

Minimizing Wiener Index for Vertex-Weighted Trees with Given Weight and Degree Sequences

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Abstract

In 1997 Klavžar and Gutman suggested a generalization of the Wiener index to vertex-weighted graphs. We minimize the Wiener index over the set of trees with the given vertex weights' and degrees' sequences and show an optimal tree to be the, so-called, Huffman tree built in a bottom-up manner by sequentially connecting vertices of the least weights.

1 Introduction

In 1947 Harold Wiener [19] employed the sum of distances between vertices in a chemical graph representing a molecule to explain boiling points of alkanes. Later the sum of distances between all vertices in a graph was called the Wiener index, which became one of the earliest topological indices.

Since then extensive research was performed on revealing connection between different topological indices of molecules and physical, chemical, pharmacological, and biological properties of substances (see, for instance, [1]), and the Wiener index appeared to be among the most useful and powerful ones (see [2]).

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For a simple connected undirected graph G with the vertex set $V(G)$ and the edge set $E(G)$ and for any pair of vertices $u, v \in V(G)$ let $d_G(u, v)$ denote the distance (the length of the shortest path) between u and v in G . Then the Wiener index of the graph G is defined as

$$WI(G) := \frac{1}{2} \sum_{u, v \in V(G)} d_G(u, v).$$

In 1997 Klavžar and Gutman [12] suggested a generalization of the Wiener index to vertex-weighted graphs. They endowed each vertex $v \in V(G)$ in graph G with some weight $\mu_G(v)$ (in contrast to integer weights, originally used in [12], below we allow for arbitrary non-negative weights) and defined the *vertex-weighted Wiener index* ($VWWI$) for such a graph as

$$VWWI(G) := \frac{1}{2} \sum_{u, v \in V(G)} \mu_G(u) \mu_G(v) d_G(u, v).$$

When the weight of each vertex in a graph G is equal to the degree of this vertex in G , this index is referred to as the *Schultz index of the second kind* [10] or the *Gutman index* [17].

One of the typical problems in topological index study is estimation of index value bounds over the certain class of graphs (molecules). In [3] a tree, which minimizes the Wiener index over the set of all trees with the given maximum vertex degree Δ has been shown to be a balanced Δ -tree (the, so-called, *Volkman tree*). Lin [13], and Furtula, Gutman, and Lin [4] explored minimizers and maximizers of the Wiener index for trees of the fixed order and all degrees odd. Wang [18] and Zhang et al. [20] have shown independently that the minimizer of the Wiener index over the set of trees with the given vertex degrees' sequence is the, so-called, *greedy tree* [18]. It is built in top-down manner by adding vertices from the highest to the lowest degree to the seed (a vertex of maximum degree) to keep the tree as balanced as possible.

In the present paper we extend the results of [18, 20] to the vertex-weighted trees and show that some generalization of the famous Huffman algorithm [11] for the optimal prefix code builds an optimal tree, which coincides with the greedy tree in case of unit weights.

The paper has the following structure. In Section 2 we describe the generalized Huffman algorithm and announce the main theorem. In Section 3 we immerse the problem

of index minimization into the space of directed trees, which is more convenient to study. We define the notion of the vector of subordinate groups' weights playing the key role in the proofs, and prove some important properties of Huffman trees. In Section 4 we follow the line of the proof from [20] establishing the relation between index minimization and the majorization problem of vectors of subordinate groups' weights. In Section 5 we introduce the notion of a proper tree and combine the above results proving that the Huffman tree minimizes $VWWI$. We discuss possible extensions in the concluding section.

2 Wiener Index and Huffman Trees

2.1 Generating Tuples

For a simple connected undirected graph G and a vertex $v \in V(G)$ let us denote with $d_G(v)$ its *degree*, i.e., the number of vertices being incident to v in G . Denote with $W(G)$ the set of *pendent vertices* (those having degree 1) of the graph G , and with $M(G) := V(G) \setminus W(G)$ the set of *internal vertices* (with degree greater than unity) of G .

Definition 1 A simple undirected graph G is called *vertex-weighted* if each vertex $v \in V(G)$ is endowed with a non-negative number $\mu_G(v) > 0$. The total vertex weight of the graph G is denoted with μ_G . \square

A connected vertex-weighted graph T with N vertices and $N - 1$ edges is called a *vertex-weighted tree*. Denote with \mathcal{T} the set of all vertex-weighted trees.

All graphs below are supposed to be vertex-weighted, unless stated otherwise.

Definition 2 Consider a vertex set V . Let the function $\mu : V \rightarrow \mathbb{R}_+$ assign a non-negative weight $\mu(v)$ to each vertex $v \in V$, while the function $d : V \rightarrow \mathbb{N}$ assigning a natural degree $d(v)$. The tuple $\langle \mu, d \rangle$ is called a *generating tuple* if the following identity holds:

$$\sum_{v \in V} d(v) = 2(|V| - 1). \quad (1)$$

Let $\mathcal{T}(\mu, d) := \{T \in \mathcal{T} : V(T) = V, d_T(v) = d(v), \mu_T(v) = \mu(v) \text{ for all } v \in V\}$ be the set of trees with the vertex set V and vertices having weights $\mu(v)$ and degrees $d(v)$, $v \in V$. Also denote with $\bar{\mu} := \sum_{v \in V} \mu(v)$ the total weight of the vertex set V . \square

It is well-known that $\mathcal{T}(\mu, d)$ is not empty if and only if identity (1) holds.

Let $V(\mu, d)$ be the domain of functions of a generating tuple $\langle \mu, d \rangle$. Introduce the set $W(\mu, d) := \{w \in V(\mu, d) : d(w) = 1\}$ of *pendent* vertices and the set $M(\mu, d) := V(\mu, d) \setminus W(\mu, d)$ of *internal* vertices.

Below we refer to the typical generating tuple as $\langle \mu, d \rangle$, which is defined on the vertex set $V := V(\mu, d)$ with the pendent vertex set $W := W(\mu, d)$ consisting of $n = |W| \geq 2$ vertices and the internal vertex set $M := M(\mu, d)$ consisting of $q = |M| \geq 1$ vertices.

We will solve the problem of characterizing the set

$$\mathcal{T}^*(\mu, d) := \operatorname{Argmin}_{T \in \mathcal{T}(\mu, d)} VWWI(T)$$

of vertex-weighted trees generated by the tuple $\langle \mu, d \rangle$, which minimize the Wiener index.

Definition 3 The vertex-weighted tree T induces the tuple $\langle \mu, d \rangle$ on the vertex set $V = V(T)$ if $\mu(v) = \mu_T(v)$, $d(v) = d_T(v)$, $v \in V(T)$. Clearly, the induced tuple $\langle \mu, d \rangle$ generates the tree T , i.e., $T \in \mathcal{T}(\mu, d)$. \square

Definition 4 We will say that in the generating tuple $\langle \mu, d \rangle$ *weights are degree-monotone* if for any pair of internal vertices $m, m' \in M$ from $d(m) < d(m')$ it follows that $\mu(m) \leq \mu(m')$. We also require pendent vertices to have positive weights: $d(v) = 1 \Rightarrow \mu(v) > 0$. \square

In this paper we show that if weights are degree-monotone in the tuple $\langle \mu, d \rangle$, then the set $\mathcal{T}^*(\mu, d)$ consists of the trees built with the simple and efficient algorithm being a generalization of the famous Huffman algorithm [11] for construction of the binary tree of an optimal prefix code.

2.2 Generalized Huffman Algorithm

Definition 5 A *star* is a complete bipartite graph $K_{1,k}$, where a distinguished vertex, called a *center*, is connected to k other vertices, called *leaves*. For a star S , the set of its leaves is denoted with $L(S)$. It is clear that $L(S) = W(S)$, except for the case of $S = K_{1,1}$, when $W(S) = V(S)$. \square

Definition 6 Consider a generating tuple $\langle \mu, d \rangle$ with degree-monotone weights. Let $m \in M$ be any internal vertex having the least degree $d(m)$ among the vertices of the least weight in M , i.e., $m \in \operatorname{Argmin}\{d(u) : u \in \operatorname{Argmin}_{v \in M} \mu(v)\}$. The *minimal star* for the tuple $\langle \mu, d \rangle$ is a vertex-weighted star $S \in \mathcal{T}$ with the center m , $\mu_S(m) = \mu(m)$, and with $d(m) - 1$ leaves having $d(m) - 1$ least weights in W , i.e., $L(S) \subseteq W$, and

$u \in L(S), v \in W \setminus L(S) \Rightarrow \mu_S(u) = \mu(u) \leq \mu(v)$. Denote with $\underline{f}(\mu, d)$ the total weight of vertices of a minimal star. \square

For a fixed tuple $\langle \mu, d \rangle$ the *generalized Huffman algorithm* builds a tree $H \in \mathcal{T}(\mu, d)$ as follows.

Setup. Define the vertex set $V_1 := V$ and the functions μ^1 and d^1 , which endow its vertices with weights $\mu^1(v) := \mu(v)$ and degrees $d^1(v) := d(v)$, $v \in V_1$.

