Wiener Polarity Index and Its Generalization in Trees

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Abstract

The Wiener polarity index of a graph G, denoted by $W_p(G)$, is defined as the number of unordered pairs of vertices that are at distance 3 in G. As one of the classic topological indices, properties of $W_p(G)$ have been extensively studied for various graphs in the recent years. In this note we limit our attention to trees. First we characterize the extremal trees with given degree sequence with respect to the Wiener polarity index. Then we compare the extremal trees with different degree sequences. As a result, extremal statements on the Wiener polarity index of different families of trees follow as immediate consequences. We also briefly discuss the generalization of the Wiener polarity index.

1 Introduction

The so-called topological indices have received much attention in recent years, as they provide a strong correlation between a chemical compound's molecular structure and

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its properties. Some examples include, but not limited to Randić index [23], degree distance [15], connective eccentricity index [33,35], Kirchhoff index [16,34], and Balaban index [11]. One of the oldest and well-studied such indices is the *Wiener index*, defined as the sum of distances over all unordered vertex pairs in a graph G [32] and denoted by

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

where $d_G(u,v)$ (or simply $d(u,v)$) is the distance between u and v in G.

Throughout the years the Wiener index has been extensively studied and has become one of the best known (if not the best known) topological indices. In the same paper, another topological index was also introduced by Wiener, called the *Wiener polarity index* $W_p(G)$, which is defined as the number of unordered pairs of vertices that are at distance 3 in G:

$$W_p(G) = |\{(u,v)|d_G(u,v) = 3, u, v \in V(G)\}|. \tag{1.1}$$

Like the Wiener index, the Wiener polarity index has attracted much attention in recent years. By using the Wiener polarity index, Lukovits and Linert demonstrated quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons in [25]. Hosoya [18] found a physical-chemical interpretation of $W_p(G)$. Du et al. [13] described a linear time algorithm for computing the Wiener polarity index of trees and characterized the trees maximizing the index among all the trees of the given order. Later, Deng, Xiao and Tang characterized the extremal trees with respect to this index among all trees of order n and diameter k [12]. While for cycle-containing graphs, the maximum Wiener polarity index of unicyclic graphs and the corresponding extremal graphs were determined in [19]. In [26] Ma et al. determined the sharp upper bound of the Wiener polarity index among all bicyclic networks based on some graph transformations. Moreover, the extremal values of catacondensed hexagonal systems, hexagonal cacti and polyphenylene chains with respect to the Wiener polarity index were computed in [6]. It was proved that the Wiener polarity index of fullerenes with n carbon atoms is $(9n - 60)/2$ in the same paper.

We will focus on the property of the Wiener polarity index in trees where a unique path exists between any pair of vertices. From the mathematical point of view, the evaluation of the Wiener polarity index may also be considered as enumerating subgraphs isomorphic to a length-3 path. More generally, consider two graphs G and H and let $N(G, H)$ denote the number of subgraphs of G that are isomorphic to H. Given an integer $m \geq 0$, define

$$N(m, H) = \max\{N(G, H) \mid G \text{ is a graph of size } m\}.$$

Erdös [14] obtained the exact value of $N(m, K_k)$ where K_k is the complete graph of order k. Alon [2] and Füredi [17] also considered $N(m, H)$ when H is isomorphic to the disjoint union of stars. Bollobás and Sarkar considered the case where H is a path of length $s \geq 2$ in [8,9]. Furthermore, Alon [1] presented the asymptotically best possible results of $N(m, H)$ if H has a spanning subgraph that is a disjoint union of cycles and isolated edges. Ahlswede and Katona [3], Bollobás and Erdös [7] also studied the case of paths of fixed length.

Due to the correlation between vertex degrees and valences of atoms, trees of given degree sequence (nonincreasing sequence of vertex degrees) appear to be an important family of structures. In Section 2, we first introduce related concepts and some previously established results. The extremal trees with respect to the Wiener polarity index then follows as a consequence. By introducing an ordering on the degree sequences, we compare the extremal trees of different degree sequences in Section 3. As a result, many extremal structures can be identified in various families of trees. Lastly, we briefly discuss the generalization of the Wiener polarity index in Section 4. In Section 5 we summarize our work and propose some open problems.

