# Distance-based graph invariants of trees and the Harary index

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**Abstract.** Introduced in 1947, the Wiener index $W(T) = \sum_{\{u,v\} \subseteq V(T)} d(u,v)$ is one of the most thoroughly studied chemical indices. The extremal structures (in particular, trees with various constraints) that maximize or minimize the Wiener index have been extensively investigated. The Harary index $H(T) = \sum_{\{u,v\} \subseteq V(T)} \frac{1}{d(u,v)}$, introduced in 1993, can be considered as the "reciprocal analogue" of the Wiener index. From recent studies, it is known that the extremal structures of the Harary index and the Wiener index coincide in many instances, i.e., the graphs that maximize the Wiener index minimize the Harary index and vice versa. In this note we provide some general statements regarding functions of distances of a tree, from which some of the extremal structures with respect to the Harary index (and a generalized version of it) are characterized. Among the results a recent conjecture of Ilić, Yu and Feng is proven. A case when the extremal structures of these two indices differ is also provided. Finally, we derive some previously known extremal results as immediate corollaries.

## 1. Introduction

So called chemical indices (also known as "topological indices" in the chemical literature) have been introduced by chemists to correlate a chemical compound's structure (the "molecular graph") with experimentally gathered data of the compound's physico-chemical properties. One of the most classical and most thoroughly studied examples is the Wiener index of a graph $G$, defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v),$$

where $d(u,v)$ is the distance between two vertices $u$ and $v$ and the sum is over all unordered pairs of vertices. Introduced in 1947 [10], the Wiener index has frequently made its appearance in both chemical and mathematical literature.

The study of chemical indices of trees is of particular interest because of the large number of chemical compounds with acyclic molecular structures. The extremal trees that maximize or minimize the Wiener index among general trees, trees with a given maximum degree, given degree sequence, and other restrictions have been vigorously studied [1, 2, 8, 13].

The Harary index $H(G)$ of a graph $G$ was introduced more recently [5, 6] and named after Frank Harary. It is defined as the "reciprocal analogue" of the Wiener index, namely

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

Rather extensive work has been done on $H(G)$ for general graphs $G$ with various parameters. See, for instance, [11] and the references therein. For general trees, it is known [3] that $H(T)$ is maximized by the star and minimized by the path among trees of given order. It is natural to imagine that $H(T)$ is larger when $W(T)$ is smaller, as indeed the star minimizes the Wiener index and the path maximizes the Wiener index among trees of given order. However, there does not exist any "functional" relation between the two concepts. This can be seen from the two trees $T$ and $T'$ in Figure 1, where we have

$$W(T') - W(T) = y - x + 1$$

and

$$H(T') - H(T) = \frac{x}{6} - \frac{y}{12} - \frac{1}{6}.$$

With proper choice of $x$ and $y$ (for instance, $x = y = 3$), we have both

$$W(T') > W(T)$$
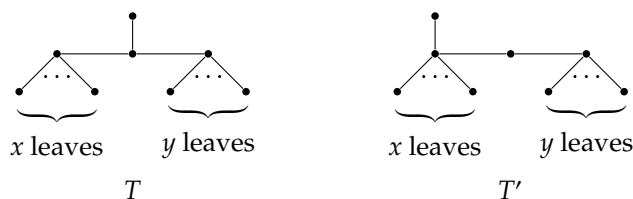
and

$$H(T') > H(T).$$



Figure 1: The trees $T$ and $T'$

In the recent work of Ilić, Yu and Feng [4], the extremal trees with respect to the Harary index are characterized for several categories of trees with restrictions on the number of vertices of degree two, matching number, independence number, radius and diameter. It was pointed out that in all the studied classes, "the trees with maximal Harary index are exactly those trees with the minimal Wiener index, and vice versa".

