Weighted Harary indices of apex trees and k-apex trees

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Abstract

If G is a connected graph, then $H_A(G) = \sum_{u \neq v}(\deg(u) + \deg(v))/d(u,v)$ is the additively Harary index and $H_M(G) = \sum_{u \neq v} \deg(u)\deg(v)/d(u,v)$ the multiplicatively Harary index of G. G is an apex tree if it contains a vertex x such that $G - x$ is a tree and is a k-apex tree if k is the smallest integer for which there exists a k-set $X \subseteq V(G)$ such that $G - X$ is a tree. Upper and lower bounds on H_A and H_M are determined for apex trees and k-apex trees. The corresponding extremal graphs are also characterized in all the cases except for the minimum k-apex trees, $k \geq 3$. In particular, if $k \geq 2$ and $n \geq 6$, then $H_A(G) \leq (k+1)(3n^2 - 5n - k^2 - k + 2)/2$ holds for any k-apex tree G, equality holding if and only if G is the join of K_k and $K_{1,n-k-1}$.

Key words: additively Harary index; multiplicatively Harary index; apex tree; k-apex tree; harmonic number

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1 Introduction

The *Harary index* $H(G)$ of a connected graph G was in 1993 independently introduced in [18, 24] as

$$H(G) = \sum_{u \neq v} \frac{1}{d(u,v)}\,.$$

Note however that the first report on the Harary index was given a year earlier in [21]. This graph invariant received a lot of attention, see recent papers [4, 15, 20, 26, 28–30, 32, 36], the new book [33] and references therein. The investigation of the Harary index is hence an established area in mathematics, but one should be aware that it was originally introduced in mathematical chemistry with a motivation that it would improve the inconsistency of the classical Wiener index caused by the fact that the contribution of close pairs of vertices to the overall value is much smaller than that of distant vertices. Since the Harary index does not resolve this inconsistency, additional modifications were proposed, several of them by including vertex degrees. In this paper we are interested in two modifications/improvements of the Harary index to be introduced next.

If G is a connected graph, then the *additively weighted Harary index* $H_A(G)$ of G is defined as

$$H_A(G) = \sum_{u \neq v} \frac{\deg(u) + \deg(v)}{d(u,v)}\,,$$

while the *multiplicatively weighted Harary index* $H_M(G)$ of G is defined as

$$H_M(G) = \sum_{u \neq v} \frac{\deg(u)\deg(v)}{d(u,v)}\,.$$

The additively weighted Harary index was first introduced by Hua and Zhang in [16] under the name *reciprocal degree distance* because this invariant can be considered as a reciprocal analogue of the degree distance [11, 12, 17] of a graph. The present name for H_A was coined by Alizadeh, Iranmanesh, and Došlić in [3] where they have independently introduced this invariant as well as the multiplicatively weighted Harary index.

Characterizing the extremal graphs from a given class of graphs with respect to a given graph invariant is an important direction in extremal graph theory. See [35] for a recent survey on the extremal graphs with respect to distance-based graph invariants. Extremal graphs with respect to the additively weighted Harary index were already studied in the seminal paper [16]. Among other results, extremal graphs were determined in the class of all connected graphs, trees, unicyclic graphs, cactuses, as well as in the class of k-connected graphs and k-edge connected graphs. Some of these extremality results were also independently proved in [3]. In particular, within the class of trees, the stars and paths have the maximum and the minimum additively weighted Harary index, respectively. For some newest results on H_A and H_M, see [10,25,34].

In this paper we extend the studies of extremal graphs with respect to weighted Harary indices to two recent but natural extensions of trees. In topological graph theory, graphs that contain a vertex whose removal yields a planar graphs play an important role, these graphs are called apex graphs [1,22]. Along these lines we say that G is an *apex tree* [37] if it contains a vertex x such that $G - x$ is a tree. The vertex x will be called an *apex vertex* of G. Note that any tree is an apex tree, hence we say that G is a *non-trivial apex tree* if G is an apex tree that is not a tree itself. Furthermore, for any $k \geq 1$ a graph G is called a *k-apex tree* [37] if there exists a k-set $X \subseteq V(G)$ such that $G - X$ is a tree, while for any $Y \subseteq V(G)$ with $|Y| < k$, $G - Y$ is not a tree. (The related concept in topological graph theory is the one of a k-apex graph [23].) A vertex from the set X is called a *k-apex vertex*. Clearly, 1-apex trees are precisely non-trivial apex trees. Apex trees and k-apex trees were introduced in [36] under the names quasi-tree graphs and k-generalized quasi-tree graphs, respectively. For any $n \geq 3$ and $k \geq 2$, let

- $\mathcal{T}(n)$ denote the set of non-trivial apex trees of order n, and let
- $\mathcal{T}_k(n)$ denote the set of k-apex trees of order n.

The paper is organized as follows. In the next section we formally introduce concepts studied here and recall several preliminary results. Then, in Section 3, we give sharp upper bounds on H_A and H_M in $\mathcal{T}(n)$ and characterize the extremal graphs. In the subsequent section we obtain related lower bounds and extremal graphs. In Section 5 we present sharp upper bounds on H_A and H_M in $\mathcal{T}_k(n)$ and again describe the extremal graphs. In the final section we obtain related lower bounds and extremal graphs in $\mathcal{T}_2(n)$. We leave an open problem to determine such lower bounds for $k \geq 3$.