2 Trees of given degree sequence

For a graph $G = (V, E)$ with $d(u)$ denoting the degree of $u \in V$, the first Zagreb index is defined as

$$M_1(G) = \sum_{v \in V} d(v)^2,$$

which is a special case of the general zeroth-order Randić index [20, 21]. The second Zagreb index is defined as

$$M_2(G) = \sum_{uv \in E} d(u)d(v),$$

which is a special case of the general Randić index [7, 23].

First note the following expression (as a corollary of Theorem 2.1 in [24]) of the Wiener polarity index in terms of M_1 and M_2, which is also provided in [22].

Theorem 2.1 *For a tree T of order n, we have*

$$W_P(T) = M_2(T) - M_1(T) + (n-1)$$

where $M_1(T)$ and $M_2(T)$ are the first and second Zagreb indices, respectively.

For trees with a given degree sequence, $M_1(T)$ and n are constants. Then $W_P(T)$ is maximized or minimized exactly when $M_2(T)$ is maximized or minimized. It has been established in [30] that $M_2(T)$ is maximized by the *greedy tree* (Definition 2.2) and minimized by the *alternating greedy tree* (Definition 2.4).

Definition 2.2 (Greedy Tree) *With given vertex degrees, the greedy tree is constructed through the following "greedy algorithm":*

(i) Label the vertex with the largest degree as v (the root);

(ii) Label the neighbors of v as $v_1, v_2, \ldots$, assign the largest degrees available to them such that $deg(v_1) \geq deg(v_2) \geq \ldots$;

(iii) Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \ldots$, such that they take all the largest degrees available and that $deg(v_{11}) \geq deg(v_{12}) \geq \ldots$, then do the same for $v_2, v_3, \ldots$;

(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.

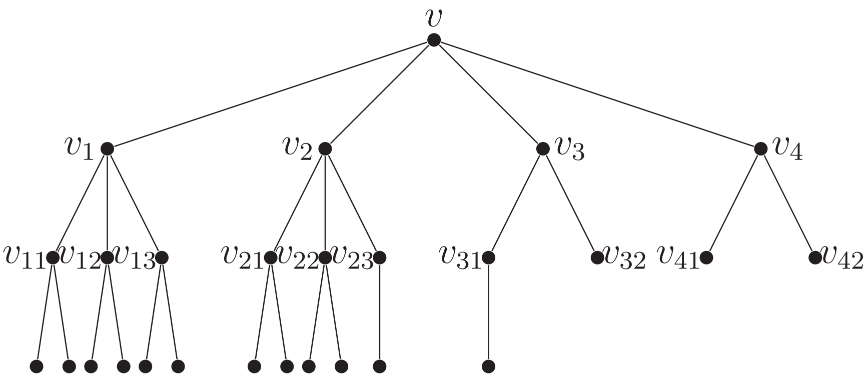

Figure 2.1. A greedy tree with degree sequence (4,4,4,3,3,3,3,3,3,3,2,2,1,. . .,1).

Figure 2.1 shows an example of a greedy tree.

The greedy tree has been shown to be extremal with respect to many topological indices, among which the Wiener index (minimized) and the second Zagreb index (maximized). Consequently we immediately have the following.

Theorem 2.3 *Among all trees with a given degree sequence, $W_P(T)$ is maximized by the greedy tree.*

With a given degree sequence, the tree with minimum M_2 was shown to be the following structure.

Definition 2.4 (Alternating greedy tree) *Given the non-increasing sequence $(d_1, d_2, \ldots, d_m)$ of internal vertex degrees, the alternating greedy tree is constructed through the following recursive algorithm:*

- *If $m-1 \leq d_m$, then the alternating greedy tree is simply obtained by a tree rooted at r with d_m children, $d_m - m + 1$ of which are leaves and the rest with degrees $d_1, \ldots, d_{m-1}$;*
- *Otherwise, $m - 1 \geq d_m + 1$. We produce a subtree T_1 rooted at r with $d_m - 1$ children with degrees $d_1, \ldots, d_{d_{m-1}}$;*

- *Consider the alternating greedy tree* S *with degree sequence* $(d_{d_m}, \ldots, d_m - 1)$*, let* v *be a leaf with the smallest neighbor degree. Identify the root of* T_1 *with* v*.*

Theorem 2.5 *Among all trees with a given degree sequence,* $W_P(T)$ *is minimized by the alternating greedy tree.*

3 Comparing greedy trees and applications

Comparing greedy trees of different degree sequences with respect to various topological indices (including the Wiener index and second Zagreb index) has been shown to be an effective way of understanding the properties of a particular topological index as well as characterizing other extremal tree structures. First we define an ordering of the degree sequences of trees of the same number of vertices.