In this note, we focus on trees with given degree sequence and maximum degree. Such classes of trees are of interest due to the relation between the degrees and the valences of atoms in a chemical compound. In Section 2, we show that the "greedy tree", which minimizes the Wiener index, indeed maximizes the Harary index among trees with given degree sequence. On the other hand, while the Wiener index and many related graph invariants are known to be maximized by a caterpillar [7], we will see from examples that this is not necessarily the case for the Harary index. This seems to be the first case of a class of

trees where the extremal structures of the two indices do not coincide. In Section 3, we first provide a "majorization result" on greedy trees with respect to distances. As a corollary, we show that the "complete *k*-ary tree" maximizes the Harary index among trees with given order and maximum degree *k*. Although "trees with given maximum degree" is interpreted in a slightly different way in [4] and in this note, this result still proves a conjecture in [4]. As applications of the main theorems, we provide in Section 4, as corollaries, some of the known extremal results concerning the Harary index. The final section summarizes our findings.

## 2. On trees with given degree sequence and the greedy tree

**Definition 2.1 (Greedy trees).** *Given a sequence of vertex degrees $(d_1, d_2, \ldots, d_n)$ such that $\sum_i d_i = 2(n-1)$ (so that it can be the degree sequence of a tree), the greedy tree is obtained through the following "greedy algorithm":*

  *(i) Label the vertex with the largest degree as $v$ (the root);*
 *(ii) Label the neighbors of $v$ as $v_1$, $v_2$, ..., and assign the largest degrees available to them such that $\deg(v_1) \geq \deg(v_2) \geq \cdots$;*
*(iii) Label the neighbors of $v_1$ (except $v$) as $v_{11}$, $v_{12}$, ... such that they take all the largest degrees available and that $\deg(v_{11}) \geq \deg(v_{12}) \geq \cdots$, then do the same for $v_2$, $v_3$, ...;*
 *(iv) Repeat (iii) for all the newly labeled vertices, always start with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.*

For example, Figure 2 displays a greedy tree with degree sequence $(4, 4, 4, 3, 3, 3, 3, 3, 3, 2, 2, 1, \ldots, 1)$.
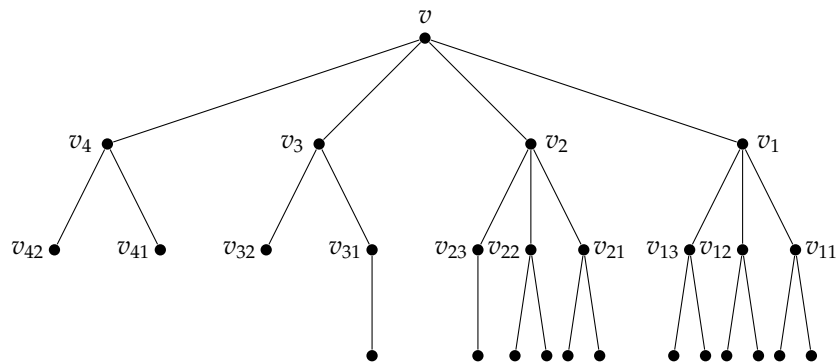


Figure 2: A greedy tree.

It has been shown in various ways that $W(T)$ is maximized by the greedy tree and minimized by a caterpillar among trees with a given degree sequence. Most recently, a general approach regarding this question for nondecreasing functions of the distances was provided in [7]. It is natural to ask for an analogue of these results with respect to the Harary index.

**Question 2.2.** *Is it true that the greedy tree maximizes $H(T)$ among all trees with given degree sequence?*

**Question 2.3.** *Does there always exist a caterpillar which minimizes $H(T)$ among trees with given degree sequence?*

We first provide a positive answer to Question 2.2 through a simple argument. The following was shown in [7].

**Theorem 2.4.** *[7] Let $d_1 \geq d_2 \geq \cdots \geq d_n$ be positive integers such that $\sum_i d_i = 2(n-1)$, and let $r$ be another arbitrary positive integer. Among all trees with degree sequence $(d_1, d_2, \ldots, d_n)$, the greedy tree has the largest number $p_r(T)$ of pairs $(u, v)$ of vertices such that $d(u, v) \leq r$.*

Let $q_r(T)$ be the number of pairs $(u, v)$ of vertices such that $d(u, v) > r$. Then $p_r(T) + q_r(T) = \binom{n}{2}$, and Theorem 2.4 implies that $q_r(T)$ is minimized by the greedy tree.