Steps $i = 1, \dots, q - 1$. Let the star S_i be a minimal star for the tuple $\langle \mu^i, d^i \rangle$. Denote its center with m_i . Define the set $V_{i+1} := V_i \setminus L(S_i)$ and functions μ^{i+1}, d^{i+1} , endowing its elements with weights and degrees as follows:

$$\begin{aligned} \mu^{i+1}(v) &:= \mu^i(v) \text{ for } v \neq m_i, \mu^{i+1}(m_i) := \mu_{S_i} = \sum_{v \in V(S_i)} \mu^i(v), \\ d^{i+1}(v) &:= d^i(v) \text{ for } v \neq m_i, d^{i+1}(m_i) := 1. \end{aligned} \quad (2)$$

Step q . Consider a vertex $m_q \in M(\mu^q, d^q)$ (such a vertex is unique by construction), and let S_q be the star with the vertex set V_q and the center m_q . We build a Huffman tree H by setting $V(H) := V$, $E(H) := E(S_1) \cup \dots \cup E(S_q)$, $\mu_H(v) := \mu(v)$, $v \in V$.

An example of Huffman tree construction is depicted in Fig. 1. Black circles correspond to pendent vertices, numbers inside circles stand for vertex weights, those under circles show the order of star sequence centers. All stars, except the last one, are surrounded by a dashed line.

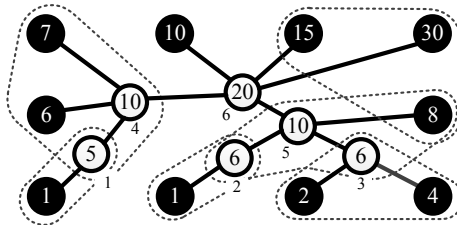


Figure 1: An example of Huffman tree construction

Thus, the Huffman tree H appears to be a union of minimal stars S_1, \dots, S_{q-1} for the corresponding generating tuples and a “finalizing” star S_q . Below we refer to the sequence S_1, \dots, S_q as the *star sequence* of a Huffman tree H . In general, the Huffman tree is not unique, as more than one star sequence is possible. Let $\mathcal{TH}(\mu, d)$ be the collection of

Huffman trees generated by the tuple $\langle \mu, d \rangle$. The main result of this paper can be stated as follows.

Theorem 1 *If weights are degree-monotone in a generating tuple $\langle \mu, d \rangle$, then $\mathcal{T}^*(\mu, d) = \mathcal{TH}(\mu, d)$. In other words, only a Huffman tree minimizes the Wiener index over the set of trees whose vertices have given weights and degrees. \square*

In the following sections we prove auxiliary results, and return to the proof of Theorem 1 at the end of Section 5.

Please note that when $\mu(v) \equiv 1$ for all $v \in V$, the Huffman tree becomes a “greedy tree” from [18]. Fig. 2 shows that weights’ monotonicity is essential for Theorem 1 (numbers inside circles are vertex weights, those under circles show the order of star sequence centers).

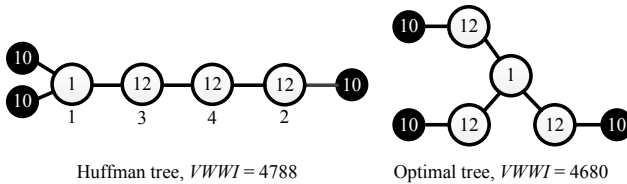


Figure 2: The counterexample for non-monotone weights

3 Properties of Huffman trees

3.1 Huffman algorithm for directed trees

The index minimization problem becomes more tractable when studied for directed trees.

Definition 7 A (weighted) *directed tree* is a connected directed graph with each vertex except the *root* having the sole outbound arc and the root having no outbound arcs. \square

An arbitrary tree $T \in \mathcal{T}$ consisting of more than two vertices can be transformed into a directed tree T_r by choosing an **internal vertex** $r \in M(T)$ as a root, and replacing all its edges with arcs directed towards the root. Let us denote with \mathcal{R} the collection of all directed trees, which can be obtained in such a way, and let $\mathcal{R}(\mu, d)$ stand for all directed trees obtained from $\mathcal{T}(\mu, d)$. Vice versa, in a directed tree $T_r \in \mathcal{R}(\mu, d)$ replacing all arcs with edges makes some tree $T \in \mathcal{T}(\mu, d)$.

Let the arcs in a directed star be directed towards its center by definition.

If in a star sequence of a Huffman tree H one replaces all stars with directed stars, then the union of the arcs of these directed stars gives a *directed Huffman tree* with the root at the center m_q of the last star in the sequence. Let $\mathcal{RH}(\mu, d) \subseteq \mathcal{R}(\mu, d)$ stand for the collection of directed Huffman trees generated by the tuple $\langle \mu, d \rangle$.

3.2 Vector of subordinate groups' weights and Wiener Index

Definition 8 For an arbitrary vertex $v \in V(T)$ of the directed tree $T \in \mathcal{R}$ define its *subordinate group* $g_T(v) \subseteq V(T)$ as the set of vertices having the directed path to the vertex v in the tree T (the vertex v itself belongs to $g_T(v)$). The *weight* $f_T(v)$ of the subordinate group $g_T(v)$ is defined as the total vertex weight of the group: $f_T(v) := \sum_{u \in g_T(v)} \mu_T(u)$. □

In particular, all vertices in a directed tree $T \in \mathcal{R}$ are subordinated to its root r , i.e., $g_T(r) = V(T)$ and $f_T(r) = \mu_T$. For example, if $T \in \mathcal{R}(\mu, d)$, then $f_T(r) = \bar{\mu}$.

Note 1 If all pendent vertices in T have strictly positive weights, then $f_T(v) > 0$ for any $v \in V(T)$. In particular, it is true for any $T \in \mathcal{R}(\mu, d)$, if weights in $\langle \mu, d \rangle$ are degree-monotone.

If some tree $T \in \mathcal{T}(\mu, d)$ is transformed into a directed tree $T_r \in \mathcal{R}(\mu, d)$ by choosing a root r , the Wiener index can be written as [12, 16]:

$$VWWI(T) = VWWI(T_r) = \sum_{v \in V \setminus \{r\}} f_{T_r}(v)(\bar{\mu} - f_{T_r}(v)) = \sum_{v \in V \setminus \{r\}} \chi(f_{T_r}(v)), \quad (3)$$

where $\chi(x) := x(\bar{\mu} - x)$.

Equality (3) implies that all directed trees obtained from one tree $T \in \mathcal{T}(\mu, d)$ share the same value of the Wiener index. Thus, if we find the collection $\mathcal{R}^*(\mu, d) := \text{Argmin}_{T \in \mathcal{R}(\mu, d)} VWWI(T)$ of directed trees minimizing the Wiener index, the collection $\mathcal{T}^*(\mu, d)$ is obtained by replacing them with corresponding undirected trees.

As the root of a directed tree $T \in \mathcal{R}(\mu, d)$ is an internal vertex, every pendent vertex has an outbound arc, so, for every pendent vertex $w \in W$ in a directed tree $T \in \mathcal{R}(\mu, d)$ $f_T(w) = \mu(w)$. Therefore, all directed trees from $\mathcal{R}(\mu, d)$ enjoy the same weights of groups subordinated to pendent vertices. Also, as noticed above, $f_T(r) = \bar{\mu}$ for the root r of any directed tree $T \in \mathcal{R}(\mu, d)$. Thus, directed trees from $\mathcal{R}(\mu, d)$ differ only in the subordinate group weights of $q - 1$ internal vertices other than root.

Definition 9 [14, 20] For the real vector $\mathbf{x} = (x_1, \dots, x_p)$, $p \in \mathbb{N}$, denote with $\mathbf{x}_\uparrow = (x_{[1]}, \dots, x_{[p]})$ the vector, where all components of \mathbf{x} are arranged in ascending order. \square

Definition 10 For a directed tree $T \in \mathcal{R}(\mu, d)$ define a $(q-1)$ -dimensional *vector* $\mathbf{f}(T) := (f_T(m) : m \in M \setminus \{r\})_\uparrow$ of *subordinate groups' weights*, where r is the root of T . \square

In the following proofs we combine the approach of [5, 6], where Huffman tree has been proved to minimize the *sum of subordinate groups' weights* in case of zero-weighted internal vertices, and that by Zhang et al [20], who minimized the Wiener index for unweighted trees having the given degree sequence.

3.3 Basic Properties of Huffman Trees

In Lemmas 1-3 we consider a Huffman tree $H \in \mathcal{RH}(\mu, d)$ with a star sequence S_1, \dots, S_q , and vertices m_1, \dots, m_q being the centers of stars S_1, \dots, S_q respectively.

Lemma 1 $\mathbf{f}(H) = (\mu^2(m_1), \mu^3(m_2), \dots, \mu^q(m_{q-1})) = (\underline{f}(\mu^1, d^1), \dots, \underline{f}(\mu^{q-1}, d^{q-1}))$, where tuples $\langle \mu^i, d^i \rangle, i = 1, \dots, q-1$, are defined by formula (2).

PROOF The definition of a minimal star implies that $\mu_{S_i} = \underline{f}(\mu^i, d^i)$. By construction of tuples $\langle \mu^i, d^i \rangle$ we have $f_H(m_i) = \sum_{v \in V(S_i)} \mu_i(v) = \mu^{i+1}(m_i)$, and thus, $f_H(m_i) = \mu^{i+1}(m_i) = \underline{f}(\mu^i, d^i), i = 1, \dots, q-1$. One can easily see that $\underline{f}(\mu^i, d^i) \leq \underline{f}(\mu^{i+1}, d^{i+1}), i = 1, \dots, q-2$, from which the statement of the lemma follows immediately. \blacksquare

Lemma 2 From $v \in L(S_i), v' \in L(S_j)$, and $i < j$ it follows that $f_H(v) \leq f_H(v')$.