Definition 3.1 (Majorization) *Given two nonincreasing degree sequences* π *and* π' *with* $\pi = (d_1, d_2, ..., d_n)$ *and* $\pi' = (d'_1, d'_2, ..., d'_n)$*, we say that* π' *majors* π *and write* $\pi \triangleleft \pi'$ *if the following conditions are met:*

- $\sum_{i=1}^{k} d_i \leqslant \sum_{i=1}^{k} d'_i$ *for* $1 \leqslant k \leqslant n-1$*;*
- $\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} d'_i$*.*

The following fact provides a convenient tool in the study related to degree sequences.

Proposition 3.2 *[31] Let* $\pi = (d_1, d_2, \ldots, d_n)$ *and* $\pi' = (d'_1, d'_2, \ldots, d'_n)$ *be two non-increasing graphical degree sequences. If* $\pi \triangleleft \pi'$*, then there exists a series of graphical degree sequences* $\pi_1, \ldots, \pi_k$ *such that* $\pi \triangleleft \pi_1 \triangleleft \ldots \pi_k \triangleleft \pi'$*, where* π_i *and* π_{i+1} *differ at exactly two entries, say* d_j (d_j^*) *and* d_k (d_k^*) *of* π_i (π_{i+1})*, with* $d_j^* = d_j + 1$*,* $d_k^* = d_k - 1$ *and* $j < k$*.*

As an example, it is known that:

Given two degree sequences $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ with $\pi \lhd \pi'$. Let T^*_π and $T^*_{\pi'}$ be the greedy trees with degree sequences π and π' respectively. Then, $M_2(T^*_\pi) \leq M_2(T^*_{\pi'})$.

3.1 Comparing greedy trees of different degree sequences

Unlike in the case of Theorems 2.3 and 2.5, we cannot directly apply the above statement to make analogous conclusions for the Wiener polarity index, as $M_1(T)$ changes with the degree sequence and hence W_p and M_2 do not have the monotonic functional relationship anymore. However, with more detailed analysis, one can still achieve the following. The proof is similar in nature as that of Theorem 2.1 in [37], but additional analysis is needed because of the change in $M_1(.)$.

Theorem 3.3 *Given two nonincreasing degree sequences $\pi = (d_1, d_2, \ldots, d_n)$ and $\pi' = (d'_1, d'_2, \ldots, d'_n)$ with $\pi \lhd \pi'$. Let T^*_π and $T^*_{\pi'}$ be the greedy trees with degree sequences π and π' respectively. Then,*

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

Proof. By Proposition 3.2 we may assume the degree sequences π and π' differ at only two entrices, say $d_{j_0}(d'_{j_0})$ and $d_{k_0}(d'_{k_0})$ with $d'_{j_0} = d_{j_0}+1$, $d'_{k_0} = d_{k_0}-1$ for some $j_0 < k_0$. Let u_1 and u_2 be the vertices of T^*_π with degrees $\mathcal{A} := d_{j_0}$ and $\mathcal{C} := d_{k_0}$ respectively (note that $\mathcal{A} \geq \mathcal{C}$). We will use the following notations:

- let the parent of u_1 have degree $\mathcal{B}$;
- let the children of u_1 have degrees $\mathcal{B}_1 \geq \mathcal{B}_2 \geq \ldots \geq \mathcal{B}_{\mathcal{A}-1}$;
- let the parent of u_2 have degree $\mathcal{D}$;
- let the children of u_2 have degrees $\mathcal{D}_1 \geq \mathcal{D}_2 \geq \ldots \geq \mathcal{D}_{\mathcal{C}-1}$.

From the structure of greedy trees it is easy to see that $\mathcal{D} \leq \mathcal{B}$ and $\mathcal{D}_i \leq \mathcal{B}_j$ for any $1 \leq i \leq \mathcal{C}-1$ and $1 \leq j \leq \mathcal{A}-1$.