Now we immediately have the following result similar to Corollary 2.2 in [7].

**Corollary 2.5.** *Let $f(x)$ be any nonnegative, nonincreasing function of $x$. Then the graph invariant*

$$W_f(T) = \sum_{\{u,v\} \subseteq V(T)} f(d(u,v))$$

*is maximized by the greedy tree among all trees with given degree sequence.*

*Proof.* Simply note that

$$W_f(T) = f(1) \cdot \binom{n}{2} + \sum_{r \geq 1} (f(r+1) - f(r)) |\{\{u, v\} \subseteq V(T) : d(u, v) > r\}|,$$

and that $f(r + 1) - f(r)$ is nonpositive for all $r$. $\square$

Hence Question 2.2 is answered positively when we set $f(x) = \frac{1}{x}$ in Corollary 2.5. By setting $f(x) = x^{-\alpha}$, one can state a somewhat generalized result as follows.

**Corollary 2.6.** *The value*

$$H^\alpha(T) = \sum_{(u,v) \subseteq V(T)} (d(u,v))^{-\alpha}$$

*is maximized by the greedy tree among trees with a given degree sequence.*

Regarding Question 2.3, the following example (similar to one in [7]) provides a negative answer.
Take a tree $T_1$ (Figure 3) of degree sequence $\{x + 1, x + 1, x + 1, 3, 1, \ldots, 1\}$. Evidently $T_1$ is not a caterpillar.
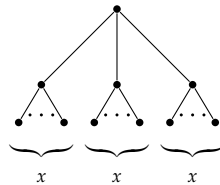


Figure 3: Tree $T_1$ of degree sequence $\{x + 1, x + 1, x + 1, 3, 1, \ldots, 1\}$

Now $T_2$ and $T_3$ in Figures 4 and 5 are the only two non-isomorphic caterpillars with the same degree sequence as $T_1$.
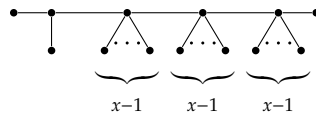


Figure 4: Caterpillar $T_2$ of degree sequence $\{x + 1, x + 1, x + 1, 3, 1, \ldots, 1\}$

Simple calculation shows that

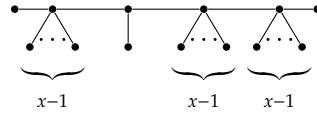$$H(T_1) = \frac{3}{2}x^2 + O(x),$$

$$H(T_2) = \frac{5}{3}x^2 + O(x),$$

Figure 5: Caterpillar $T_3$ of degree sequence $\{x+1, x+1, x+1, 3, 1, \ldots, 1\}$

and

$$H(T_3) = \frac{23}{15}x^2 + O(x).$$

Hence

$$H(T_1) < \min\{H(T_2), H(T_3)\}$$

when $x$ is sufficiently large. It follows that the tree that minimizes the Harary index is not always a caterpillar. However, the following simple minimization result is easy to prove:

**Theorem 2.7.** *Among all trees of order n, the path $P_n$ has the smallest number $p_r(T)$ of pairs $(u, v)$ of vertices such that $d(u, v) \leq r$ $(0 < r < n)$.*

*Proof.* By induction on $n$, the initial cases ($n \leq 3$) being trivial. Let $D$ be the diameter of a tree $T$ of order $n$, and let $v$ be one of the ends of a diametral path (thus $v$ is necessarily a leaf of $T$). For any $r \leq D$, there are clearly at least $r$ vertices whose distance to $v$ is $\leq r$ (namely vertices on the diametral path). Together with the induction hypothesis, it follows that

$$p_r(T) \geq p_r(T \setminus v) + r \geq p_r(P_{n-1}) + r$$

for $r < D$ and

$$p_r(T) = p_r(T \setminus v) + n - 1 \geq p_r(T \setminus v) + r \geq p_r(P_{n-1}) + r$$

for $D \leq r < n$. Since $p_r(P_n) = p_r(P_{n-1}) + r$ for all $r < n$, this completes the induction. $\square$