PROOF Suppose, by contradiction, that $f_H(v) > f_H(v')$. As $v \in L(S_i), v' \in L(S_j)$, and $i < j$, a vertex $v'' \in g_H(v')$ exists, which also belongs to $W(\mu^i, d^i)$ (otherwise the vertex v' cannot belong to the set $W(\mu^j, d^j)$, as the tuple $\langle \mu^j, d^j \rangle$ is defined later, at the $(j-1)$ -th step of the algorithm).

By definition of a subordinate group, a path exists from the vertex v'' to v' in H , which immediately implies that $f_H(v') \geq f_H(v'')$, and, by assumption, $f_H(v) > f_H(v'')$. Then the vertex v cannot be a leaf of S_i by definition of a minimal star, as the set $W(\mu^i, d^i)$ contains the vertex v'' , which does not belong to the minimal star S_i , but has the weight $\mu^i(v'') < \mu^i(v)$ (since, by Lemma 1, $\mu^i(v'') = f_H(v''), \mu^i(v) = f_H(v)$). We obtain a contradiction, so the lemma is correct. \blacksquare

Lemma 3 *If weights are degree-monotone in $\langle \mu, d \rangle$, then for any $H \in \mathcal{RH}(\mu, d)$*

$$[vm, v'm' \in E(H), m \neq m', f_H(v) < f_H(v')] \Rightarrow f_H(m) < f_H(m'). \quad (4)$$

PROOF Suppose, by contradiction, that a pair of arcs $vm_i, v'm_j \in E(H)$ exists, such that $m_i \neq m_j$, $f_H(v) < f_H(v')$, but $f_H(m_i) \geq f_H(m_j)$. In case of strict inequality $f_H(m_i) > f_H(m_j)$, from Lemma 1, it follows that $i > j$. Then (since presence of the arcs vm_i and $v'm_j$ implies that $v \in L(S_i)$ and $v' \in L(S_j)$), by Lemma 2, $f_H(v) \geq f_H(v')$. We obtain a contradiction, and, since $m_i \neq m_j$, we are left with the sole case of $i < j$ and $f_H(m_i) = f_H(m_j)$.

Since, by Lemma 2, for every pair of vertices $u \in L(S_i)$, $u' \in L(S_j)$ we have $f_H(u) \leq f_H(u')$, and, by construction of the Huffman tree, $\mu(m_i) \leq \mu(m_j)$, and also, from degree-monotonicity of weights in $\langle \mu, d \rangle$ we have $d(m_i) \leq d(m_j)$, the equality $f_H(m_i) = f_H(m_j)$ is possible only if $\mu(m_i) = \mu(m_j)$, and $f_H(u) = f_H(u')$ for all $u \in L(S_i), u' \in L(S_j)$. However, by assumption, $v \in L(S_i), v' \in L(S_j)$ and $f_H(v) < f_H(v')$. The obtained contradiction completes the proof. ■

3.4 Vector of subordinate groups' weights in Huffman Trees

In this paragraph we show that all directed Huffman trees share the same vector of subordinate groups' weights, and no other tree enjoys this vector of subordinate groups' weights. These results allow us to move the index minimization problem into the space of vectors of subordinate groups' weights for directed trees from $\mathcal{R}(\mu, d)$.

Definition 11 Consider a tuple $\langle \mu, d \rangle$ of functions (not necessarily the generating one) defined on the set V , and a tuple $\langle \mu', d' \rangle$ defined on the set V' . A bijection $\sigma : V \rightarrow V'$ preserves weights and degrees if $\mu(v) = \mu'(\sigma(v))$, $d(v) = d'(\sigma(v))$, $v \in V$. □

Lemma 4 *Consider a generating tuple $\langle \mu, d \rangle$ on the set V , a tuple $\langle \mu', d' \rangle$ on the set V' , and a bijection $\sigma : V \rightarrow V'$ preserving weights and degrees. If $H \in \mathcal{RH}(\mu, d)$ is a directed Huffman tree, then there exists a Huffman tree $H' \in \mathcal{RH}(\mu', d')$ such that $\mathbf{f}(H) = \mathbf{f}(H')$.*

PROOF Consider a star sequence S_1, \dots, S_q of the Huffman tree H , with m_1, \dots, m_q being the centers of stars S_1, \dots, S_q respectively. The Huffman algorithm takes care only of vertex weights and degrees, so, replacing all vertices in stars S_1, \dots, S_q with their images

under the bijection $\sigma(\cdot)$, we obtain the sequence $\sigma(S_1), \dots, \sigma(S_q)$ of stars, which give some Huffman tree $H' \in \mathcal{RH}(\mu', d')$ as their union.

As the group $g_{H'}(\sigma(m_i))$ subordinated in the directed tree H' to the image $\sigma(m_i)$ of the vertex m_i coincides with the image $\sigma(g_H(m_i))$ of the subordinate group of the vertex m_i in the directed tree H , we obtain $f_H(m_i) = f_{H'}(\sigma(m_i))$. So, according to Definition 10, $\mathbf{f}(H) = \mathbf{f}(H')$. ■

Lemma 5 *If S and S' are two different minimal stars for the tuple $\langle \mu, d \rangle$, then a bijection $\sigma : L(S) \rightarrow L(S')$ preserving weights and degrees can be established between the leaf sets $L(S)$ and $L(S')$ of these stars.*

PROOF By definition of a minimal star, sets $L(S)$ and $L(S')$ consist of the same number of elements. Define the vectors $\mathbf{w} := (\mu(v) : v \in L(S))_{\uparrow}$ and $\mathbf{w}' := (\mu(v) : v \in L(S'))_{\uparrow}$. Since both $L(S)$ and $L(S')$ include the same number of vertices having the minimum weight in W , it is clear that $\mathbf{w} = \mathbf{w}'$. The desired bijection is built by matching sequentially vertices inducing the first, the second, etc, components of the vectors \mathbf{w} and \mathbf{w}' . ■

Definition 12 A directed star S with the center $m \in M(T)$ is called the *lower star* of a directed tree $T \in \mathcal{R}$, if $V(S) = g_T(m)$ and $\mu_S(v) = \mu_T(v), v \in V(S)$. □

Definition 13 Let $m \in M(T)$ be an internal vertex in a directed tree $T \in \mathcal{R}$. The *m -rollup* of T is a directed tree $\underline{T} \in \mathcal{R}$ obtained from T by deleting the set of vertices $g_T(m) \setminus \{m\}$ along with their incident arcs, and setting $\mu_{\underline{T}}(m) := f_T(m)$. □

Please note that if a directed tree R is a contraction of T to the vertex set $V(R) := g_T(m)$, and m is not a root of T , then $\mathbf{f}(T) = (\mathbf{f}(R), f_T(m), \mathbf{f}(\underline{T}))_{\uparrow}$.

Lemma 6 *Consider the star sequence S_1, \dots, S_q of a Huffman tree $H \in \mathcal{RH}(\mu, d)$ with the vertex m_1 being the center of the star S_1 . If the tuple $\langle \mu', d' \rangle$ is induced by the m_1 -rollup \underline{H} of the Huffman tree H , then $\underline{H} \in \mathcal{RH}(\mu', d')$. In other words, the m_1 -rollup of a Huffman tree appears to be a Huffman tree for the induced generating tuple.*

PROOF By construction of the Huffman tree the tuple $\langle \mu', d' \rangle$ coincides with the tuple $\langle \mu^2, d^2 \rangle$ from the Huffman algorithm. Thus, S_2 is a minimal star for $\langle \mu', d' \rangle$, which implies that the stars S_3, \dots, S_q are minimal stars for the corresponding generating tuples defined with formula (2). As $E(\underline{H}) = E(S_2) \cup \dots \cup E(S_q)$, by definition of a Huffman tree we obtain $\underline{H} \in \mathcal{RH}(\mu', d')$. ■

Lemma 7 *All Huffman trees share the same vector of subordinate groups' weights, i.e., if $T, H \in \mathcal{RH}(\mu, d)$, then $\mathbf{f}(T) = \mathbf{f}(H)$.*

PROOF Employ induction on the number of internal vertices q . For $q = 1$ the vector of subordinate groups' weights has zero components, thus, the lemma obviously holds.

Suppose the lemma holds for all $q' < q$. Let us prove that it also holds for the set V with q internal vertices. Denote $\mathbf{f}(T) = (f_1, \dots, f_{q-1})$, $\mathbf{f}(H) = (f'_1, \dots, f'_{q-1})$. On the first step of the Huffman algorithm some minimal stars S and S' with the centers m and m' are added to the trees T and H respectively, thus, $f_1 = f'_1 = \underline{f}(\mu, d)$. Consider the m_1 -rollup \underline{T} of the tree T and the m'_1 -rollup \underline{H} of the tree H . Let \underline{T} induce the tuple $\langle \mu', d' \rangle$ and \underline{H} induce the tuple $\langle \mu'', d'' \rangle$. From Lemma 6, $\underline{T} \in \mathcal{RH}(\mu', d')$, $\underline{H} \in \mathcal{RH}(\mu'', d'')$. By Lemma 1, $\mathbf{f}(\underline{T}) = (f_2, \dots, f_{q-1})$, $\mathbf{f}(\underline{H}) = (f'_2, \dots, f'_{q-1})$.