2 Preliminaries

All graphs considered in this paper are finite, simple and, unless stated otherwise, also connected. For a vertex $v \in V(G)$, we denote by $N_G(v)$ the neighborhood of v in G. The degree of v is $\deg_G(v) = |N_G(v)|$; if G will be clear from the context we will simplify the notation to $\deg(v)$. The minimum degree of G will be denoted with $\delta(G)$. For $X \subseteq V(G)$, let $G - X$ be the subgraph of G obtained from G by removing the vertices from X and the edges incident with them, in particular, $G - \{v\}$ will be briefly denoted by $G - v$. Similarly, for $F \subseteq E(G)$, $G - F$ is the spanning subgraph of G obtained by removing the edges of F and if $e \in E(G)$ then we will write $G - e$ for $G - \{e\}$. The distance $d_G(u, v)$ is the usual shortest-path distance between u and v in G. Again, if G will be clear from the context we will write $d(u, v)$. If G and H are graphs, then their *join* $G \oplus H$ is the graph obtained from the disjoint union of G

and H by adding all edges between $V(G)$ and $V(H)$. The complete bipartite graph $K_{1,n-1}$ is also known as the *n-star* and denoted with S_n. We denote by $C_k(n-k)$ the graph obtained from the cycle C_k by attaching a path of length $n-k$ to a vertex of C_k.

The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ of a graph G are, respectively, defined as follows [13, 14]:

$$M_1(G) = \sum_{v \in V(G)} \deg(v)^2, \quad M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v)\,.$$

The first Zagreb index can be equivalently expressed as follows:

$$M_1(G) = \sum_{uv \in E(G)} (\deg(u) + \deg(v)). \tag{1}$$

We will need the following upper bounds on the Zagreb indices:

Lemma 2.1 [9] *If T is a tree of order n, then*

(1) *$M_1(T) \le n(n-1)$ with equality holding if and only if $T = S_n$;*

(2) *$M_2(T) \le (n-1)^2$ with equality holding if and only if $T = S_n$.*

See [7–9, 19, 27, 31] for some new results on Zagreb indices.

The *first Zagreb coindex* $\overline{M}_1(G)$ and the *second Zagreb coindex* $\overline{M}_2(G)$ of a graph G are defined as follows [5]:

$$\overline{M}_1(G) = \sum_{\substack{uv \notin E(G) \\ u \ne v}} (\deg(u) + \deg(v)), \quad \overline{M}_2(G) = \sum_{\substack{uv \notin E(G) \\ u \ne v}} \deg(u)\deg(v)\,.$$

We next recall two relations between the Zagreb indices and the Zagreb coindices.

Lemma 2.2 [6] *If G is a connected graph of order n and size m, then*

(1) *$\overline{M}_1(G) = 2m(n-1) - M_1(G)$;*

(2) *$\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G)$.*

We now turn to the weighted Zagreb indices. The following lemma easily follows from the definitions.

Lemma 2.3 *If G is a graph and $u, v \in V(G)$ are not adjacent, then*

(1) *$H_M(G + uv) > H_M(G)$;*

(2) *$H_A(G + uv) > H_A(G)$.*

If G is a graph and $x \in V(G)$, then set

$$h_G(x) = \sum_{u \in V(G-x)} \frac{\deg(u)}{d(u,x)}\,.$$

The quantity $h(x)$ plays a similar role with respect to H_A as the distance $d_G(x)$ of $x \in V(G)$ (that is, the sum of the distances from x to all other vertices) with respect to the Wiener index $W(G)$, cf. [2]. Indeed, it can be easily seen that

$$H_A(G) = \frac{1}{2} \sum_{x \in V(G)} h_G(x)\,.$$

We will apply the following result on the Harary index of k-apex trees.

Lemma 2.4 [36] *If $k \geq 2$ and $G \in \mathcal{T}_k(n)$, $n \geq 6$, then*

$$H(G) \leq \frac{n(n-1)}{4} + \frac{(k+1)(n-k-1)}{2} + \frac{(k+1)k}{4}$$

with equality holding if and only if $G = K_k \oplus S_{n-k}$.

Finally, the *n-th harmonic number* is $H_n = \sum\limits_{k=1}^{n} \frac{1}{k}$.

3 Maximal apex trees

Before presenting the main result of this section (Theorem 3.4), we prove two lemmas and recall another one.

Lemma 3.1 *If $G \in \mathcal{T}(n)$ is a graph with H_A as large as possible and x is an apex vertex of G, then* (1) $\delta(G) = 2$ *and* (2) $\deg_G(x) = n-1$.

Proof. (1) We first prove that the $\delta(G) \geq 2$. Suppose on the contrary that y is a pendant vertex of G. Then clearly $xy \notin E(G)$ and hence $G + xy \in \mathcal{T}(n)$. But then $H_A(G+xy) > H_A(G)$ holds by Lemma 2.3, a contradiction. We next show that $\delta(G) \leq 2$ and assume by way of contradiction that all the vertices in G have degree at least 3. But then for any vertex v the minimum degree of $G - v$ is at least 2 which implies that $G - v$ is not a tree and so G is not an apex tree, a contradiction.

(2) This follows immediately from Lemma 2.3, the maximality of $H_A(G)$, and the fact that x is an apex vertex. □

Analogously we obtain the next lemma, hence its proof is omitted.

Lemma 3.2 *If $G \in \mathcal{T}(n)$ is a graph with H_M as large as possible and x is an apex vertex of G, then* (1) $\delta(G) = 2$ *and* (2) $\deg_G(x) = n-1$.

Lemma 3.3 [3] *If for $i = 1, 2$, G_i is a graph of order n_i and size m_i, then*

$$\begin{aligned} H_A(G_1 \oplus G_2) &= \frac{1}{2}\left(M_1(G_1) + M_1(G_2)\right) + (n_1 + n_2 - 1)(m_1 + m_2) \\ &+ \frac{1}{2} n_1 n_2 (3n_1 + 3n_2 - 2) + 2n_1 m_2 + 2n_2 m_1 \,. \end{aligned}$$

We are now ready for the main result of this section. Note that $\mathcal{T}(3) = \{C_3\}$, hence in the following we consider $\mathcal{T}(n)$ for $n \geq 4$.