**Corollary 2.8.** *Let $f(x)$ be any nonnegative, nonincreasing (nondecreasing) function of x. Then the graph invariant*

$$W_f(T) = \sum_{\{u,v\} \subseteq V(T)} f(d(u, v))$$

*is minimized (maximized) by the path $P_n$ among all trees of order n. If the function $f(x)$ is strictly decreasing/increasing, then the path is the unique extremal tree.*

*Proof.* Essentially identical to the proof of Corollary 2.5. If the function is strictly monotone, then $P_n$ is the unique extremal tree since it is the only tree of diameter $n - 1$, so that one has strict inequality $p_{n-2}(T) > p_{n-2}(P_n)$ for all trees $T$ of order $n$ that are not isomorphic to $P_n$. $\square$

## 3. Majorization of greedy trees with respect to distances

The *complete k-ary tree* with a given maximum degree $k$ (also called the "*Volkmann tree*") is defined in a similar way as the greedy tree, except that the vertices $v, v_1, \ldots$ take the maximum degree $k$ until there are not enough vertices (Figure 6). As a result, the complete $k$-ary tree has degree sequence $(k, k, \ldots, k, m, 1, \ldots, 1)$ for some $1 < m \leq k$.

The complete $k$-ary tree is known to minimize the Wiener index among trees with a given maximum degree $k$. It was conjectured in [4], in accordance with other observations, that

**Conjecture 3.1.** *[4] The complete k-ary tree maximizes the Harary index among trees with given order and maximum degree k.*
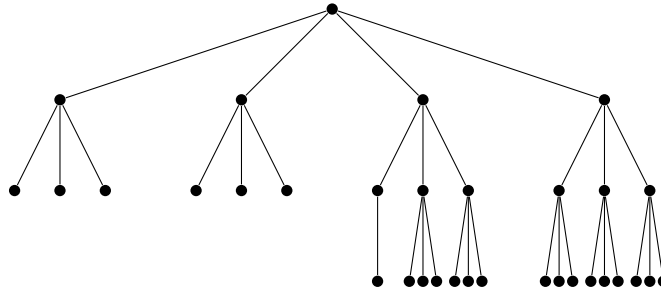
Figure 6: A complete 4-ary tree

We will use Theorem 2.4 and Theorem 3.3 below to show that the complete $k$-ary tree maximizes $p_r(T)$ for all $r > 0$ among such trees. Then the conjecture follows as a corollary.

Consider two nonincreasing sequences $\pi = (d_0, \cdots, d_{n-1})$ and $\pi' = (d'_0, \cdots, d'_{n-1})$. If

$$\sum_{i=0}^{k} d_i \leq \sum_{i=0}^{k} d'_i$$

for $k = 0, \cdots, n - 2$ and

$$\sum_{i=0}^{n-1} d_i = \sum_{i=0}^{n-1} d'_i,$$

then $\pi'$ is said to *majorize* the sequence $\pi$, which we denote by

$$\pi \lhd \pi'.$$

**Lemma 3.2.** *[9] Let $\pi = (d_0, \cdots d_{n-1})$ and $\pi' = (d'_0, \cdots, d'_{n-1})$ be two nonincreasing graphic degree sequences. If $\pi \lhd \pi'$, then there exists a series of graphic degree sequences $\pi_1, \cdots, \pi_\ell$ such that $\pi = \pi_1 \lhd \cdots \lhd \pi_\ell = \pi'$, where $\pi_i$ and $\pi_{i+1}$ differ at exactly two entries, say $d_j$ ($d'_j$) and $d_k$ ($d'_k$) of $\pi_i$ ($\pi_{i+1}$), with $d'_j = d_j + 1$, $d'_k = d_k - 1$ and $j < k$.*

**Theorem 3.3.** *Given two different degree sequences $\pi$ and $\pi'$, if $\pi \lhd \pi'$, then*

$$p_r(T^*_\pi) \leq p_r(T^*_{\pi'})$$

*for any $r > 0$, where $T^*_\pi$ and $T^*_{\pi'}$ are the greedy trees with degree sequences $\pi$ and $\pi'$ respectively. The inequality is strict for at least one $r$ unless $\pi = \pi'$.*

*Proof.* By Lemma 3.2, it is sufficient to show the statement for two degree sequences

$$\pi = (d_0, \cdots d_{n-1}) \lhd (d'_0, \cdots, d'_{n-1}) = \pi'$$

that differ only at the $j$-th and $k$-th entries, with $d'_j = d_j + 1$, $d'_k = d_k - 1$ for some $j < k$.