From Lemma 5, a bijection can be established between elements of the sets $L(S)$ and $L(S')$, which preserves weights and degrees. So, obviously, an analogous bijection σ can be established between the elements of the residual sets $V(\underline{T}) = V \setminus L(S)$ (with the generating tuple $\langle \mu', d' \rangle$) and $V(\underline{H}) = V \setminus L(S')$ (with the generating tuple $\langle \mu'', d'' \rangle$), which also preserves weights and degrees. Thus, by Lemma 4, there exists such a Huffman tree $\underline{H} \in \mathcal{RH}(\mu', d')$ that $\mathbf{f}(\underline{H}) = \mathbf{f}(\underline{T})$.

There are $q-1$ internal vertices in the tree \underline{T} , so, by inductive assumption $(f_2, \dots, f_{q-1}) = (f'_2, \dots, f'_{q-1})$ and, since $f_1 = f'_1$, the proof is complete. \blacksquare

Lemma 8 *If a tree has the same vector of subordinate groups' weights as some Huffman tree, it has to be a Huffman tree itself. In other words, for $H \in \mathcal{RH}(\mu, d), T \in \mathcal{R}(\mu, d)$ from $\mathbf{f}(H) = \mathbf{f}(T)$ it follows that $T \in \mathcal{RH}(\mu, d)$.*

PROOF We again employ induction on the number of internal vertices q . For $q = 1$ the vector of subordinate groups' weights has zero components, but $H = T$, since the collection $\mathcal{R}(\mu, d)$ consists of the sole directed tree (the star). Assume the lemma is valid for all $q' < q$; let us prove that it also holds for the vertex set V with q internal vertices.

Denote for short $\mathbf{f}(H) = \mathbf{f}(T) = (f_1, \dots, f_{q-1})$. By construction of the Huffman tree H , $f_1 = \underline{f}(\mu, d)$. Every star with the total vertex weight $\underline{f}(\mu, d)$ is minimal, so, some minimal star S_1 for the tuple $\langle \mu, d \rangle$ must be a part of the tree T ; H contains some minimal star S'_1 by definition. Denote with m_1, m'_1 respectively the centers of these stars.

Let the tuple $\langle \mu', d' \rangle$ be induced by the m_1 -rollup \underline{T} of the directed tree T , and the tuple $\langle \mu'', d'' \rangle$ be induced by the m'_1 -rollup \underline{H} of the directed Huffman tree H . By Lemma 6, $\underline{H} \in \mathcal{RH}(\mu'', d'')$. Moreover, by Lemma 1, $\mathbf{f}(\underline{T}) = \mathbf{f}(\underline{H}) = (f_2, \dots, f_{q-1})$.

By analogy with the proof of Lemma 7, between the vertex sets $V(\underline{T})$ (with the tuple $\langle \mu', d' \rangle$) and $V(\underline{H})$ (with the tuple $\langle \mu'', d'' \rangle$) one can establish a bijection σ preserving weights and degrees, so, by Lemma 4, such a Huffman tree $\underline{H} \in \mathcal{RH}(\mu', d')$ exists that $\mathbf{f}(\underline{H}) = \mathbf{f}(\underline{T})$. Then we have $\mathbf{f}(\underline{H}) = \mathbf{f}(\underline{T}) = (f_2, \dots, f_{q-1})$, and, by inductive assumption, \underline{T} is a Huffman tree for the tuple $\langle \mu', d' \rangle$. Let S_2, \dots, S_q be its star sequence. Then the tree T can be obtained as a union of \underline{T} and the minimal star S_1 , and, thus, $T \in \mathcal{RH}(\mu, d)$. ■

To sum up, Lemmas 7 and 8 say that if some Huffman tree H has the vector $\mathbf{f}(H)$ of subordinate groups' weights, then all Huffman trees, and only they, have this vector of subordinate groups' weights.

Corollary 1 *If $H, H' \in \mathcal{RH}(\mu, d)$ are two directed Huffman trees, then $VWWI(H) = VWWI(H')$.*

PROOF From equation (3) we know that the value of the index is determined by the components of vectors $\mathbf{f}(H), \mathbf{f}(H')$, and also by the weights of pendent vertices of trees H and H' . From Lemma 7 we learn that $\mathbf{f}(H) = \mathbf{f}(H')$, so, since the trees H and H' enjoy the same weights of pendent vertices, we induce that the index has the same value for both trees. ■

Therefore, to justify Theorem 1 it is enough to prove that the vector of subordinate groups' weights originated from some Huffman tree minimizes $VWWI$ over all directed trees in the collection $\mathcal{R}(\mu, d)$. We postpone the proofs to the next section.

4 Huffman Trees and Majorization

4.1 Notion of Vectors' Majorization

Let us recall that notation $\mathbf{x}_\uparrow = (x_{[1]}, \dots, x_{[p]})$ stands for the vector where all components of a real vector $\mathbf{x} = (x_1, \dots, x_p), p \in \mathbb{N}$, are arranged in the ascending order.

Definition 14 [14, 20] A non-negative vector $\mathbf{x} = (x_1, \dots, x_p), p \in \mathbb{N}$, *weakly majorizes* a non-negative vector $\mathbf{y} = (y_1, \dots, y_p)$ (which is denoted with $\mathbf{y} \preceq^w \mathbf{x}$ or $\mathbf{x} \succeq^w \mathbf{y}$) if

$$\sum_{i=1}^k x_{[i]} \leq \sum_{i=1}^k y_{[i]} \text{ for all } k = 1, \dots, p.$$

Moreover, if $\mathbf{x}_\uparrow \neq \mathbf{y}_\uparrow$, then \mathbf{x} is said to *strictly weakly majorize* \mathbf{y} (which is denoted with $\mathbf{y} \prec^w \mathbf{x}$ or $\mathbf{x} \succ^w \mathbf{y}$). \square

We will need the following properties of weak majorization.

Lemma 9 [14, 20] *Consider a positive number $b > 0$ and two non-negative vectors, $\mathbf{x} = (x_1, \dots, x_k, y_1, \dots, y_l)$ and $\mathbf{y} = (x_1 + b, \dots, x_k + b, y_1 - b, \dots, y_l - b)$, such that $0 \leq k \leq l$. If $x_i \geq y_i$ for $i = 1, \dots, k$, then $\mathbf{x} \prec^w \mathbf{y}$. \square*

Lemma 10 [14, 20] *If $\mathbf{x} \preceq^w \mathbf{y}$ and $\mathbf{x}' \preceq^w \mathbf{y}'$, then $(\mathbf{x}, \mathbf{x}') \preceq^w (\mathbf{y}, \mathbf{y}')$, where $(\mathbf{x}, \mathbf{x}')$ means concatenation of vectors \mathbf{x} and \mathbf{x}' . Moreover, if $\mathbf{x}' \prec^w \mathbf{y}'$, then $(\mathbf{x}, \mathbf{x}') \prec^w (\mathbf{y}, \mathbf{y}')$. \square*

Lemma 11 [14, 20] *If $\chi(x)$ is an increasing concave function, and $(x_1, \dots, x_p) \preceq^w (y_1, \dots, y_p)$, then $\sum_{i=1}^p \chi(x_i) \geq \sum_{i=1}^p \chi(y_i)$, and equality is possible only when $(x_1, \dots, x_p)_\uparrow = (y_1, \dots, y_p)_\uparrow$. \square*

4.2 Transformations of Trees and Majorization

The following lemmas play the same role in our proofs as Lemmas 3.1-3.5 in [20]. Some novelty is originated from accounting for variations in internal vertex weights.

Lemma 12 *Suppose a directed tree $T \in \mathcal{R}(\mu, d)$ contains the disjoint paths (v, m_1, \dots, m_k, m) and $(v', m'_1, \dots, m'_l, m)$ from vertices $v, v' \in V$ to some vertex $m \in M$, and suppose that $1 \leq k \leq l$, $f_T(v) < f_T(v')$, $f_T(m_i) \geq f_T(m'_i)$, $i = 1, \dots, k$. If the directed tree T' is obtained from T by deleting the arcs $vm_1, v'm'_1$ and adding the arcs $v'm_1$ and vm'_1 instead, then $T' \in \mathcal{R}(\mu, d)$ and $\mathbf{f}(T') \succ^w \mathbf{f}(T)$.*

PROOF Clearly, $T' \in \mathcal{R}(\mu, d)$, since vertex degrees and weights do not change during the transformation. Denote $b := f_T(v') - f_T(v) > 0$. In the tree T' weights of the groups subordinated to the vertices $m_1, \dots, m_k \in M$ increase by b (i.e., $f_{T'}(m_i) = f_T(m_i) + b$, $i = 1, \dots, k$), weights of the groups subordinated to the vertices $m'_1, \dots, m'_l \in M$ decrease by b (i.e., $f_{T'}(m'_i) = f_T(m'_i) - b$, $i = 1, \dots, l$), weights of all other vertices (including m) do not change. Therefore, by Lemma 9,

$$\begin{aligned} \mathbf{y} &:= (f_{T'}(m_1), \dots, f_{T'}(m_k), f_{T'}(m'_1), \dots, f_{T'}(m'_l)) = \\ &= (f_T(m_1) + b, \dots, f_T(m_k) + b, f_T(m'_1) - b, \dots, f_T(m'_l) - b) \succ^w \\ &\succ^w (f_T(m_1), \dots, f_T(m_k), f_T(m'_1), \dots, f_T(m'_l)) =: \mathbf{x}. \end{aligned}$$

If one denotes with \mathbf{z} the vector of (unchanged) weights of groups subordinated to all other internal vertices of T distinct from the root, then, by Lemma 10, $\mathbf{f}(T') = (\mathbf{y}, \mathbf{z}) \succ^w (\mathbf{x}, \mathbf{z}) = \mathbf{f}(T)$. \blacksquare

Lemma 13 *Consider a directed tree $T \in \mathcal{R}(\mu, d)$ containing the disjoint paths (v, m_1, \dots, m_k, m) and $(v', m'_1, \dots, m'_l, m)$ from vertices $v, v' \in V$ to some vertex $m \in M$, and suppose that $1 \leq l \leq k$, $f_T(v) < f_T(v')$, $f_T(m_1) = f_T(m'_1)$, and $f_T(m_i) \leq f_T(m'_i)$, $i = 2, \dots, l$. Then such a directed tree $T' \in \mathcal{R}(\mu, d)$ exists that $\mathbf{f}(T') \succ^w \mathbf{f}(T)$.*

PROOF Introduce the notation

$$u = \begin{cases} m_2, & \text{if } k \geq 2 \\ m, & \text{if } k = 1, \end{cases} \quad u' = \begin{cases} m'_2, & \text{if } l \geq 2 \\ m, & \text{if } l = 1, \end{cases}$$

and consider the tree T' obtained from T by deleting the arcs $vm_1, v'm'_1, m_1u, m'_1u'$ and adding the arcs $v'm_1, vm'_1, m_1u'$, and m'_1u instead. We have $T' \in \mathcal{R}(\mu, d)$, since vertex degrees and weights do not change during the transformation.