Theorem 3.4 *If $n \geq 4$ and $G \in \mathcal{T}(n)$, then*

(1) *$H_A(G) \leq 3n^2 - 5n$ with equality holding if and only if $G = K_1 \oplus S_{n-1}$;*

(2) *$H_M(G) \leq 6n^2 - 19n + 15$ with equality holding if and only if $G = K_1 \oplus S_{n-1}$.*

Proof. (1) Select $G \in \mathcal{T}(n)$ with $H_A(G)$ as large as possible. Then Lemma 3.1 (2) implies that $G = K_1 \oplus T_{n-1}$, where T_{n-1} is a tree of order $n - 1$. Therefore, using Lemma 3.3 we have

$$\begin{aligned} H_A(G) &= \frac{1}{2}(M_1(K_1) + M_1(T_{n-1})) + (n-1)(n-2) \\ &+ \frac{1}{2}(n-1)(3n-2) + 2(n-2) \\ &\leq \frac{1}{2}(n-2)(n-1) + (n-1)(\frac{5}{2}n - 3) + 2(n-2) \\ &= 3n^2 - 5n. \end{aligned}$$

Moreover, using Lemma 2.1 (1) we infer that the equality holds if and only if $T_{n-1} = S_{n-1}$. Hence $G = K_1 \oplus S_{n-1}$.

(2) Select now $G \in \mathcal{T}(n)$ such that $H_M(G)$ is as large as possible and let x be an apex vertex of G. In view of Lemma 3.2 (2) we can easily get that $G = K_1 \oplus T_{n-1}$, where $V(K_1) = \{x\}$. Obviously, $G - x = T_{n-1}$ and G has $2n - 3$ edges. From Lemmas 2.2 and 2.1, and having in mind the equivalent formulation of the first Zagreb index from Equation (1), we get

$$\begin{aligned} H_M(G) &= \sum_{u \neq x} \frac{(n-1)\deg_G(u)}{d_G(u,x)} + \sum_{u,v \in V(G-x)} \frac{\deg_G(u)\deg_G(v)}{d_G(u,v)} \\ &= \sum_{u \neq x} (n-1)\deg_G(u) + \sum_{uv \in E(T_{n-1})} \deg_G(u)\deg_G(v) \\ &+ \sum_{uv \notin E(T_{n-1})} \frac{\deg_G(u)\deg_G(v)}{d_G(u,v)} \end{aligned}$$

$$
\begin{aligned}
&\le (n-1)[2m-(n-1)] + \sum_{uv\in E(T_{n-1})} [\deg_{T_{n-1}}(u)+1][\deg_{T_{n-1}}(v)+1] \\
&\quad + \sum_{uv\notin E(T_{n-1})} \frac{[\deg_{T_{n-1}}(u)+1][\deg_{T_{n-1}}(v)+1]}{2} \\
&= (n-1)[2m-(n-1)] + M_1(T_{n-1}) + M_2(T_{n-1}) + (n-2) \\
&\quad + \frac{1}{2}\overline{M}_1(T_{n-1}) + \frac{1}{2}\overline{M}_2(T_{n-1}) + \frac{1}{2}\frac{(n-2)(n-3)}{2} \\
&= (n-1)[2m-(n-1)] + M_1(T_{n-1}) + M_2(T_{n-1}) + (n-2) \\
&\quad + \frac{1}{2}\left(2(n-2)^2 - M_1(T_{n-1}) + 2(n-2)^2 - M_2(T_{n-1}) - \frac{1}{2}M_1(T_{n-1})\right) \\
&\quad + \frac{(n-2)(n-3)}{4} \\
&= (n-1)(3n-5) + \frac{1}{4}M_1(T_{n-1}) + \frac{1}{2}M_2(T_{n-1}) + (n-2) + 2(n-2)^2 \\
&\quad + \frac{(n-2)(n-3)}{4} \\
&\le (n-1)(3n-5) + \frac{1}{4}(n-2)(n-1) + \frac{1}{2}(n-2)^2 + (n-2)(2n-3) \\
&\quad + \frac{(n-2)(n-3)}{4} \\
&= 6n^2 - 19n + 15.
\end{aligned}
$$

Having in mind Lemma 2.1, equality holds in the above inequalities if and only if the distance between any two nonadjacent vertices in T_{n-1} is precisely 2, hence $T_{n-1} = S_{n-1}$. We conclude that $G = K_1 \oplus S_{n-1}$. □

4 Minimal apex trees

In this section we determine graphs from $\mathcal{T}(n)$ with minimal H_A and H_M. To present the main results of this section (Theorems 4.5 and 4.6), we need several lemmas. First, in parallel to Lemma 2.3, we have the following result for h_G:

Lemma 4.1 *Let G be a graph with $x \in V(G)$ and non-adjacent vertices u, v. Then $h_G(x) < h_{G+uv}(x)$.*

Proof. Set $G' = G + uv$ and distinguish the following two cases.

Case 1: $x \in \{u, v\}$.
Assume without loss of generality that $x = v$. Then $\deg_{G'}(x) = \deg_G(x) + 1$, $\deg_{G'}(u) = \deg_G(u) + 1$, and $d_{G'}(u, x) = 1 < d_G(u, x)$. Moreover, any vertex other

than u in G' has the same degree as that in G and $d_{G'}(w,x) \leq d_G(w,x)$ for any vertex $w \in V(G-x)$ different from u. From the definition of $h_G(x)$, it follows that $h_G(x) < h_{G'}(x)$.

Case 1: $x \neq u, v$.
In this case $d_{G'}(w,x) \leq d_G(w,x)$ for any vertex $w \in V(G-x)$. Furthermore, $\deg_{G'}(v) = \deg_G(v) + 1$ and $\deg_{G'}(u) = \deg_G(u) + 1$. Thus $h_G(x) < h_{G'}(x)$. $\square$

Lemma 4.2 *If T is a tree of order $n \geq 2$ and x is a pendant vertex of T, then*

$$h_T(x) \geq 2H_{n-1} - \frac{1}{n-1}$$

with equality holding if and only if $T = P_n$.