Now let

$$T_{\pi'} = T^*_\pi - \{u_2u_3\} + \{u_1u_3\}$$

as in Figure 3.2, where u_3 is a child of u_2 with degree $\mathcal{D}_1$. Note that $T_{\pi'}$ has degree sequences π' but is not necessarily a greedy tree.

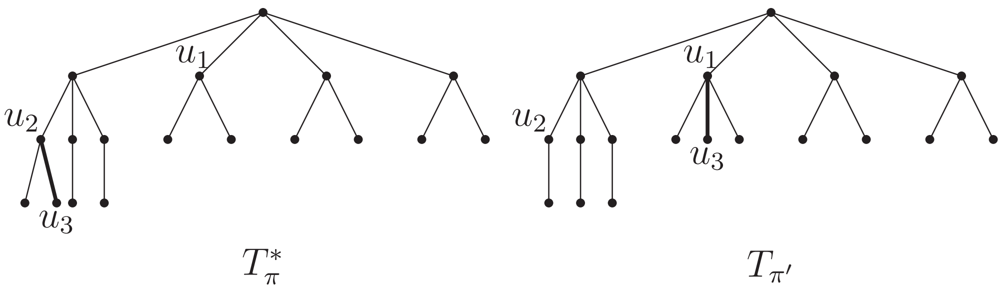

Figure 3.2. π=$(4, 4, 3, 3, 3, 3, 2, 2, 1, \ldots, 1)$ and π'=$(4, 4, 4, 3, 3, 2, 2, 2, 1, \ldots, 1)$.

From T^*_π to $T_{\pi'}$, the change in $M_1(.)$ is

$$M_1(T_{\pi'}) - M_1(T^*_\pi) = (\mathcal{A} + 1)^2 + (\mathcal{C} - 1)^2 - (\mathcal{A}^2 + \mathcal{C}^2) = 2(\mathcal{A} - \mathcal{C} + 1).$$

The change in $M_2(.)$ can also be directly computed. We make use Theorem 2.1 of [37] and have

$$M_2(T_{\pi'}) - M_2(T^*_\pi) = \mathcal{B} - \mathcal{D} + (\mathcal{A} - \mathcal{C} + 1)\mathcal{D}_1 + \sum_{i=1}^{\mathcal{A}-1} \mathcal{B}_i - \sum_{j=2}^{\mathcal{C}-1} \mathcal{D}_j.$$

Thus

$$\begin{aligned} W_P(T'_\pi) - W_P(T^*_\pi) =& (M_2(T_{\pi'}) - M_1(T_{\pi'}) + n - 1) - (M_2(T^*_\pi) - M_1(T^*_\pi) + n - 1) \\ =& M_2(T_{\pi'}) - M_2(T^*_\pi) - (M_1(T_{\pi'}) - M_1(T^*_\pi)) \\ =& \mathcal{B} - \mathcal{D} + (\mathcal{D}_1 - 2)(\mathcal{A} - \mathcal{C} + 1) + \sum_{i=1}^{\mathcal{A}-1} \mathcal{B}_i - \sum_{j=2}^{\mathcal{C}-1} \mathcal{D}_j. \end{aligned} \quad (2.1)$$

Note that $\mathcal{B} - \mathcal{D} \geq 0$ and $\sum_{i=1}^{\mathcal{A}-1} \mathcal{B}_i - \sum_{j=2}^{\mathcal{C}-1} \mathcal{D}_j \geq 0$ from the definition of a greedy tree. We now consider two cases:

- $\mathcal{D}_1 \geq 2$. Clearly, (2.1) ≥ 0;

- $\mathcal{D}_1 = 1$. In this case, we have $\mathcal{D}_j = 1$ for $2 \le j \le \mathcal{C} - 1$. Then (2.1) can be rewritten as

$$\begin{aligned} W_P(T'_\pi) - W_P(T^*_\pi) =& \mathcal{B} - \mathcal{D} - (\mathcal{A} - \mathcal{C} + 1) + \sum_{i=1}^{\mathcal{A}-1} \mathcal{B}_i - (\mathcal{C} - 2) \\ \ge& \mathcal{B} - \mathcal{D} - (\mathcal{A} - \mathcal{C} + 1) + \mathcal{A} - 1 - (\mathcal{C} - 2) = \mathcal{B} - \mathcal{D} \ge 0. \end{aligned}$$