Let $T^*_\pi$ be the greedy tree corresponding to degree sequence $\pi$, and let $u$ and $v$ be the vertices corresponding to $d_j$ and $d_k$ respectively. Moreover, let us denote the number of vertices whose distance from a vertex $x$ in a tree $T$ is at most $r$ by $p_r(T, x)$. We first prove that

$$p_r(T^*_\pi, u) \geq p_r(T^*_\pi, v)$$

for all $r > 0$. It suffices to do so in the case that $k = j + 1$. There are two possible cases: $u$ and $v$ are either next to each other on the same level, or they are on subsequent levels. We start with the former case: $u$ and $v$ are on the same level. Let $S$ be the subtree formed by the common ancestor of $u$ and $v$ and all its descendants (thus including $u$ and $v$). All vertices outside of $S$ have the same distance from $u$ and $v$ and can

thus be ignored. In view of the "greedy" construction, there are more vertices at any given distance from $u$ in the branch of $S$ that contains $u$ than vertices at the same distance from $v$ in the branch that contains $v$. The stated inequality follows.

In the case that $u$ and $v$ are on consecutive levels ($u$ being the last vertex on its level and $v$ the first), we can apply the same idea, however we consider the tree $T^*_\pi$ as edge-rooted at the edge between the root and its first (rightmost) child. Then $u$ and $v$ are on the same level, and an analogous argument applies.

Now let $T'$ be the tree obtained from $T^*_\pi$ by removing a child $w$ of $v$ and all its descendants. Since all these (removed) vertices are closer to $v$ than to $u$, it is clear that

$$p_r(T', u) \geq p_r(T', v)$$

for all $r > 0$, and that strict inequality holds for some $r$. Now let $T''$ be the tree achieved from $T^*_\pi$ by removing the edge $vw$ and adding an edge $uw$ (see Figure 7 for an example).
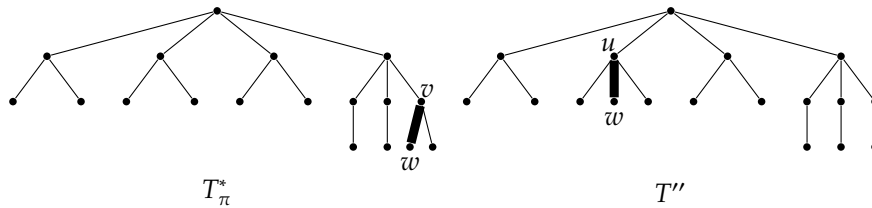


Figure 7: $\pi = (4, 4, 3, 3, 3, 3, 2, 2, 1, \ldots, 1)$ and $\pi' = (4, 4, 4, 3, 3, 2, 2, 2, 1, \ldots, 1)$

Let $S_w$ be the subtree formed by $w$ and its descendants. Distances between vertices outside of $S_w$ clearly remain the same in $T^*_\pi$ and $T''$. Furthermore, for any $x$ in $S_w$ such that $d(w, x) = h$, we have

$$p_r(T'', x) = p_r(S_w, x) + p_{r-h-1}(T', u)$$

and

$$p_r(T^*_\pi, x) = p_r(S_w, x) + p_{r-h-1}(T', v),$$

which shows that $p_r(T'', x) \geq p_r(T^*_\pi, x)$ for all $x$ in $S_w$, and at least one of these inequalities is strict. Since the degree sequence of $T''$ is $\pi'$, it follows that

$$p_r(T^*_{\pi'}) \geq p_r(T'') \geq p_r(T^*_\pi)$$

for all $r > 0$, again with at least one strict inequality. □

Among all trees with given order and maximum degree $k$, evidently the degree sequence

$$(k, k, \ldots, k, m, 1, \ldots, 1)$$

majorizes all other degree sequences. Hence Theorem 3.3 and Theorem 2.4 immediately imply the following.