Denote $b := f_T(v') - f_T(v) > 0$. In the tree T' weights of the groups subordinated to the vertices $m'_1, m_2, \dots, m_k \in M$ decrease by b (i.e., $f_{T'}(m'_1) = f_T(m'_1) - b$, $f_{T'}(m_i) = f_T(m_i) - b$, $i = 2, \dots, k$), weights of the groups subordinated to the vertices $m_1, m'_2, \dots, m'_l \in M$ increase by b (i.e., $f_{T'}(m_1) = f_T(m_1) + b$, $f_{T'}(m'_i) = f_T(m'_i) + b$, $i = 2, \dots, l$), while weights of all other vertices (including m) do not change. Therefore, by Lemma 9,

$$\begin{aligned} \mathbf{y} &:= (f_{T'}(m'_1), f_{T'}(m_2), \dots, f_{T'}(m_k), f_{T'}(m_1), f_{T'}(m'_2), \dots, f_{T'}(m'_l)) = \\ &= (f_T(m'_1) - b, f_T(m_2) - b, \dots, f_T(m_k) - b, f_T(m_1) + b, f_T(m'_2) + b, \dots, f_T(m'_l) + b) \succ^w \\ &\succ^w (f_T(m_1), \dots, f_T(m_k), f_T(m'_1), \dots, f_T(m'_l)) =: \mathbf{x}. \end{aligned}$$

If one denotes with \mathbf{z} the vector of weights of groups subordinated to all other internal vertices of T distinct from the root, then, by Lemma 10, $\mathbf{f}(T') = (\mathbf{y}, \mathbf{z}) \succ^w (\mathbf{x}, \mathbf{z}) = \mathbf{f}(T)$. \blacksquare

Lemma 14 *Consider a directed tree $T \in \mathcal{R}(\mu, d)$, which contains the paths (v, m) and $(v', m'_1, \dots, m'_l, m)$ from vertices $v, v' \in V$ to some vertex $m \in M$, and suppose that $l \geq 1$ and $f_T(v) < f_T(v')$. If the directed tree T' is obtained from T by deleting the arcs $vm, v'm'_1$ and adding the arcs $v'm$ and vm'_1 instead, then $T' \in \mathcal{R}(\mu, d)$ and $\mathbf{f}(T') \succ^w \mathbf{f}(T)$.*

PROOF Since vertex degrees and weights do not change during the transformation, $T' \in \mathcal{R}(\mu, d)$. Denote $b := f_T(v') - f_T(v) > 0$. In the tree T' weights of the groups subordinated to the vertices $m'_1, \dots, m'_l \in M$ decrease by b (i.e., $f_{T'}(m'_i) = f_T(m'_i) - b, i = 1, \dots, l$), while weights of all other vertices do not change. Therefore, by Lemma 9,

$$\mathbf{y} := (f_{T'}(m'_1), \dots, f_{T'}(m'_l)) = (f_T(m'_1) - b, \dots, f_T(m'_l) - b) \succ^w (f_T(m'_1), \dots, f_T(m'_l)) =: \mathbf{x}.$$

If \mathbf{z} is the vector of weights of groups subordinated to all other internal vertices of T distinct from the root, then, by Lemma 10, $\mathbf{f}(T') = (\mathbf{y}, \mathbf{z}) \succ^w (\mathbf{x}, \mathbf{z}) = \mathbf{f}(T)$. \blacksquare

Lemma 15 *Suppose weights are degree-monotone in a generating tuple $\langle \mu, d \rangle$ and consider a directed tree $T \in \mathcal{R}(\mu, d)$ containing the disjoint paths (v, m_1, \dots, m_k, m) and $(v', m'_1, \dots, m'_l, m)$ from vertices $v, v' \in M$ to some vertex $m \in M$. Suppose that $0 \leq k \leq l$, $d_T(v') - d_T(v) = \Delta > 0$, $f_T(v) \geq f_T(v')$, $f_T(m_i) \geq f_T(m'_i)$, $i = 1, \dots, k$. Then there exists a directed tree $T' \in \mathcal{R}(\mu, d)$ such that $\mathbf{f}(T') \succ^w \mathbf{f}(T)$.*

PROOF Let the vertex v have $d > 0$ inbound arcs in T . Introduce the notation

$$u = \begin{cases} m_1, & \text{if } k \geq 1 \\ m, & \text{if } k = 0, \end{cases} \quad u' = \begin{cases} m'_1, & \text{if } l \geq 1 \\ m, & \text{if } l = 0, \end{cases}$$

and consider the tree T' obtained from T by replacing the arcs $vu, v'u'$ with the arcs $v'u, vu'$, redirecting all d inbound arcs of the vertex v in T to the vertex v' , and redirecting arbitrary d inbound arcs of the vertex v' in T to the vertex v . We have $T' \in \mathcal{R}(\mu, d)$, since vertex degrees and weights do not change during the transformation.

Let u_1, \dots, u_Δ be those Δ vertices, for which outbound arcs to the vertex v' in the tree T survived in the tree T' , and introduce $b := f_T(u_1) + \dots + f_T(u_\Delta) + [\mu(v') - \mu(v)]$. Weights are degree-monotone in $\langle \mu, d \rangle$, so we have $\mu(v') - \mu(v) \geq 0$. Since $\Delta > 0$, from Note 1 it follows that $b > 0$.

In the tree T' weights of the groups subordinated to the vertices m_1, \dots, m_k (when $k > 0$) increase by b , weights of the groups subordinated to the vertices m'_1, \dots, m'_l (when $l > 0$) decrease by b . Also we have $f_{T'}(v') - f_T(v) = -[f_{T'}(v) - f_T(v')] = b$. Weights of all other vertices (including m) do not change. Therefore, by Lemma 9,

$$\begin{aligned} \mathbf{y} &:= (f_{T'}(v'), f_{T'}(m_1), \dots, f_{T'}(m_k), f_{T'}(v), f_{T'}(m'_1), \dots, f_{T'}(m'_l)) = \\ &= (f_T(v) + b, f_T(m_1) + b, \dots, f_T(m_k) + b, f_T(v') - b, f_T(m'_1) - b, \dots, f_T(m'_l) - b) \succ^w \end{aligned}$$

$$\succ^w (f_T(v), f_T(m_1), \dots, f_T(m_k), f_T(v'), f_T(m'_1), \dots, f_T(m'_l)) =: \mathbf{x}.$$

If \mathbf{z} is the vector of weights of groups subordinated to all other internal vertices of T distinct from the root, then, by Lemma 10, $\mathbf{f}(T') = (\mathbf{y}, \mathbf{z}) \succ^w (\mathbf{x}, \mathbf{z}) = \mathbf{f}(T)$. ■

Lemma 16 Consider a directed tree $T \in \mathcal{R}(\mu, d)$ containing the disjoint paths (v, m_1, \dots, m_k, m) and $(v', m'_1, \dots, m'_l, m)$ from vertices $v, v' \in M$ to some vertex $m \in M$, and suppose that $0 \leq k \leq l$, $d(v) = d(v')$, $\mu(v) < \mu(v')$, $f_T(v) \geq f_T(v')$, and $f_T(m_i) \geq f_T(m'_i)$, $i = 1, \dots, k$. If the directed tree T' is obtained from T by swapping all incident arcs of vertices v and v' , then $T' \in \mathcal{R}(\mu, d)$ and $\mathbf{f}(T') \succ^w \mathbf{f}(T)$.

PROOF It is clear that $T' \in \mathcal{R}(\mu, d)$. Denote $b := \mu(v') - \mu(v) > 0$. The rest of the proof repeats the one of Lemma 15. ■

Lemma 17 Consider a path (v', m_1, \dots, m_k, v) , $k \geq 0$, in a directed tree $T \in \mathcal{R}(\mu, d)$, and suppose that $d(v) = d(v')$, $\mu(v') > \mu(v)$. If the directed tree T' is obtained from T by swapping all incident arcs of vertices v and v' , then $T' \in \mathcal{R}(\mu, d)$ and $\mathbf{f}(T') \succ^w \mathbf{f}(T)$.