Hence,

$$W_P(T^*_\pi) \le W_P(T_{\pi'}).$$

We have $W_P(T_{\pi'}) \le W_P(T^*_{\pi'})$ by Theorem 2.3. Therefore

$$W_P(T^*_\pi) \le W_P(T^*_{\pi'}).$$

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3.2 Applications

As mentioned earlier, the importance of Theorem 3.3 lies in the fact that the characterization of many other extremal structures follows immediately. We list a few of them here. For convenience we say that a degree sequence is *optimal* if it majorizes all other degree sequences under the given constraints. The key to all the proofs below is to identify the optimal degree sequence and apply Theorems 2.3 and 3.3.

- Among all trees of order n, the degree sequence $(n-1, 1, \ldots, 1)$ is optimal. The corresponding greedy tree, the star, maximizes $W_P(.)$;

- Among all trees of order n with given maximum degree Δ, the degree sequence $(\Delta, \Delta, \ldots, \Delta, q, 1, \ldots, 1)$ (where $1 \le q \le \Delta - 1$) is optimal. Hence the corresponding greedy tree maximizes $W_P(.)$. In different literatures such a tree is also called a "complete Δ-ary tree", "good Δ-ary tree", or "Volkmann trees".

- Among all trees of order n with s leaves, the degree sequence $\left(s, 2, \ldots, 2, \underbrace{1, \ldots, 1}_{s \text{ 1's}} \right)$ is optimal, the corresponding "star like tree" maximizes $W_P(.)$.

- Among all trees of order n with independence number α, the greedy tree with degree sequence $(\alpha, 2, \ldots, 2, 1, \ldots, 1)$ maximizes $W_P(.)$. This is because:
  - If I is an independent set of T of exactly α vertices. For any leaf $u \notin I$, the unique neighbor v of u must be in I and $I \cup \{u\} - \{v\}$ is also an independent set of T. Hence there exists an independent set of α vertices that contains all leaves. Consequently there are at most α leaves. Under this condition, the degree sequence $(\alpha, 2, \ldots, 2, 1, \ldots, 1)$ is optimal.
- Among all trees of order n with matching number β, the greedy tree with degree sequence $(n - \beta, 2, \ldots, 2, 1, \ldots, 1)$ maximizes $W_P(.)$. This is because:
  - If M is a matching of T of exactly β edges, each of these edges contains at least one vertex of degree at least 2. Hence there are at least β vertices of degree at least 2. Under this condition, the degree sequence $(n - \beta, 2, \ldots, 2, 1, \ldots, 1)$ is optimal.

4 Generalizations

In [22], the authors introduced the generalized Wiener polarity index $W_{P_k}(G)$ as the number of unordered pairs of vertices $\{u, v\}$ at distance k in G. This is, in fact, the k-th coefficient in the Wiener polynomial. In the case of $k = 3$ this is exactly the original Wiener polarity index. For a tree T, $W_{P_k}(T)$ is just the number of paths with length k in T. If the diameter of T is less than k, then $W_{P_k}(T) = 0$. Thus the minimum value of $W_{P_k}(T)$ is zero, achieved by all trees with $diam(T) < k$. In [22], the authors proved that the maximum value of $W_{P_k}(T)$ is achieved for a tree with diameter k and with all pendent vertices with eccentricity (the largest distance from a vertex to any other vertex) k. A linear algorithm for computing $W_{P_k}(T)$ of trees was also designed. Bollobás and Tyomkyn [10] considered the maximum number of walks or paths of certain lengths in trees and they proved the following.

Theorem 4.1 *[10] For a tree T of order n and every integer k, there is a p such that the maximal value of $W_{P_k}(T)$ is attained for a p-broom.*

To continue the effort of understanding the generalized Wiener polarity index, we start with finding expressions that relate it to other topological indices. We will generalize Theorem 2.1 for $k \geq 4$. First we define a generalization of the Zagreb indices

$$M_k(T) = \sum_{d(u,v)=k-1} d(u)d(v)$$

for $k \geq 3$.