Proof. We choose a tree T of order n and a pendant vertex $x \in V(T)$ such that $h_T(x)$ is as small as possible. To prove the lemma it suffices to prove that T has only one pendant vertex in $V(G-x)$. Indeed, then the assertion follows immediately from the fact that $h_{P_n}(x) = 2H_{n-1} - \frac{1}{n-1}$.

Assume on the contrary that there exist at least two pendant vertices in $V(G-x)$. Let y be a vertex that is furthest from x and let P_{xy} be the x,y-path. (So the length of P_{xy} is the eccentricity of x in T.) Clearly, y is also a pendant vertex of T. By our assumption, there exists at least one vertex $z \in P_{xy}$ such that $\deg_T(z) \geq 3$. Let T_z be the maximal subtree of T which is rooted at z and for which $V(T_z) \cap P_{xy} = \{z\}$. Now we construct a new tree T' of order n by removing T_z (but keeping z) and attaching it to y, see Figure 1.

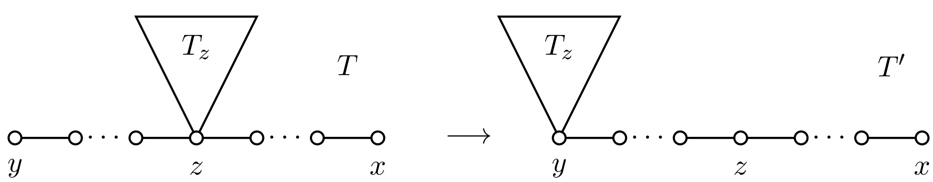

Figure 1: Trees T and T' from the proof of Lemma 4.2

Setting $Y = h_T(x) - h_{T'}(x)$ we have:

$$\begin{aligned} Y &= \frac{\deg_T(z) - 2}{d_T(z,x)} + \frac{1 - (1 + \deg_T(z) - 2)}{d_T(y,x)} + \sum_{u \in V(T_z)\setminus\{z\}} \left[\frac{\deg_T(u)}{d_T(u,x)} - \frac{\deg_T(u)}{d_{T'}(u,x)}\right] \\ &= \frac{\deg_T(z) - 2}{d_T(z,x)} + \frac{2 - \deg_T(z)}{d_T(y,x)} \\ &\quad + \sum_{u \in V(T_z)\setminus\{z\}} \left[\frac{\deg_T(u)}{d_T(u,z) + d_T(z,x)} - \frac{\deg_T(u)}{d_{T'}(u,y) + d_{T'}(y,x)}\right] \end{aligned}$$

$$
\begin{aligned}
&> \frac{\deg_T(z)-2}{d_T(y,x)} + \frac{2-\deg_T(z)}{d_T(y,x)} \\
&\quad + \sum_{u\in V(T_z)\setminus\{z\}} \left[\frac{\deg_T(u)}{d_T(u,z)+d_T(z,x)} - \frac{\deg_T(u)}{d_{T'}(u,y)+d_{T'}(y,x)}\right] \\
&> \sum_{u\in V(T_z)\setminus\{z\}} \left[\frac{\deg_T(u)}{d_T(u,z)+d_T(z,x)} - \frac{\deg_T(u)}{d_{T'}(u,y)+d_{T'}(y,x)}\right] \\
&= \sum_{u\in V(T_z)\setminus\{z\}} \left[\frac{\deg_T(u)}{d_G(u,z)+d_T(z,x)} - \frac{\deg_T(u)}{d_T(u,z)+d_T(y,x)}\right] \\
&> 0\,.
\end{aligned}
$$

This is a contradiction to the choice of T. $\square$

Lemma 4.3 *If x is a pendant vertex of a graph $G\in\mathcal{T}(n)$, then*

$$h_G(x) \geq 2H_{n-2} + \frac{2}{n-2} + \frac{1}{n-3}$$

with equality holding if and only if $G = C_3(n-3)$.

Proof. Select $G\in\mathcal{T}(n)$ with a pendant vertex x such that $h_G(x)$ is as small as possible. Let w be an apex vertex of G. We claim that $\deg_G(w)=2$. Suppose not, then $\deg_G(w)\geq 3$. Let w_1 be an arbitrary neighbor of w and set $G_0 = G - ww_1$. Note that $G_0\in\mathcal{T}(n)$. However, by Lemma 4.1, $h_{G_0}(x) < h_G(x)$, a contradiction with the choice of G.

Applying Lemma 4.2 and the fact that $G-w$ is a tree of order $n-1$ we can estimate as follows:

$$
\begin{aligned}
h_G(x) &= \sum_{u\in V(G-x)} \frac{\deg_G(u)}{d_G(u,x)} \\
&= \sum_{u\in V(G-\{w,x\})} \frac{\deg_G(u)}{d_G(u,x)} + \frac{\deg_G(w)}{d_G(w,x)} \\
&\geq \sum_{u\in V(G-\{w,x\})} \frac{\deg_G(u)}{d_{G-w}(u,x)} + \frac{2}{n-2} \\
&\geq \sum_{u\in V(G-\{w,x\})} \frac{\deg_{G-w}(u)}{d_{G-w}(u,x)} + \frac{1}{n-2} + \frac{1}{n-3} + \frac{2}{n-2} \\
&\geq 2H_{n-2} + \frac{2}{n-2} + \frac{1}{n-3}\,.
\end{aligned}
$$

In the above three inequalities, equality holds simultaneously if and only if $d_G(w,x) = n-2$, w is adjacent to two vertices at distance $n-2$ and $n-3$ from x, respectively, and $G - w = P_{n-1}$. Thus we have $G = C_3(n-3)$. $\square$

The last lemma we need is the following technical lemma on the harmonic numbers:

Lemma 4.4 *If $n \geq 6$, then*

$$4\sum_{i=1}^{n-2} H_i + 4H_{n-2} + 6 - \frac{2}{n-2} < \begin{cases} 4nH_{\frac{n-1}{2}} & if\ n\ is\ odd; \\ \\ 4nH_{\frac{n}{2}} - 4 & if\ n\ is\ even. \end{cases}$$

Proof. Note first that $\frac{1}{n-i} < \frac{1}{i+1}$ when $i < \frac{n-1}{2}$. Hence $H_i + H_{n-i} < H_{i+1} + H_{n-i-1}$ and consequently

- if n is odd, $H_1 + H_{n-2} < H_2 + H_{n-3} < \cdots < H_{\frac{n-3}{2}} + H_{\frac{n+1}{2}} < 2H_{\frac{n-1}{2}}$;
- if n is even, $H_1 + H_{n-1} < H_2 + H_{n-2} < \cdots < H_{\frac{n-2}{2}} + H_{\frac{n+2}{2}} < 2H_{\frac{n}{2}}$.

It can be verified directly that the result holds for $n \in \{6, 7, 8, 10\}$. So we only need to consider odd integers $n \geq 9$ and even integers $n \geq 12$. Set $A = 4\sum_{i=1}^{n-2} H_i + 4H_{n-2}$.

Suppose first that n is odd. Then for any $n \geq 9$,

$$4H_{\frac{n-1}{2}} - 2H_{n-2} = 2\left(1 + \frac{1}{2} + \cdots + \frac{1}{\frac{n-1}{2}}\right) - 2\left(\frac{1}{\frac{n+1}{2}} + \cdots + \frac{1}{n-2}\right) > 3 - \frac{1}{n-2}$$

and therefore

$$\begin{aligned} A &< 4\left(2 \times \frac{n-3}{2} + 1\right) H_{\frac{n-1}{2}} + 4H_{n-2} \\ &= 4nH_{\frac{n-1}{2}} - 2\left(4H_{\frac{n-1}{2}} - 2H_{n-2}\right) \\ &< 4nH_{\frac{n-1}{2}} - 6 + \frac{2}{n-2}. \end{aligned}$$

Assume now that n is even. Since $2H_{\frac{n}{2}} + \frac{2}{n-1} + \frac{1}{n-2} > 5$ for $n \geq 12$, we have

$$\begin{aligned} A &= 4\left(H_1 + H_2 + \cdots + H_{n-2} + H_{n-1}\right) - \frac{4}{n-1} \\ &< 4\left(2 \times \frac{n-2}{2} + 1\right) H_{\frac{n}{2}} - \frac{4}{n-1} \\ &= 4nH_{\frac{n}{2}} - 2\left(2H_{\frac{n}{2}} + \frac{2}{n-1}\right) \\ &< 4nH_{\frac{n}{2}} - \left(10 - \frac{2}{n-2}\right), \end{aligned}$$

which completes the proof of this lemma. $\square$

It can be easily checked that $\mathcal{T}(4) = \{K_1 \oplus S_3, C_3(1), C_4\}$ and that $H_A(K_1 \oplus S_3) > H_A(C_3(1)) > H_A(C_4)$. In addition, the minimal extremal graphs in $\mathcal{T}(5)$ with respect to H_A are C_5 and $C_3(2)$. In the following theorem we thus restrict our attention to $n \geq 6$.

Theorem 4.5 *If $n \geq 6$ and $G \in \mathcal{T}(n)$, then*

$$H_A(G) \geq 4\sum_{i=1}^{n-2} H_i + 4H_{n-2} + 6 - \frac{2}{n-2}$$

with equality holding if and only if $G = C_3(n-3)$.

Proof. We prove this result by induction on n, the case $n = 6$ can be checked by computer. Let now $n \geq 7$ and select $G \in \mathcal{T}(n)$ with $H_A(G)$ as small as possible.

We claim that G contains a pendant vertex. If not, then $\delta(G) \geq 2$ and G contains a cycle. From [3] we recall that $H_A(C_n) = 4nH_{\frac{n-1}{2}}$ if n is odd, and $H_A(C_n) = 4nH_{\frac{n}{2}} - 4$ when n is even. Using Lemma 4.4 it follows $H_A(C_n) > 4\sum_{i=1}^{n-2} H_i + 4H_{n-2} - \frac{2}{n-2}$. Since on the other hand the graph $C_3(n-3)$ attains the lower bound of the theorem we infer that $G \neq C_n$. So G contains at least two cycles and let e be an edge of G that lies in a cycle. Then $G - e \in \mathcal{T}(n)$ but $H_A(G-e) < H_A(G)$ by Lemma 2.3 (2). This contradiction proves the claim.

Let x be a pendant vertex of G and let y be its unique neighbor. Clearly, $G - x \in \mathcal{T}(n-1)$. By the induction hypothesis and Lemma 4.3, we obtain

$$\begin{aligned}
H_A(G) &= \sum_{u \in V(G-x)} \frac{\deg_G(u)+1}{d_G(u,x)} + \sum_{u,v \in V(G-x)} \frac{\deg_G(u)+\deg_G(v)}{d_G(u,v)} \\
&= \sum_{u \in V(G-x)} \frac{\deg_G(u)+1}{d_G(u,x)} + \sum_{u,v \in V(G-x)} \frac{\deg_{G-x}(u)+\deg_{G-x}(v)}{d_{G-x}(u,v)} \\
&\quad + \sum_{u \in V(G-\{x,y\})} \frac{1}{d_G(u,y)} \\
&= H_A(G-x) + h_G(x) + \sum_{u \in V(G-x)} \frac{1}{d_G(u,x)} + \sum_{u \in V(G-\{x,y\})} \frac{1}{d_G(u,y)} \\
&\geq 4\sum_{i=1}^{n-3} H_i + 4H_{n-3} + 6 - \frac{2}{n-3} + 2H_{n-2} + \frac{2}{n-2} + \frac{1}{n-3} \\
&\quad + H_{n-2} + \frac{1}{n-2} + H_{n-3} + \frac{1}{n-3} \\
&= 4\sum_{i=1}^{n-2} H_i + 4H_{n-2} + 6 - \frac{2}{n-2}\,.
\end{aligned}$$