PROOF It is clear that $T' \in \mathcal{R}(\mu, d)$. Denote $b := \mu(v') - \mu(v) > 0$. Then $f_{T'}(v') = f_T(v)$, $f_{T'}(v) = f_T(v') - b$, $f_{T'}(m_i) = f_T(m_i) - b$, $i = 1, \dots, k$. Weights of all other vertices do not change. Therefore, by Lemmas 9 and 10,

$$\begin{aligned} \mathbf{y} &:= (f_{T'}(v), f_{T'}(m_1), \dots, f_{T'}(m_k), f_{T'}(v')) = \\ &= (f_T(v') - b, f_T(m_1) - b, \dots, f_T(m_k) - b, f_T(v)) \succ^w \\ &\succ^w (f_T(v'), f_T(m_1), \dots, f_T(m_k), f_T(v)) =: \mathbf{x}. \end{aligned}$$

If \mathbf{z} is the vector of weights of groups subordinated to all other internal vertices of T distinct from the root, then, by Lemma 10, $\mathbf{f}(T') = (\mathbf{y}, \mathbf{z}) \succ^w (\mathbf{x}, \mathbf{z}) = \mathbf{f}(T)$. ■

Lemma 18 Suppose weights are degree-monotone in a generating tuple $\langle \mu, d \rangle$ and consider a directed tree $T \in \mathcal{R}(\mu, d)$. Let T contain an arc $mm' \in E(T)$, and suppose that $d_T(m) - d_T(m') = \Delta > 0$. Then such a directed tree $T' \in \mathcal{R}(\mu, d)$ exists that $\mathbf{f}(T') \succ^w \mathbf{f}(T)$.

PROOF If the vertex m' has an outbound arc in the tree T , denote this arc with $m'u$. Let the vertex m' have $d \geq 0$ inbound arcs from the vertices other than m . Consider

a directed tree T' obtained from T by replacing the arc mm' with the inverse arc $m'm$, replacing the arc $m'u$ (if it presents) with the arc mu , redirecting to the vertex m all d arcs entering the vertex m' from the vertices other than m in T , and redirecting to the vertex m' as many (arbitrary) inbound arcs of the vertex m in T as needed to restore its degree $d(m')$ (we are enough to redirect d arcs in case of m' being a root in T , and $d + 1$ arcs otherwise). Since vertex degrees and weights do not change during the transformation, we have $T' \in \mathcal{R}(\mu, d)$.

Let u_1, \dots, u_Δ be those Δ vertices, for which outbound arcs to the vertex m in the tree T survived in the tree T' , and introduce $b := f_T(u_1) + \dots + f_T(u_\Delta) + [\mu(m') - \mu(m)]$. Weights are degree-monotone in $\langle \mu, d \rangle$, so we have $\mu(m') - \mu(m) \geq 0$, and, since $\Delta > 0$, from Note 1 it follows that $b > 0$.

By construction of T' we have $f_{T'}(m') = f_T(m)$, $f_T(m') - f_{T'}(m) = b$. Therefore, by Lemma 9,

$$\mathbf{y} := (f_{T'}(m)) = (f_T(m') - b) \succ^w (f_T(m')) =: \mathbf{x}.$$

Weights of groups subordinated to all other vertices do not change, so, by analogy with Lemmas 12-17, by Lemma 10 we obtain $\mathbf{f}(T') \succ^w \mathbf{f}(T)$. ■

Please note that only Lemmas 15 and 18 require degree-monotonicity of the generating tuple $\langle \mu, d \rangle$.

As we show below, conditions of Lemmas 12-18 are never satisfied for directed Huffman trees (an only for directed Huffman trees), and the above transformations cannot result in a tree with the vector of subordinate groups' weights majorizing the one of some directed Huffman tree.

4.3 Huffman Trees and Majorization

Let us define the following useful tree transformations.

Definition 15 A directed tree $T \in \mathcal{R}(\mu, d)$ induces the Huffman tree H , if $H \in \mathcal{RH}(\mu, d)$. A directed tree $H' \in \mathcal{R}(\mu, d)$ is an *augmentation* of a Huffman tree for the m -rollup of the tree $T \in \mathcal{R}(\mu, d)$ if H' is obtained by joining, firstly, the Huffman tree \underline{H} induced by an m -rollup \underline{T} of the directed tree T , and, secondly, the contraction $R \in \mathcal{R}$ of the tree T to the vertex set $V(R) := g_T(m)$, i.e. $E(R) := E(T) \cap (g_T(m) \times g_T(m))$, $V(H') := V, E(H') := E(\underline{H}) \cup E(R)$, $\mu_{H'}(v) := \mu(v), v \in V$. □

Note 2 If the vertex $m \in M$ is not the root of T , then, clearly, $\mathbf{f}(H') = (\mathbf{f}(R), f_T(m), \mathbf{f}(\underline{H}))_1$. Moreover, formula (4) from Lemma 3 holds for those vertices of the augmented tree H' , which also belong to the Huffman tree \underline{H} induced by the m -rollup of T .

Theorem 2 If weights are degree-monotone in a generating tuple $\langle \mu, d \rangle$, and $H \in \mathcal{RH}(\mu, d)$ is a directed Huffman tree, then for any directed tree $T \in \mathcal{R}(\mu, d)$ $\mathbf{f}(H) \succeq^w \mathbf{f}(T)$.

PROOF Let us employ induction on the number of internal vertices q . If $q = 1$, the statement of the theorem is straightforward, since the collection $\mathcal{R}(\mu, d)$ consists of the sole tree (a directed star). Assume the theorem is valid for all directed trees with less than q internal vertices. Let us prove that it is also valid for directed trees with q internal vertices.

The relation \succ^w is a strict partial ordering on the set of $(q - 1)$ -dimensional vectors, and, hence, a strict partial ordering on a narrower set of vectors of subordinate groups' weights of all directed trees from $\mathcal{R}(\mu, d)$. Therefore, the set

$$\bar{\mathcal{R}}(\mu, d) := \{T \in \mathcal{R}(\mu, d) : \nexists T' \in \mathcal{R}(\mu, d) \text{ such that } \mathbf{f}(T') \succ^w \mathbf{f}(T)\}$$

of trees whose vector of subordinate groups' weights is "maximal" with respect to the partial ordering \succ^w , is not empty. Without loss of generality suppose that $T \in \bar{\mathcal{R}}(\mu, d)$.

Among all lower stars of the tree T , one or more has the least total weight. One or more centers of these least-weight lower stars has the least degree. Let $\underline{v} \in M$ be one of these least-degree centers having the least vertex weight $\mu(\cdot)$, and let \underline{S} be the \underline{v} -centered lower star in T .

Note that, since $q > 1$, the vertex \underline{v} (being a center of a lower star) cannot be the root of T . The following four steps prove that the star \underline{S} is minimal for the tuple $\langle \mu, d \rangle$, i.e., that $f_T(\underline{v}) = \underline{f}(\mu, d)$. Below the shorthand notation $d := \min_{u \in M} d(u)$ is used.

Step I. First we prove that the tree T contains a lower star with $d - 1$ pendent vertices. Suppose, by contradiction, that centers of all lower stars in T have more than $d - 1$ pendent vertices and, thus, have degree greater than d . Then the tree T must contain a vertex $m' \in M$ of degree $d_T(m') = d$, which has an inbound arc from some vertex $m \in M$ of degree $d_T(m) > d$. But Lemma 18 says that then the tree $T' \in \mathcal{R}(\mu, d)$ exists, such that $\mathbf{f}(T') \succ^w \mathbf{f}(T)$, so T cannot belong to the collection $\bar{\mathcal{R}}(\mu, d)$. The obtained contradiction proves that T contains some lower star (denote it with S) containing $d - 1$ pendent vertices. Let $v \in M$ be the center of S .

Step II. Let us prove that the star \underline{S} has exactly $d - 1$ leaves. Suppose, by contradiction, that $|L(\underline{S})| > d - 1$. In particular, this implies that $S \neq \underline{S}$ and $f_T(v) > f_T(\underline{v})$ ($f_T(v) \geq f_T(\underline{v})$ by construction of the star \underline{S} , and the case of $f_T(v) = f_T(\underline{v})$ contradicts the fact that \underline{v} has the least degree among all least-weight lower stars).

It is clear that the star S is still a lower star in a \underline{v} -rollup of the tree T , so, let $H^\clubsuit \in \mathcal{R}(\mu, d)$ stand for the augmentation of a Huffman tree \underline{H} induced by the (v, \underline{v}) -rollup \underline{T} of the tree T . Since neither v , nor \underline{v} , are the roots of T , by Definition 13 we have $\mathbf{f}(T) = (f_T(v), f_T(\underline{v}), \mathbf{f}(\underline{T}))$. By Note 2, $\mathbf{f}(H^\clubsuit) = (f_T(v), f_T(\underline{v}), \mathbf{f}(\underline{H}))$. By inductive assumption we have $\mathbf{f}(\underline{H}) \succeq^w \mathbf{f}(\underline{T})$, so, by Lemma 10, $\mathbf{f}(H^\clubsuit) \succeq^w \mathbf{f}(T)$. Since $T \in \bar{\mathcal{R}}(\mu, d)$, the case of $f(H^\clubsuit) \succ^w f(T)$ is impossible, and, thus, $\mathbf{f}(H^\clubsuit) = \mathbf{f}(T)$, i.e., $H^\clubsuit \in \bar{\mathcal{R}}(\mu, d)$.