**Corollary 3.4.** *The complete $k$-ary tree maximizes $p_r(T)$ for all $r > 0$ among trees with maximum degree $k$.*

Now, similar to Corollaries 2.5 and 2.6, the statement of Conjecture 3.1 follows as a special case of the following.

**Corollary 3.5.** *Let $f(x)$ be any nonnegative, nonincreasing (nondecreasing) function of $x$. Then the graph invariant*

$$W_f(T) = \sum_{\{u,v\} \subseteq V(T)} f(d(u, v))$$

*is maximized (minimized) by the complete $k$-ary tree among all trees with given order and maximum degree $k$.*

## 4. Some applications

In this section, we use Corollary 2.5 and Theorem 3.3 to characterize extremal graphs with the largest Harary index of trees in several classes of graphs. In particular, we obtain some results from [4] as corollaries.

**Corollary 4.1.** *Let $f(x)$ be any nonnegative, nonincreasing (nondecreasing) function of $x$. Then the graph invariant*

$$W_f(T) = \sum_{\{u,v\} \subseteq V(T)} f(d(u,v))$$

*is maximized (minimized) by the star $K_{1,n-1}$ among all trees of order $n$.*

*Proof.* For any tree of order $n$, its degree sequence $\pi$ is majorized by $\pi' = (n-1, 1, \ldots, 1)$, and the only tree with degree sequence $\pi'$ is $K_{1,n-1}$. By Corollary 2.5 and Theorem 3.3, the assertion holds. $\square$

Let $\mathcal{T}_{n,s}^{(1)}$ be the set of all trees of order $n$ with $s$ leaves, $\mathcal{T}_{n,\alpha}^{(2)}$ be the set of all trees of order $n$ with independence number $\alpha$ and $\mathcal{T}_{n,\beta}^{(3)}$ be the set of all trees of order $n$ with matching number $\beta$.

Similar to Corollary 4.1, some other useful consequences follow from Corollary 2.5 and Theorem 3.3. The proofs of them are very similar to those in [14] and are skipped here.

**Corollary 4.2.** *Let $f(x)$ be any nonnegative, nonincreasing (nondecreasing) function of $x$. Then the graph invariant*

$$W_f(T) = \sum_{\{u,v\} \subseteq V(T)} f(d(u,v))$$

*is maximized (minimized) by the tree $T_{n,s}^{(1)}$ in $\mathcal{T}_{n,s}^{(1)}$, which is the greedy tree $T_\pi^*$ with degree sequence*

$$(s, 2, \ldots, 2, 1, \ldots, 1)$$

*($2$ being repeated $n - s - 1$ times and $1$ being repeated $s$ times). $T_{n,s}^{(1)}$ is obtained from $t$ paths of order $q + 2$ and $s - t$ paths of order $q + 1$ by identifying one end of each of the $s$ paths. Here $n - 1 = sq + t, 0 \le t < s$.*

**Corollary 4.3.** *Let $f(x)$ be any nonnegative, nonincreasing (nondecreasing) function of $x$. Then the graph invariant*

$$W_f(T) = \sum_{\{u,v\} \subseteq V(T)} f(d(u,v))$$

*is maximized (minimized) by the tree $T_{n,\alpha}^{(2)}$ in $\mathcal{T}_{n,\alpha}^{(2)}$, which is the greedy tree $T_\pi^*$ with degree sequence*

$$\pi = (\alpha, 2, \ldots, 2, 1, \ldots, 1)$$

*($2$ being repeated $n - \alpha - 1$ times and $1$ being repeated $\alpha$ times). In other words, $T_{n,\alpha}^{(2)}$ is obtained from the star $K_{1,\alpha}$ by adding $n - \alpha - 1$ pendent edges to $n - \alpha - 1$ leaves of $K_{1,\alpha}$.*

