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On the generalized Wiener polarity index for some classes of graphs

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***Abstract*—The generalized Wiener polarity index $W_k(G)$ of a graph $G = (V, E)$ is defined as a number of unordered pairs $\{u, v\}$ of G such that the shortest distance between u and v is equal to k:**

$$W_k(G) = |\{\{u, v\}, d(u, v) = k, u, v \in V(G)\}|$$

In this paper we give some results for 2-trees in case of mentioned index. We present an infinite family of 2-trees with maximum value of generalized Wiener polarity index.

I. Introduction

Let $G = (V(G), E(G))$ be a connected, simple graph with $V(G)$ the vertex set and $E(G)$ the edge set. Let n be the number of vertices and m the number of edges. By $d(u, v)$ we denote the distance between two vertices u and v in the graph G. What we call a diameter $diam(G)$ is the longest distance between two vertices of G. The degree of the vertex u in the graph G is denoted by $deg(u)$. Other definitions, not mentioned here can be found in [1].

The Wiener polarity index of a graph $G = (V(G), E(G))$ is defined as

$$WP(G) = |\{\{u, v\} : d(u, v) = 3; u, v \in V(G)\}|$$

which is a number of unordered pairs of vertices $\{u, v\}$ of G such that $d(u, v) = 3$. Authors of [4, 5, 7, 13] studied this index for trees with different parameters such that number of pendant vertices, diameter or maximum degree. Additionally, in [12] there are described algorithms for counting $W_k(T)$ for trees.

The generalized Wiener polarity index of a graph $G = (V(G), E(G))$ is defined as

$$W_k(G) = |\{\{u, v\}, d(u, v) = k, u, v \in V(G)\}|$$

which is a number of unordered pairs of vertices $\{u, v\}$ of G such that the distance between u and v is equal to k.

Let us now remind the definition of the Wiener index $W(G)$

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v) = \frac{1}{2} \sum_{v \in V(G)} D(v),$$

where $D(v) = \sum_{u \in V(G)} d(u, v)$ is the sum of all distances from the vertex v. As we can see $W(G)$ is defined as the sum of the distances between all pairs of vertices in the graph G. Note that: $W(G) = \sum_{k=1}^{diam(G)} kW_k(G)$. The Hosoya polynomial (Wiener polynomial) of G in x is defined as follows

$$W(G, x) = \sum_{u,v \in V(G)} x^{d(u,v)} = \sum_{k=1}^{diam(G)} W_k(G) \cdot x^k$$

More information about Hosoya polynomial the reader can find in [9].

The applications of mentioned indices are described in the papers [2, 3] and also in [9, 10]. Probably the best known topological index is the Wiener index and this is the one described by many authors, for example [2, 8].

II. Generalized Wiener polarity index

In case of generalized Wiener polarity index for trees there are some known results presented in [12]. Let T be a tree. If $k = 1$ then $W_1(T) = m$, where m is the number of edges. If $k = 2$ then

$$W_2(T) = \sum_{v \in V(T)} \binom{deg(v)}{2} = \frac{\sum_{v \in V(T)} deg^2(v)}{2} - m = \frac{M_1(G)}{2} - m$$

where $M_1(G)$ is the first Zagreb index of a graph. For detailed information on Zagreb indices the reader is referred to [11].

If $k = 3$ we have

$$W_3(T) = \sum_{uv \in E(T)} (deg(v) - 1)(deg(u) - 1) = \sum_{uv \in E(T)} deg(u)deg(v) - \sum_{v \in V(T)} deg^2(v) + m = M_2(T) - M_1(T) + m$$

where $M_2(T)$ is the second Zagreb index of a graph.

Let us now assume that $k \geq 3$. In a situation when diameter of T is less than k we have $W_k(T) = 0$ and that is why the minimum value of $W_k(T)$ is equal to zero. This is achieved for all trees for which $diam(T) < k$. Actually, this is simple fact for each graph.

Now we will study the generalized Wiener polarity index for 2-trees. Let us define a 2-tree first. The smallest 2-tree is a complete graph K_3 of order $n = 3$. A 2-tree of order n is obtained from a 2-tree G of order $n-1$ by attaching a new vertex v and two edges $\{vx, vy\}$ such that $\{x, y\} \in E(G)$. Concerning 2-trees with $diam(G) \geq k$ is more difficult than for trees.

Let G be a 2-tree of order n and size m. A pendant vertex in a 2-tree is a vertex with degree equal to 2. Now, for $k = 1$ the value of $W_1(G)$ stays the same as for trees. For $k = 2$ we have

$$W_2(G) = \sum_{v \in V(G)} \left(\binom{deg(v)}{2} - m \right)$$

But let us move on to what will be considered now and this are the maximum values of $W_k(G)$ where G is a 2-tree.