In the above inequality, equality holds if and only if $G - x = C_3(n-4)$ and y is a pendant vertex in $G - x$, that is, if and only if $G = C_3(n-3)$. $\square$

As already mentioned, $\mathcal{T}(4) = \{K_1 \oplus S_3, C_3(1), C_4\}$. Just as for H_A we have $H_M(K_1 \oplus S_3) > H_M(C_3(1)) > H_M(C_4)$. Similarly we can check that the graphs in $\mathcal{T}(5)$ and in $\mathcal{T}(6)$ with minimal H_M are C_5 and C_6, respectively. In the following theorem we thus restrict our attention to $n \geq 7$.

Theorem 4.6 *If $n \geq 7$ and $G \in \mathcal{T}(n)$, then*

$$H_M(G) \geq 4\sum_{i=1}^{n-2} H_i + 4H_{n-3} - \frac{1}{n-3} + 8$$

with equality holding if and only if $G = C_3(n-3)$.

Proof. We proceed as in the proof of Theorem 4.5 by induction on n, verifying the base case, and selecting $G \in \mathcal{T}(n)$ such that $H_M(G)$ is as small as possible. Note that $H_A(C_n) = H_M(C_n)$. Similarly way as in the proof of Lemma 4.4 we then find that $H_M(C_n) > 4\sum_{i=1}^{n-2} H_i + 4H_{n-3} - \frac{1}{n-3} + 8$ for $n \geq 7$. Then we infer that G contains a pendant vertex, say x, and that $G - x \in \mathcal{T}(n-1)$. If y is the neighbor of x, then by the induction hypothesis and Lemma 4.3,

$$\begin{aligned}
H_M(G) &= \sum_{u \in V(G-x)} \frac{\deg_G(u)}{d_G(u,x)} + \sum_{u,v \in V(G-x)} \frac{\deg_G(u) d_G(v)}{\deg_G(u,v)} \\
&= \sum_{u \in V(G-x)} \frac{\deg_G(u)}{d_G(u,x)} + \sum_{u,v \in V(G-x)} \frac{\deg_{G-x}(u)\deg_{G-x}(v)}{d_{G-x}(u,v)} \\
&\quad + \sum_{u \in V(G-x-y)} \frac{\deg_{G-x}(u)}{d_{G-x}(u,y)} \\
&= H_M(G-x) + h_G(x) + h_{G-x}(y) \\
&\geq 4\sum_{i=1}^{n-3} H_i + 4H_{n-4} - \frac{1}{n-4} + 8 + 2H_{n-2} + \frac{2}{n-2} + \frac{1}{n-3} \\
&\quad + 2H_{n-3} + \frac{2}{n-3} + \frac{1}{n-4} \\
&= 4\sum_{i=1}^{n-2} H_i + 4H_{n-3} - \frac{1}{n-3} + 8\,.
\end{aligned}$$

In the above inequality, equality holds if and only if $G - x = C_3(n-4)$ and x is a new vertex adjacent to the pendant vertex of $C_3(n-4)$, that is, if and only if $G = C_3(n-3)$. $\square$

5 Maximal k-apex trees

In this section we determine the graphs maximizing H_A and H_M within the families $\mathcal{T}_k(n)$, $k \geq 1$. Since $\mathcal{T}(n) = \mathcal{T}_1(n)$, the case $n = 1$ has already been solved in Theorem 3.4. The next result is thus an extension of Theorem 3.4 from apex trees to all k-apex trees.

Theorem 5.1 *If $k \geq 2$, $n \geq 6$, and $G \in \mathcal{T}_k(n)$, then*

$$H_A(G) \leq \frac{(k+1)(3n^2 - 5n - k^2 - k + 2)}{2}$$

with equality holding if and only if $G = K_k \oplus S_{n-k}$, and

$$H_M(G) \leq \frac{(k+1)^2(7n^2 - 6nk - 15n + k^2 + 7k + 8)}{4} - \frac{(k+1)(n-1)^2}{2}$$

with equality holding if and only if $G = K_k \oplus S_{n-k}$.

Proof. As already mentioned, the result holds for $k = 1$ by Theorem 3.4. We proceed by induction. Let $k \geq 2$ and assume that the result holds for all $(k-1)$-apex trees. Suppose that $G \in \mathcal{T}_k(n)$ has the largest H_A (or H_M) and let $V_k \subseteq V(G)$ be the set of k k-apex vertices. From Lemma 2.3 it follows that V_k induces a complete graph and that for any vertex $u \in V_k$, $\deg_G(u) = n - 1$, so the number m of edges of G is

$$m = \binom{k}{2} + k(n-k) + (n-k-1) = \frac{(k+1)k}{2} + (k+1)(n-k-1)\,. \tag{2}$$

Select now $x \in V_k \subseteq V(G)$ and set $V_{k-1} = V_k \setminus x$. Note that $G - x$ is a $(k-1)$-apex tree.