**Corollary 4.4.** *Let $f(x)$ be any nonnegative, nonincreasing (nondecreasing) function of $x$. Then the graph invariant*

$$W_f(T) = \sum_{\{u,v\} \subseteq V(T)} f(d(u,v))$$

*is maximized (minimized) by the tree $T_{n,\beta}^{(3)}$ in $\mathcal{T}_{n,\beta}^{(3)}$, which is the greedy tree $T_\pi^*$ with degree sequence*

$$\pi = (n - \beta, 2, \ldots, 2, 1, \ldots, 1)$$

*($2$ being repeated $\beta - 1$ times and $1$ being repeated $n - \beta$ times). In other words, $T_{n,\beta}^{(3)}$ is obtained from the star $K_{1,n-\beta}$ by adding $\beta - 1$ pendent edges to $\beta - 1$ leaves of $K_{1,n-\beta}$.*

**Remark 4.5.** *In all the above corollaries, the extremal tree is unique if the function $f(x)$ is strictly monotone. This is because one has strict inequality for at least one r in Theorem 3.3 as well as in Theorem 2.4 (the latter follows from the fact that $T_\pi$ is the unique tree with degree sequence $\pi$ that minimizes the Wiener index, see [8]).*

As special cases, the following results from [4] follow. Theorem 2.7 is also used here.

**Corollary 4.6.** *[4] Let T be a tree with n vertices. Then*

$$n(H_n - 1) \leq H(T) \leq \frac{(n+2)(n-1)}{4},$$

*where $H_n$ stands for the harmonic number $\sum_{i=1}^{n} 1/i$. Equality holds on the left hand side if and only if T is a path of order n and equality holds on the right hand side if and only if T is the star of order n.*

**Corollary 4.7.** *[4] Let T be any tree of order n with s leaves. Then*

$$H(T) \leq H(T_{n,s}^{(1)}) = (s-1)\left(n-1+\frac{s}{2}\right)H_{2q+1} - (s-2)(n-1+s)H_{q+1} + s\left(\frac{s-3}{2} - q\right) + \frac{t(t-1)}{4(q+1)},$$

*where $T_{n,s}^{(1)}$ is defined as in Corollary 4.2 ($n - 1 = sq + t$, $0 \leq t < s$). Equality holds if and only if T is isomorphic to $T_{n,s}^{(1)}$.*

**Corollary 4.8.** *[4] Let T be a tree of order n with independence number $\alpha$. Then*

$$H(T) \leq H(T_{n,\alpha}^{(2)}) = \frac{1}{24}[3n^2 + (2\alpha + 19)n + \alpha^2 - 9\alpha - 22],$$

*where $T_{n,\alpha}^{(2)}$ is defined as in Corollary 4.3. Equality holds if and only if T is isomorphic to $T_{n,\alpha}^{(2)}$.*

**Corollary 4.9.** *[4] Let T be any tree of order n with matching number $\beta$. Then*

$$H(T) \leq H(T_{n,\beta}^{(3)}) = \frac{1}{24}[6n^2 - (4\beta - 10)n + \beta^2 + 9\beta - 22],$$

*where $T_{n,\beta}^{(3)}$ is defined as in Corollary 4.4. Equality holds if and only if T is isomorphic to $T_{n,\beta}^{(3)}$.*

## 5. Summary

Motivated by the concept of the Wiener index and the Harary index, we provided some general statements regarding maximizing or minimizing functions of distances of trees. A number of corollaries follow, including new and previously known results. As some of the consequences, we characterized trees that maximize the Harary index among trees with given degree sequence or maximum degree. The extremal structures found coincide with the ones that minimize the Wiener index. However, examples are provided showing that there is no functional relation between these two indices. Furthermore, among trees with a given degree sequence, the tree that minimizes the Harary index is not necessarily the same that also maximizes the Wiener index. Some "partial" characterization of the trees that minimize the Harary index among trees with given degree sequence might be an interesting subject of further investigation.

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