4.1). At 10000 samples EFT perfectly recovers at least 50% of the models and 25% already for 250 samples. Since the RP algorithm and EFT differ only in their second phases, these results suggest that meaningful gains can be had by replacing CI-tests in the second phase of RP with a greedy search over the edges of CIM$_T$ when the data-generating distribution is approximately normal.

As shown in Proposition 3.12, the moves used by EFT in its second phase generalize the moves of the turning phase of GES, which uses only single edge reversals. Hence, it is of interest to see if the additional moves provided by using all edges of CIM$_T$ yield substantial gains over the turning phase of GES. To test this, we generated 100 random linear Gaussian polytree models (as described above) and drew random samples of size $n = 15, 20, 250, 500, 1000, 10000$ from each model. We then
had EFT and the turning phase of GES estimate the data-generating polytree for each model with the true skeleton given as background knowledge. The accuracies of the estimated essential graphs is presented in the box plots in Figure 3.

Intuitively, we expect that the additional moves provided to EFT over GES by using all edges of $\text{CIM}_T$ when searching (as opposed to only turn pairs) does not substantially boost performance. This is because GES is known to perform quite well when the data-generating system is sparse. The results presented in Figure 3 confirm this intuition. The accuracy rates are highly comparable, especially as the sample size grows. This suggests that one could replace phase two of EFT with the turning phase of GES to obtain a comparable, but perhaps slightly more efficient hybrid algorithm for estimating polytrees. The results also suggest interesting features of the geometry of $\text{CIM}_G$. For instance, the subgraph consisting only of (polytope) edges corresponding to (essential graph) edge reversals of the edge graph of $\text{CIM}_G$ appears to provide as good of a search mechanism as the entire graph. It would be interesting to have a deeper understanding of how the essential graph edge reversals are distributed along the edge graph of $\text{CIM}_G$ for $G$ a tree. It would also be of interest to understand if this phenomenon occurs for denser choices of $G$, in which one would generalize EFT by replacing the search phase based on essential flips with a corresponding characterization of edges of $\text{CIM}_G$ for the given skeleton. Since GES tends to perform increasingly worse as the density of the graph
increases, one might observe that GES’s competitiveness with a such generalized version EFT decreases as the graphs become increasingly dense. Since the set of moves used by the search phase of such a generalization of EFT would necessarily include edge reversals, such an algorithm would be expected to be consistent at least as often as GES. It is possible that, for certain skeletons, we see improvements in accuracy over GES in the finite sample setting. As well, such moves could possibly improve efficiency if they offer substantially faster paths between two graphs than any corresponding sequence of edge reversals. Such complexity questions could be better understood via an analysis of the diameter of the edge graph of CIM versus the diameter of its subgraph with edges corresponding to edge reversals.

4.2.2. Real Data Analysis. The protein signaling dataset of Sachs et al. [17] is a standard benchmark dataset in causal inference consisting of 7466 abundance measurements of phospholipids and phosphoproteins taken under varying experimental conditions in primary human immune system cells. The different experimental conditions are produced by reagents that inhibit or activate different sets of signaling proteins within the system before measurements are taken. Such measurements are termed “samples from an interventional distribution” [12] since the reagents are altering the data-generating distribution. To learn a (probabilistic) DAG model for the system we work with only observational data; i.e., samples drawn from the unaltered data-generating distribution. An observational dataset can be extracted from the Sachs data as described in [27], which results in a sample size of 1755.

We compared the accuracy of the essential graphs estimated by EFT, the RP algorithm, GES and GreedySP for the protein signaling system based on these 1755 samples in Figure 4. Here, accuracy of the estimated essential graphs was computed relative to the accepted ground-truth network depicted in Figure 5a. Since the ground-truth network is not a polytree, only GES and GreedySP could
potentially learn the network exactly. However, the results presented in Figure 4a show that both EFT and the RP-algorithm tend to perform best in regards to accuracy. In this analysis, the cut-off threshold for CI-testing in the RP-algorithm was set to $\alpha = 0.05$, and GES and the second phase of EFT were conducted using a Gaussian MLE in the BIC computations. GreedySP (GSP) was implemented with depth and run parameters $d = 4$ and $r = 5$ and a Gaussian (partial correlation) test for conditional independence. Since the data is believed to be highly non-Gaussian [17], the Gaussianity assumptions on EFT, GES and GreedySP can result in suboptimal performance. Hence, we also assessed the performance of GreedySP with varying cut-off thresholds for CI-testing ranging over $\alpha \in \{0.05, 0.025, 0.005, 0.0005, 0.00005, 0.000005\}$. In the first phase of EFT and the RP-algorithm, where the skeleton is estimated, the data (which is drawn from a continuous distribution) is binned to yield a discrete approximation of the sampling distribution that is used to calculate the empirical mutual information weights. The results for different numbers of bins were analyzed, ranging over \{5, 10, 15, \ldots, 50\}. We see in Figure 4a that the best accuracy of both EFT and the RP-algorithm is achieved simultaneously by 25 and 30 bins, with both achieving identical accuracy measurements. In this plot, we report GreedySP’s highest accuracy rate, which was achieved with $\alpha = 0.0001$ along with the results for $\alpha = 0.05, 0.025$ (the default choice in causaldag [21] and the best performing threshold value in Figure 4b, respectively). Figure 4b presents an ROC plot, which shows the false positive rates versus the true positive rates, of the different experiments. (Here, for the sake of space, we only report GreedySP’s best performing value $\alpha = 0.025$ and the default value in causaldag $\alpha = 0.05$.) Despite tying with EFT in optimal accuracy scores in Figure 4a, we see in Figure 4b that the RP-algorithm outperforms EFT, GES and GreedySP, having lower false positive rates and higher true positive rates. One possible explanation for this is that the data is known to be highly non-Gaussian, contrary to the implemented assumptions for EFT, GES and GreedySP. On the other hand, the RP algorithm works directly with a discrete approximation of the data. To test this, we implemented a version of EFT, denoted discEFT in Figure 4, that discretizes the data according to the specified number of bins and computes the BIC score of the discretized data set. Due to computational complexity limitations, this was done only for numbers of bins ranging over \{5, 10, 15, 20, 25, 30\}. We see that EFT assuming discrete data (discEFT) then performs equally as well as the RP-algorithm in Figure 4b for the optimal numbers of bins (25 and 30) identified in Figure 4a. We note that the accuracy of EFT on discretized data for these numbers of bins is 0.8, tying with that of Gaussian EFT and the RP-algorithm. All details of this real data analysis and the simulations are available for reproduction at [15] (https://github.com/soluslab/causalCIM). Overall, these analyses suggest that EFT performs equally well as the RP-algorithm on the real data example and outperforms it in the linear Gaussian model regime.

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Figure 5. The ground-truth essential graph for the protein signaling system and the optimal learned essential graphs for each algorithm according to the ROC plot in Figure 4b. Here, undirected edges in essential graphs are represented by bidirected edges.

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