We first consider H_A. By the induction hypothesis for H_A, Lemma 2.4, and Equality (2), we obtain

$$\begin{aligned}
H_A(G) &= \sum_{u,v \in V(G-x)} \frac{\deg_G(u) + \deg_G(v)}{d_G(u,v)} + \sum_{u \in V(G-x)} \frac{\deg_G(u) + \deg_G(x)}{d_G(u,x)} \\
&= \sum_{u,v \in V(G-x)} \frac{\deg_{G-x}(u) + 1 + \deg_{G-x}(v) + 1}{d_{G-x}(u,v)} + \sum_{u \in V(G-x)} \deg_G(u) + (n-1)^2 \\
&= H_A(G-x) + 2H(G-x) + 2m - \deg_G(x) + (n-1)^2 \\
&\leq \frac{k[3n^2 - 5n - (k-1)^2 - k + 3]}{2} + 2\left[\frac{n(n-1)}{4} + \frac{k(n-k)}{2} + \frac{(k-1)k}{4}\right] \\
&\quad + 2\left[\frac{(k+1)k}{2} + (k+1)(n-k-1)\right] - (n-1) + (n-1)^2 \\
&= \frac{(k+1)(3n^2 - 5n - k^2 - k + 2)}{2}\,.
\end{aligned}$$

The above equality holds if and only if $G - x = K_{k-1} \oplus S_{n-k}$ and $m = \frac{(k+1)k}{2} + (k+1)(n-k-1)$, that is, if and only if $G = K_k \oplus S_{n-k}$.

Consider next H_M. By the induction hypotheses for H_M and H_A, Lemma 2.4, and Equality (2), we obtain:

$$\begin{aligned}
H_M(G) &= \sum_{u,v \in V(G-x)} \frac{\deg_G(u)\deg_G(v)}{d_G(u,v)} + \sum_{u \in V(G-x)} \frac{(n-1)\deg_G(u)}{d_G(u,x)} \\
&= \sum_{u,v \in V(G-x)} \frac{(\deg_{G-x}(u)+1)(\deg_{G-x}(v)+1)}{d_{G-x}(u,v)} + \sum_{u \in V(G-x)} \deg_G(u)(n-1) \\
&= H_M(G-x) + H_A(G-x) + H(G-x) + [2m - \deg_G(x)](n-1) \\
&\le \frac{k^2[7(n-1)^2 - 6(n-1)(k-1) - 15(n-1) + (k-1)^2 + 7(k-1) + 8]}{4} \\
&\quad - \frac{k(n-2)^2}{2} + \frac{k[3n^2 - 5n - (k-1)^2 - k + 3]}{2} \\
&\quad + \left[\frac{n(n-1)}{4} + \frac{k(n-k)}{2} + \frac{(k-1)k}{4}\right] \\
&\quad + [(k+1)k + 2(k+1)(n-k-1) - (n-1)]\,(n-1) \\
&= \frac{(k+1)^2(7n^2 - 6nk - 15n + k^2 + 7k + 8)}{4} - \frac{(k+1)(n-1)^2}{2}.
\end{aligned}$$

The above inequality is equality if and only if $G - x = K_{k-1} \oplus S_{n-k}$ and $m = \frac{(k+1)k}{2} + (k+1)(n-k-1)$, that is, if and only if $G = K_k \oplus S_{n-k}$. □

6 Minimal 2-apex trees

In this final section we consider the minimal H_A and H_M within the class 2-apex tress $\mathcal{T}_2(n)$. Let $C_{3,3}^{n-5}$ denote the graph obtained from two disjoint triangles by connecting with a path of length $n-5$ a vertex in one triangle with a vertex in the other triangle; see Figure 2.

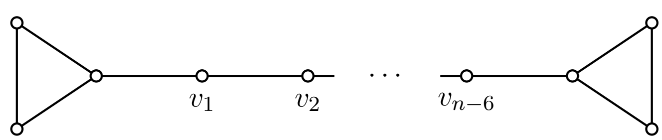

Figure 2: The graph $C_{3,3}^{n-5}$

Lemma 6.1 *If $G \in \mathcal{T}_2(n)$ and x, y are non-adjacent 2-apex vertices, then*

$$h_G(x) \geq 2H_{n-3} + \frac{2}{n-3} + \frac{1}{n-4} + 3$$

with equality holding if and if $G = C_{3,3}^{n-5}$ and x is a vertex of degree 2.

Proof. Select $G \in \mathcal{T}_2(n)$ with a 2-apex vertex x such that $h_G(x)$ is as small as possible. Let $y \neq x$ be a 2-apex vertex. Note first that $\deg_G(x) \geq 2$, because otherwise the graph $G - y$ would be a tree, contradicting the assumption that $G \in \mathcal{T}_2(n)$. Analogously, $\deg_G(y) \geq 2$. Similarly as in the proof of Lemma 4.3 we obtain

$$\begin{aligned}
h_G(x) &= \sum_{u \in V(G-x)} \frac{\deg_G(u)}{d_G(u,x)} \\
&= \sum_{u \in V(G-\{y,x\})} \frac{\deg_G(u)}{d_G(u,x)} + \frac{\deg_G(y)}{d_G(y,x)} \\
&\geq \sum_{u \in V(G-\{y,x\})} \frac{\deg_{G-y}(u)}{d_{G-y}(u,x)} + \frac{1}{n-4} + \frac{1}{n-3} + \frac{2}{n-3} \\
&\geq 2H_{n-3} + 3 - \frac{1}{n-3} + \frac{1}{n-4} + \frac{3}{n-3} \\
&= 2H_{n-3} + \frac{2}{n-3} + \frac{1}{n-4} + 3\,.
\end{aligned}$$

Moreover, equalities hold simultaneously if and only if $\deg_G(x) = \deg_G(y) = 2$, $d_G(x,y) = n-3$, and $G - \{x,y\} = P_{n-2}$, that is, if and only if $G = C_{3,3}^{n-5}$. $\square$

Theorem 6.2 *If $n \geq 4$ and $G \in \mathcal{T}_2(n)$, then*

$$H_A(G) \geq 4\sum_{i=1}^{n-3} H_i + 9H_{n-3} + H_{n-4} + \frac{3}{n-3} + \frac{2}{n-4} + 12$$

with equality holding if and only if $G = C_{3,3}^{n-5}$.