What we are going to do is to decompose all vertices v in G with $deg(v) = 2$ into some number of groups. Each group has the following property

$$A_i = \{v \in V(G) : deg(v) = 2 \wedge \exists_{e_i = \{u_i, w_i\}}; vu_i, vw_i \in E(G)\}$$

for $i = 1, 2, ...$

We have at least two such groups. Let us say that the distance between two arbitrary pendant vertices from different groups is not equal to k. Distances between vertices in each group are equal to 2.

Let p_1 and p_2 be the numbers of vertices on distance k from an arbitrary pendant vertex from A_1 and A_2, respectively. We can ssume that $p_1 \geq p_2$ with no loss of generality. After removal of all pendant vertices from A_2 and addition to the group A_1 we get the transformed 2-tree G'

$$\begin{aligned} &W_k(G') - W_k(G) \geq \\ &\quad = (|A_1|p_1 + |A_2|p_1) - (|A_1|p_1 + |A_2|p_2) = \\ &\quad = |A_2|(p_1 - p_2) \geq 0 \end{aligned} \tag{1}$$

Note this is true for two groups. If there are more of them inequality in (1) may not hold.

By repetition of this transformation we will get a new 2-tree with possibly greater generalized Wiener polarity index. The diameter of G' after each transformation is less or stays the same as the one for G. Each transformation gives us also one new pendant vertex. If we will choose the most distant groups of pendant vertices we will get a 2-tree with diameter equal to k. After that we can apply the transformation finitely many times until all pendant vertices are on distance k and no other vertex of the final 2-tree has eccentricity equal to k. During this process the $W_k(G)$ may be changing by decreasing or increasing. Some example is presented in $Fig.1$.

Let us assume we have p groups of pendant vertices with sizes: $a_1, a_2, ..., a_p$ and $a_1 + a_2 + ... + a_p = q$. We consider a 2-tree with $diam(G) = k$. We have then $n - 2(k-1) \geq q \geq 2$. Assume that the distance between any two pendant vertices not from the same group is equal to k and that is why

$$W_k(G) = \frac{1}{2} \sum_{i=1}^{p} a_i(q - a_i) = \frac{1}{2}\left(q^2 - \sum_{i=1}^{p} a_i^2\right) \tag{2}$$

In the case when the distance between the group A_i and A_j for $i \neq j$ is less than k the generalized Wiener polarity index is less than the one presented above. If $p = 2$ we have $W_k(G) = a_1 a_2$. This value is maximum for $a_1 + a_2 = n - 2(k-1)$, $a_1 = \left\lfloor \frac{n-2(k-1)}{2} \right\rfloor$ and $a_2 = \left\lceil \frac{n-2(k-1)}{2} \right\rceil$.

$$\begin{aligned} W_k(G) &= \left\lfloor \frac{n-2(k-1)}{2} \right\rfloor \left\lceil \frac{n-2(k-1)}{2} \right\rceil = \\ &= \left(\left\lfloor \frac{n}{2} \right\rfloor - (k-1) \right) \left(\left\lceil \frac{n}{2} \right\rceil - (k-1) \right) = \\ &= \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil - (k-1) \left(\left\lfloor \frac{n}{2} \right\rfloor + \left\lceil \frac{n}{2} \right\rceil \right) + (k-1)^2 \end{aligned}$$

so

$$W_k(G) = \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil - (k-1)(n - (k-1)) \tag{3}$$

Let $p > 2$ and $k > 2$. First we consider the even k. By $n \geq 2 + p(k-2) + q$ and $2 < p \leq q$ we have $p \leq \frac{n-2-q}{k-2}$, so

$$p < \frac{n-2}{k-2}. \tag{4}$$

We have the following

$$q = \sum_{i=1}^{p} a_i,$$

$$n = 2 + 2p\left(\frac{k}{2} - 1\right) + \sum_{i=1}^{p} a_i = 2 + p(k-2) + \sum_{i=1}^{p} a_i.$$

Hence

$$n \geq 2 + p(k-2) + q. \tag{5}$$

We apply Cauchy - Schwarz ineqality to the formula (2) with $q \leq n - 2 - p(k-2)$

$$W_k(G) = \frac{1}{2}\left(q^2 - \sum_{i=1}^{p} a_i^2\right) \leq \frac{1}{2}\left(q^2 - \frac{q^2}{p}\right) \leq \frac{1}{2} f(p) \tag{6}$$

where

$$f(p) = (n - 2 - p(k-2))^2 \left(1 - \frac{1}{p}\right).$$

The extremal generalized Wiener polarity index $W_k(G)$ is obtained for the case when we have equality in (6). We are going to study this case. We will give some examples of extremal 2-trees and then we will state the final result in Theorem 1.