Definitely, disjoint paths (v, m_1, \dots, m_k, m) and $(\underline{v}, m'_1, \dots, m'_l, m)$ to some vertex $m \in M$ present in H^\clubsuit , where $k, l \geq 0$. Again recall Note 2: since $f_T(v) > f_T(\underline{v})$, formula (4) makes $f_{H^\clubsuit}(m_i) > f_{H^\clubsuit}(m'_i), i = 1, \dots, \min[k, l]$. It also follows from (4) that $k \leq l$, since otherwise $f_{H^\clubsuit}(m_{l+1}) > f_{H^\clubsuit}(m)$, which is impossible, as $m_{l+1} \in g_{H^\clubsuit}(m)$. Thus, the considered pair of paths satisfies conditions of Lemma 15, and a tree exists whose vector of subordinate groups' weights majorizes the appropriate vector of the tree H^\clubsuit , which contradicts the fact that $H^\clubsuit \in \bar{\mathcal{R}}(\mu, d)$.

The obtained contradiction proves that the star \underline{S} has $d - 1$ pendent vertices.

Step III. Let us prove that the vertex \underline{v} (the center of the star \underline{S}) has the least weight $\mu(\cdot)$ in the set M . Assume, by contradiction, that a vertex $\underline{v} \in M$ exists such that $\mu(\underline{v}) < \mu(v)$. Since weights are degree-monotone in the tuple (μ, d) , this implies that $d(\underline{v}) = d(\underline{v}) = d$. By construction of the vertex \underline{v} we have $f_T(\underline{v}) \leq f_T(v)$. Moreover, we can discard the case of $f_T(\underline{v}) = f_T(v)$, since then the vertex \underline{v} would be the center of a lower star, and, because $d(v) = d(\underline{v})$, we would not have $\mu(\underline{v}) < \mu(v)$ by construction of the vertex v . Consequently, only the case of $f_T(\underline{v}) > f_T(v)$ is left.

If $\underline{v} \in g_T(\underline{v})$, a path exists from \underline{v} to \underline{v} in T , and, by Lemma 17, $T \notin \bar{\mathcal{R}}(\mu, d)$. Otherwise consider an augmentation $H^\diamond \in \mathcal{R}(\mu, d)$ of a Huffman tree \underline{H} induced by the (\underline{v}, v) -rollup \underline{T} of the tree T . If \underline{R} is a contraction of T to the vertex set $g_T(\underline{v})$, then, by Note 2, we have $\mathbf{f}(H^\diamond) = (f_T(\underline{v}), \mathbf{f}(\underline{R}), f_T(\underline{v}), \mathbf{f}(\underline{H}))_{\uparrow}$. On the other hand, by Definition 13, $\mathbf{f}(T) = (f_T(\underline{v}), \mathbf{f}(\underline{R}), f_T(\underline{v}), \mathbf{f}(\underline{T}))_{\uparrow}$. By inductive assumption, $\mathbf{f}(\underline{H}) \succeq^w \mathbf{f}(\underline{T})$, i.e., by Lemma 10, $\mathbf{f}(H^\diamond) \succeq^w \mathbf{f}(T)$. Since, by assumption, $T \in \bar{\mathcal{R}}(\mu, d)$, the case of $\mathbf{f}(H^\diamond) \succ^w \mathbf{f}(T)$ is impossible, so, $\mathbf{f}(H^\diamond) = \mathbf{f}(T)$, and $H^\diamond \in \bar{\mathcal{R}}(\mu, d)$. Again, H^\diamond contains

disjoint paths (v, m_1, \dots, m_k, m) and $(v, m'_1, \dots, m'_l, m)$, $k, l \geq 0$ to some vertex $m \in M$. Since $f_T(\underline{v}) > f_T(\underline{v})$, applying formula (4) we deduce that $k \leq l$, $f_{H^\diamond}(m_i) > f_{H^\diamond}(m'_i)$, $i = 1, \dots, k$. Then, by Lemma 16, the vector of subordinate group weights of H^\diamond is majorized by the appropriate vector of some tree from $\mathcal{R}(\mu, d)$, and H^\diamond cannot be in $\bar{\mathcal{R}}(\mu, d)$. The obtained contradiction proves that the vertex \underline{v} has the least weight in M .

Step IV. Now to prove the minimality of the star \underline{S} we are left to show that its pendent vertices have the least possible weights $\mu(\cdot)$. Assume, by contradiction, that it is not true, i.e., such vertices $w \in W \setminus L(\underline{S})$ and $w' \in L(\underline{S})$ exist that $\mu(w) < \mu(w')$. The vertex w has an outbound arc in T to some vertex $\tilde{v} \in M$. There are two possible alternatives:

1. $\underline{v} \in g_T(\tilde{v})$. By assumption, $f_T(w) = \mu(w) < \mu(w') = f_T(w')$ and thus, by Lemma 14 we conclude that $T \notin \bar{\mathcal{R}}(\mu, d)$, which contradicts the above assumption.
2. $\underline{v} \notin g_T(\tilde{v})$. Let H^\heartsuit be the augmentation of a Huffman tree induced by a $(\underline{v}, \tilde{v})$ -rollup of the tree T . By analogy to the step II we show that $H^\heartsuit \in \bar{\mathcal{R}}(\mu, d)$.

By construction, there are disjoint paths (w, m_1, \dots, m_k, m) and $(w', m'_1, m'_2, \dots, m'_l, m)$ (where $k \geq 1$, $l \geq 1$, $m_1 = \tilde{v}, m'_1 = \underline{v}$), in H^\heartsuit to some vertex $m \in M$. We have $f_T(\underline{v}) \leq f_T(\tilde{v})$ by construction of the vertex \underline{v} . If this inequality is strict, then we also have $f_{H^\heartsuit}(\underline{v}) < f_{H^\heartsuit}(\tilde{v})$ and, using formula (4), conclude that $k \leq l$, $f_{H^\heartsuit}(m_i) > f_{H^\heartsuit}(m'_i)$, $i = 1, \dots, k$. Since $\mu(w) < \mu(w')$, Lemma 12 predicates the existence of a tree, whose vector of subordinate groups' weights majorizes the appropriate vector of the tree H^\heartsuit , which contradicts to the assumption that $H^\heartsuit \in \bar{\mathcal{R}}(\mu, d)$. In case of $f_T(\underline{v}) = f_T(\tilde{v})$ we cannot use formula (4) to compare subordinate groups' weights of elements of both chains, since all possible alternatives of $k = 1$, or $l = 1$, or any sign of the expression $f_{H^\heartsuit}(m_2) - f_{H^\heartsuit}(m'_2)$ in case of $k, l \geq 2$ are possible. On the other hand, if $f_{H^\heartsuit}(m_2) > f_{H^\heartsuit}(m'_2)$, then formula (4) can be used to show that $k \leq l$, $f_{H^\heartsuit}(m_i) > f_{H^\heartsuit}(m'_i)$, $i = 2, \dots, k$. In case of the opposite inequality, $f_{H^\heartsuit}(m_2) < f_{H^\heartsuit}(m'_2)$, formula (4) says that, by contrast, $k \geq l$, $f_{H^\heartsuit}(m_i) < f_{H^\heartsuit}(m'_i)$, $i = 2, \dots, l$. Repeating this argument through the chain, we see that only two alternatives are possible:

- $1 \leq p \leq k \leq l$, $f_{H^\heartsuit}(m_i) = f_{H^\heartsuit}(m'_i)$, $i = 1, \dots, p$, $f_{H^\heartsuit}(m_i) > f_{H^\heartsuit}(m'_i)$, $i = p + 1, \dots, k$. Since $\mu(w) < \mu(w')$, Lemma 12 gives $H^\heartsuit \notin \bar{\mathcal{R}}(\mu, d)$, which is a

contradiction.

- $1 \leq p \leq l \leq k$, $f_{H^\heartsuit}(m_i) = f_{H^\heartsuit}(m'_i)$, $i = 1, \dots, p$, $f_{H^\heartsuit}(m_i) < f_{H^\heartsuit}(m'_i)$, $i = p + 1, \dots, l$. In this case the same conclusion that $H^\heartsuit \notin \widehat{\mathcal{R}}(\mu, d)$ follows from Lemma 13.

The obtained contradictions prove the minimality of the star \underline{S} having the center \underline{v} . In other words, we have $f_T(\underline{v}) = \underline{f}(\mu, d)$.

Let H^\spadesuit be the augmentation of the Huffman tree \underline{H} induced by the \underline{v} -rollup \underline{T} of the tree T . Since $|M(\underline{H})| = |M(\underline{T})| = q - 1$, by inductive assumption we have $f(\underline{H}) \succeq^w f(\underline{T})$. Since $\mathbf{f}(T) = (\underline{f}(\mu, d), \mathbf{f}(\underline{T}))$, $f(H^\spadesuit) = (\underline{f}(\mu, d), \mathbf{f}(\underline{H}))$, by Lemma 10 obtain $\mathbf{f}(H^\spadesuit) \succeq^w \mathbf{f}(T)$. As H^\spadesuit is constructed by adding a minimal star \underline{S} to the Huffman tree \underline{H} , by Lemmas 1 and 8 it appears to be a Huffman tree itself, i.e., $H^\spadesuit \in \mathcal{RH}(\mu, d)$. Then Lemma 7 says that $\mathbf{f}(H^\spadesuit) = \mathbf{f}(H)$, and, therefore, $\mathbf{f}(H) \succeq^w \mathbf{f}(T)$. ■

5 Huffman Tree Minimizes Wiener Index

Definition 16 A directed tree $T \in \mathcal{R}(\mu, d)$ with the vector (f_1, \dots, f_{q-1}) of subordinate groups' weights is called a *proper tree* if $f_i \leq \bar{\mu}/2$, $i = 1, \dots, q - 1$. □

Lemma 19 *Each tree $T \in \mathcal{T}(\mu, d)$ has a corresponding proper tree, and vice versa.*

PROOF For a tree with $q < 2$ internal vertices the lemma is trivial, since the vector of subordinate groups' weights is empty, therefore, suppose that $q \geq 2$. Consider a vertex $u \in V(T)$ with incident edges $uw_1, \dots, uw_d \in E(T)$, where $d := d_T(u)$. Deleting the vertex u and the edges uw_1, \dots, uw_d we break the tree T into disjoint components T_1, \dots, T_d .