Proof. Select $G \in \mathcal{T}_2(n)$ with $H_A(G)$ as small as possible. Let x, y be 2-apex vertices of G. Then $G - x, G - y \in \mathcal{T}(n-1)$. By Lemma 2.3 (1), x, y are not adjacent in G. As in the proof of Lemma 6.1 we observe that $\deg_G(x) \geq 2$ and $\deg_G(y) \geq 2$. Let $\{w, z\} \subseteq N_G(x)$. Then by Theorem 4.5 and Lemma 6.1,

$$H_A(G) \geq \sum_{u \in V(G-x)} \frac{\deg_G(u) + 2}{d_G(u,x)} + \sum_{u,v \in V(G-x)} \frac{\deg_G(u) + \deg_G(v)}{d_G(u,v)}$$

$$\begin{aligned}
&\geq \sum_{u\in V(G-x)} \frac{\deg_G(u)+2}{d_G(u,x)} + \sum_{u,v\in V(G-x)} \frac{\deg_{G-x}(u)+\deg_{G-x}(v)}{d_{G-x}(u,v)} \\
&\quad + \sum_{u\in V(G-\{x,w\})} \frac{1}{d_G(u,w)} + \sum_{u\in V(G-\{x,w,z\})} \frac{1}{d_G(u,z)} + 1 \\
&= h_G(x) + 2\sum_{u\in V(G-x)} \frac{1}{d_G(u,x)} + H_A(G-x) + \sum_{u\in V(G-\{x,w\})} \frac{1}{d_G(u,w)} + 1 \\
&\quad + \sum_{u\in V(G-\{x,w,z\})} \frac{1}{d_G(u,z)} \\
&\geq 2H_{n-3} + \frac{2}{n-3} + \frac{1}{n-4} + 3 + 2(H_{n-3} + \frac{1}{n-3} + 1) + 4\sum_{i=1}^{n-3} H_i + 4H_{n-3} \\
&\quad + 6 - \frac{2}{n-3} + H_{n-3} + \frac{1}{n-3} + 1 + H_{n-4} + \frac{1}{n-4} \\
&= 4\sum_{i=1}^{n-3} H_i + 9H_{n-3} + H_{n-4} + \frac{3}{n-3} + \frac{2}{n-4} + 12\,.
\end{aligned}$$

In addition, equalities hold simultaneously if and only if in G, the vertex x is adjacent to the pendant vertex and its neighbor of $G-x = C_3(n-4)$. This holds if and only if $G = C_{3,3}^{n-5}$. □

Theorem 6.3 *If $n \geq 4$ and $G \in \mathcal{T}_2(n)$, then*

$$H_M(G) \geq 4\sum_{i=1}^{n-3} H_i + 12H_{n-3} + \frac{4}{n-4} + \frac{1}{n-5} + 16$$

with equality holding if and only if $G = C_{3,3}^{n-5}$.

Proof. Again select $G \in \mathcal{T}_2(n)$ such that $H_M(G)$ is as small as possible. By a similar reasoning as that in the proof of Theorem 6.2 we find two non-adjacent 2-apex vertices x and y, so that $G-x, G-y \in \mathcal{T}(n-1)$. Let $\{w,z\} \subseteq N_G(x)$, then by Theorem 4.6 and Lemma 6.1,

$$\begin{aligned}
H_M(G) &\geq 2\sum_{u\in V(G-x)} \frac{\deg_G(u)}{d_G(u,x)} + \sum_{u,v\in V(G-x)} \frac{\deg_G(u)\deg_G(v)}{d_G(u,v)} \\
&= 2h_G(x) + \sum_{u,v\in V(G-x)} \frac{\deg_{G-x}(u)\deg_{G-x}(v)}{d_{G-x}(u,v)} + \sum_{u\in V(G-\{x,w\})} \frac{\deg_{G-x}(u)}{d_{G-x}(u,w)} \\
&\quad + \sum_{u\in V(G-\{x,w,z\})} \frac{\deg_{G-x}(u)}{d_{G-x}(u,z)} + \deg_{G-x}(w) + 1
\end{aligned}$$

$$
\begin{aligned}
&= 2h_G(x) + H_M(G-x) + h_{G-x}(w) \\
&\quad + \sum_{u\in V(G-\{x,w,z\})} \frac{\deg_{G-x}(u)}{d_{G-x}(u,z)} + \deg_{G-x}(w) + 1 \\
&\geq 2\left(2H_{n-3} + \frac{2}{n-3} + \frac{1}{n-4} + 3\right) + (4\sum_{i=1}^{n-3} H_i + 4H_{n-4} - \frac{1}{n-4} + 8) + 2H_{n-3} \\
&\quad + \frac{2}{n-2} + \frac{1}{n-4} + 2H_{n-4} + \frac{2}{n-4} + \frac{1}{n-5} + 2 \\
&= 4\sum_{i=1}^{n-3} H_i + 12H_{n-3} + \frac{4}{n-4} + \frac{1}{n-5} + 16\,.
\end{aligned}
$$

Moreover, equalities hold if and only if $N_G(x) = \{w, z\}$ and $G - x = C_3(n-4)$, that is, if and only if $G = C_{3,3}^{n-5}$. □

To conclude the paper we pose:

Problem 6.4 *Extend Theorems 6.2 and 6.3 to k-apex graphs, $k \geq 3$.*

What is the exact form of the extremal graphs in the above problem? Suppose that G is the above extremal graph with $V_k \subseteq V(G)$ of all k-apex vertices. By Lemma 2.3 the subset V_k must be an independent set in G. Moreover, any two vertices from V_k are at the distance as large as possible in G. Probably $G - V_k$ is just P_{n-k}. For $k = 1, 2$, our statements above are all confirmed to be correct from Theorems 4.5, 4.6, 6.2 and 6.3, respectively. But for general value of k, it seems more difficult to solve this problem completely.

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