Theorem 4.2 *For a tree T and integer $k \geq 3$, we have Moreover,*

$$W_{P_k}(T) = (-1)^k \left(\frac{k-1}{2} M_1(T) + \sum_{i=2}^{k-1} (-1)^{i+1}(k-i)M_i(T) - (n-1) \right).$$

Proof. First we also define

$$L_k(T) = \sum_{d(u,v)=k-1} (d(u) + d(v)) = \sum_{u \in V} \sum_{d(u,w)=k-1} d(u),$$

then

$$\begin{aligned} W_{P_k}(T) &= \sum_{d(u,v)=k-2} (d(u)-1)(d(v)-1) \\ &= \sum_{d(u,v)=k-2} d(u)d(v) - \sum_{d(u,v)=k-2} (d(u)+d(v)) + \sum_{d(u,v)=k-2} 1 \\ &= M_{k-1}(T) - L_{k-1}(T) + W_{P_{k-2}}(T). \end{aligned} \tag{4.1}$$

Further examining $L_{k-1}(T)$ shows

$$\begin{aligned} L_k(T) = \sum_{d(u,v)=k-1} (d(u)+d(v)) &= \sum_{u \in V} \left(d(u) \cdot \sum_{d(u,w)=k-2} (d(w)-1) \right) \\ &= \sum_{u \in V} \sum_{d(u,w)=k-2} d(u)d(w) - \sum_{u \in V} \sum_{d(u,w)=k-2} d(u) \\ &= 2M_{k-1}(T) - L_{k-1}(T). \end{aligned} \tag{4.2}$$

For even k, repeatedly applying (4.1) yields

$$W_{P_k}(T) = \sum_{i=3,odd}^{k-1} M_i(T) - \sum_{i=3,odd}^{k-1} L_i(T) + W_{P_2}(T). \tag{4.3}$$

Similarly, by (4.2), we have for odd $i \geq 3$

$$L_i = 2\sum_{j=2}^{i-1}(-1)^j M_j(T) - M_1(T). \tag{4.4}$$

Substitute (4.4) into (4.3), then

$$\begin{aligned}
W_{P_k}(T) &= \sum_{i=3,odd}^{k-1} M_i(T) - \sum_{i=3,odd}^{k-1}\left(2\sum_{j=2}^{i-1}(-1)^j M_j(T) - M_1(T)\right) + W_{P_2}(T) \\
&= \sum_{i=3,odd}^{k-1} M_i(T) - 2\sum_{i=3,odd}^{k-1}\sum_{j=2}^{i-1}(-1)^j M_j(T) + \frac{k-2}{2}M_1(T) + \frac{M_1(T)}{2} - (n-1) \\
&= \sum_{i=3,odd}^{k-1} M_i(T) - \sum_{i=2,even}^{k-2}(k-i)M_i(T) + \sum_{i=3,odd}^{k-3}(k-i-1)M_i(T) \\
&\quad + \frac{k-1}{2}M_1(T) - (n-1) \\
&= \sum_{i=2}^{k-1}(-1)^{i+1}(k-i)M_i(T) + \frac{k-1}{2}M_1(T) - (n-1).
\end{aligned}$$

Similarly, for odd k we have

$$W_{P_k}(T) = \sum_{i=2}^{k-1}(-1)^i(k-i)M_i(T) - \frac{k-1}{2}M_1(T) + (n-1).$$

Hence

$$W_{P_k}(T) = (-1)^k\left(\sum_{i=2}^{k-1}(-1)^{i+1}(k-i)M_i(T) + \frac{k-1}{2}M_1(T) - (n-1)\right).$$

∎

5 Concluding remarks

In this note we examined the properties of the Wiener polarity index of trees. In particular, we point out that the extremal trees with a given degree sequence with respect to the Wiener polarity index are the greedy trees and alternating greedy trees. This follows directly from the correlation between the Wiener polarity index and other previously studied indices such as the Zagreb indices. We then compared the values of the Wiener polarity index of greedy trees with different degree sequences. As immediate consequences we listed a number of extremal results for different families of trees. Lastly, we discussed the generalization of the Wiener polarity index, for which some basic extremal results were established before. We provided formulas that express the generalized Wiener polarity index in terms of other graph invariants.

Characterizing the extremal trees for the generalization of the Wiener polarity index appears to be difficult. For instance, it is easy to find counter examples to Theorems 2.3 and 3.3 for $W_{P_4}(T)$. Among trees with a given degree sequence, the extremal problems for general $W_{P_k}(T)$ and $M_k(T)$ remain wide open.

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