Let us prove that in any tree $T \in \mathcal{T}(\mu, d)$ deletion of some vertex $v \in V(T)$ results in components of the weight no more than $\bar{\mu}/2$. Assume, by contradiction, that for every vertex $u \in V(T)$ such an incident vertex $\pi(u) \in V(T)$ exists that deletion of the edge $u\pi(u)$ gives rise to the component including the vertex $\pi(u)$ and having the weight greater than $\bar{\mu}/2$. Clearly, the weight of the second component (the one including the vertex u) does not exceed $\bar{\mu}/2$. Then, since the tree T has finite number of vertices, it inevitably contains a cycle (u_1, \dots, u_k, u_1) , where $k > 2$, $u_{i+1} = \pi(u_i)$, $i = 1, \dots, k - 1$, $u_1 = \pi(u_k)$, which contradicts to the fact that T is a tree.

If v is an internal vertex, then we choose the root $r = v$, otherwise let the vertex incident to v be the root r of the corresponding directed tree $P \in \mathcal{R}(\mu, d)$ ($r \in M(T)$, since $q \geq 1$). One can easily see that P is a proper tree. The inverse statement is trivial. ■

Let $\mathcal{P} \subseteq \mathcal{R}$ stand for the collection of all proper directed trees, and let $\mathcal{P}(\mu, d) \subseteq \mathcal{R}(\mu, d)$ be the collection of proper trees, which correspond to the trees from $\mathcal{T}(\mu, d)$.

Lemma 20 *If weights are degree-monotone in the tuple $\langle \mu, d \rangle$, all directed Huffman trees from $\mathcal{RH}(\mu, d)$ are proper trees.*

PROOF Consider a directed Huffman tree $H \in \mathcal{RH}(\mu, d)$ with a star sequence S_1, \dots, S_q and let m_1, \dots, m_q be the centers of stars S_1, \dots, S_q respectively. To prove the lemma we are enough to show that $f_{q-1}(H) = f_H(m_{q-1}) \leq \bar{\mu}/2$. Assume, by contradiction, that $f_H(m_{q-1}) > \bar{\mu}/2$. Since $f_H(m_q) = \bar{\mu}$, we have

$$\begin{aligned} \sum_{v \in L(S_q) \setminus \{m_{q-1}\}} f_H(v) &= \bar{\mu} - f_H(m_{q-1}) - \mu(m_q) < \\ < \bar{\mu}/2 - \mu(m_q) < f_H(m_{q-1}) - \mu(m_q) = \mu(m_{q-1}) + \sum_{v \in L(S_{q-1})} f_H(v) - \mu(m_q). \end{aligned}$$

Since $H \in \mathcal{RH}(\mu, d)$, by construction of the Huffman tree we have $\mu(m_{q-1}) \leq \mu(m_q)$, so,

$$\sum_{v \in L(S_q) \setminus \{m_{q-1}\}} f_H(v) < \sum_{v \in L(S_{q-1})} f_H(v). \quad (5)$$

From the fact that $H \in \mathcal{RH}(\mu, d)$ and from degree-monotonicity of weights in $\langle \mu, d \rangle$ it follows that $d_H(m_{q-1}) \leq d_H(m_q)$. Introduce the notation $\Delta := d_H(m_{q-1}) - 1$. Choose any Δ vertices from the set $L(S_q) \setminus \{m_{q-1}\}$ and denote them with v_1, \dots, v_Δ . Transform the tree H by redirecting outbound arcs of vertices v_1, \dots, v_Δ to the vertex m_{q-1} and by redirecting all Δ outbound arcs from the vertices of the set $L(S_{q-1})$ to the vertex m_q . Vertex degrees and weights do not change during the transformation, thus, the transformed tree H' belongs to $\mathcal{R}(\mu, d)$. Using inequality (5) it is easy to show that the weight of the group subordinated to the vertex m_{q-1} decreases by

$$b := \sum_{v \in L(S_{q-1})} f_H(v) - \sum_{i=1}^{\Delta} f_H(v_i) \geq \sum_{v \in L(S_{q-1})} f_H(v) - \sum_{v \in L(S_q) \setminus \{m_{q-1}\}} f_H(v) > 0,$$

while the weights of groups subordinated to all other vertices in a tree do not change. Then, by Lemma 9, $f(H') \succ^w f(H)$, which is impossible by Theorem 2. The obtained contradiction proves that $f_H(m_{q-1}) \leq \bar{\mu}/2$ and H is a proper tree. ■

Theorem 3 *Let a function $\chi(x)$ be concave and increasing on the range $x \in [0, \bar{\mu}/2]$. If $H \in \mathcal{RH}(\mu, d)$, $T \in \mathcal{P}(\mu, d)$, then $\sum_{v \in V \setminus \{r\}} \chi(f_H(v)) \leq \sum_{v \in V \setminus \{r'\}} \chi(f_T(v))$, where r and r' are the roots of the trees H and T respectively. The equality is possible only if $T \in \mathcal{RH}(\mu, d)$.*

PROOF By Theorem 2, if $H \in \mathcal{RH}(\mu, d)$, $T \in \mathcal{P}(\mu, d) \subseteq \mathcal{R}(\mu, d)$, then $\mathbf{f} := \mathbf{f}(H) \succeq^w \mathbf{f}' := \mathbf{f}(T)$. From Lemma 20 we know that $H \in \mathcal{P}(\mu, d)$, so both f_i and f'_i ($i = 1, \dots, q-1$), belong to the range $[0, \bar{\mu}/2]$, where the function $\chi(x)$ is increasing and concave. Then, by Lemma 11, $\sum_{i=1}^{q-1} \chi(f_{[i]}) \leq \sum_{i=1}^{q-1} \chi(f'_{[i]})$, and the equality is possible only if $\mathbf{f} = \mathbf{f}'$. Since trees from $\mathcal{R}(\mu, d)$ differ only in weights of groups subordinated to internal vertices, we immediately obtain the desired inequality. In case of equality, Lemma 8 proves that $T \in \mathcal{RH}(\mu, d)$. ■

Now we are ready to prove the **Theorem 1**.

PROOF From Lemma 19, each tree in $T \in \mathcal{T}(\mu, d)$ has a corresponding proper directed tree P , and vice versa. From equation (3) it follows that trees P and T share the same value of the Wiener index, so, if $\mathcal{P}^*(\mu, d) := \text{Argmin}_{T \in \mathcal{P}(\mu, d)} VWWI(T)$, then the collection $\mathcal{T}^*(\mu, d)$ of vertex-weighted trees minimizing the Wiener index is a collection of trees corresponding to trees from $\mathcal{P}^*(\mu, d)$. Since $VWWI$ satisfies the conditions of Theorem 3 with function $\chi(x) = x(\bar{\mu} - x)$, which is concave and increasing on the range $[0, \bar{\mu}/2]$, we deduce that $\mathcal{P}^*(\mu, d) = \mathcal{RH}(\mu, d)$ and, since $\mathcal{TH}(\mu, d)$ is the collection of all trees corresponding to directed trees from $\mathcal{RH}(\mu, d)$, we finally deduce that $\mathcal{T}^*(\mu, d) = \mathcal{TH}(\mu, d)$. ■

6 Conclusion

In the conclusion, let us discuss possible applications and extensions of the considered model. In [7, 8, 9] a technique was suggested to optimize abstract degree-based topological indices of the form $C_{deg}(G) := C_1(G) + C_2(G)$, where

$$C_1(G) = \sum_{v \in V(G)} c_1(d_G(v)), \quad C_2(G) = \sum_{uv \in E(G)} c_2(d_G(u), d_G(v)),$$

over the set of trees with the given number of pendent vertices. Together with the results of this paper the technique from [7] can be seen as a step towards optimization of joint linear combinations of degree-based and distance-based indices over the set of trees with the given total number of vertices or the given number of pendent vertices.

For the fixed degree sequence optimization of the linear combination of $C_1(G)$ and $VWWI(G)$ reduces to building a Huffman tree, and then we are just to find an optimal degree sequence, which is an integer program with linear constraint (1). The efficient algorithms for joint index optimization problems would contribute to the methods of designing materials with extremal characteristics.

In the definition of $VWWI(G)$ each distance from $u \in V(G)$ to $v \in V(G)$ is weighted with the product $\mu_G(u)\mu_G(v)$ of positive vertex weights. The obvious extension assumes endowing each path in a tree (i.e., each pair $u, v \in V$) with its own weight $\mu_G(u, v)$. Such an extended index would give more freedom to build models relating physical and chemical properties of substances to the topology of their molecules. For instance, we would be able to assign independently unique weights to OH-OH, C-OH and C-C paths in polyhydric alcohol molecules.

This settings seems to be closer to NP-hard problems of hierarchical graph clustering (see [15] for a survey) and merits a more detailed study in the future.

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