So for real variable p we study

$$\begin{aligned} f(p) = &\left((n-2)^2 + p^2(k-2)^2\right)\left(1 - \frac{1}{p}\right) \\ &- 2(k-2)(n-2)(p-1). \end{aligned} \tag{7}$$

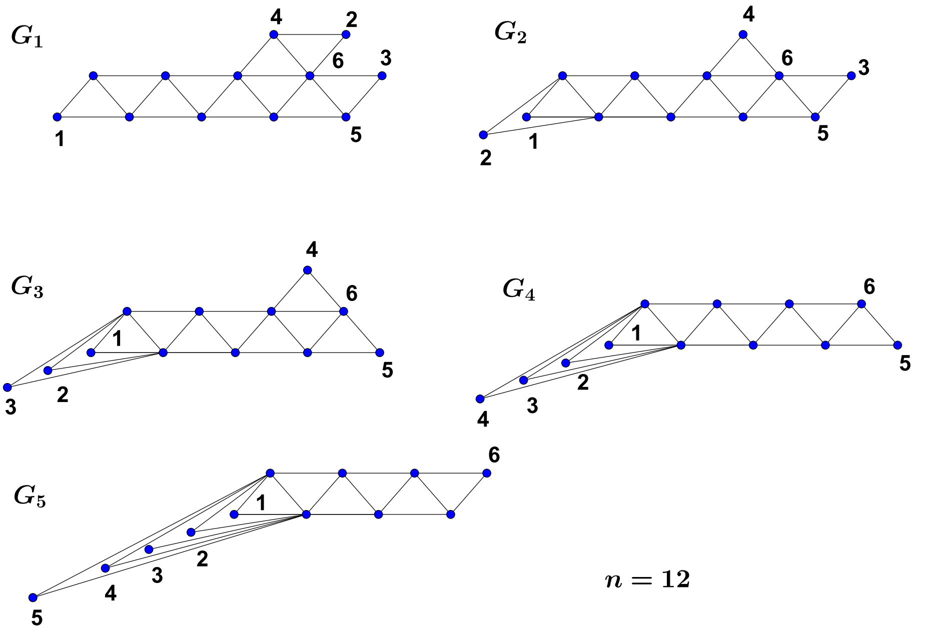

Fig. 1. A process of moving pendant vertices $G_1 \to G_2 \to G_3 \to G_4 \to G_5$. $W_4(G_1) = 8$, $W_4(G_2) = 9$, $W_4(G_3) = 10$, $W_4(G_4) = 9$, $W_4(G_5) = 5$.

Let $h(p) = 2(2-k)(1-\frac{1}{p}) + \frac{n-2-p(k-2)}{p^2}$. Then the first derivative equals

$$f'(p) = (n-2-p(k-2))h(p)$$

By (4) we have $f'(p) = 0$ if and only if $p = \hat{p}$, where

$$\hat{p} = \frac{1}{4} + \frac{1}{4}\sqrt{\frac{8n+k-18}{k-2}} \tag{8}$$

Similarly $f'(p) > 0$ if and only if $h(p) > 0$. This is equivalent to the inequality

$$g(p) = 2p^2 - p - \frac{n-2}{k-2} < 0.$$

So $g(p) < 0$ if and only if $p < \hat{p}$.
Let

$$s = 4\hat{p} = 1 + \sqrt{\frac{8n+k-18}{k-2}}.$$

Then

$$\frac{1}{\hat{p}} = \frac{\sqrt{(k-2)(8n+k-18)} - (k-2)}{2n-4} = \frac{(k-2)(s-2)}{2n-4}.$$

By (6) we can write

$$f(\hat{p}) = \left(n-2-\frac{1}{4}(k-2)s\right)^2 \left(1 - \frac{(k-2)(s-2)}{2n-4}\right).$$

Then

$$f(\hat{p}) = \left((n-2)^2 - \frac{(n-2)(k-2)}{2}s + \frac{(k-2)^2}{16}s^2\right) \cdot \left(1 - \frac{(k-2)(s-2)}{2n-4}\right). \tag{9}$$

We are interested in the case with $\hat{p} \geq 3$. By (8) we get $n \geq 15k - 28$.

Example 1:
By the formula (9) for $k = 6$ we get

$$f(\hat{p}) = \left((n-2)^2 - 2(n-2)\left(1+\sqrt{2n-3}\right) + \left(1+\sqrt{2n-3}\right)^2\right) \cdot \left(1 - \frac{2\sqrt{2n-3}-2}{n-2}\right).$$

Let us set

$$n = 2t^2 + 2 \geq 15k - 28 = 62. \tag{10}$$

By (8) for even t we have

$$\lfloor \hat{p} \rfloor = \left\lfloor \frac{1}{4} + \frac{1}{4}\sqrt{4t^2+1} \right\rfloor = \left\lfloor \frac{1}{4} + \frac{t}{2} \right\rfloor = \frac{t}{2}. \tag{11}$$

Note that by (7)

$$f(\lfloor \hat{p} \rfloor) = 4t(t-1)^2(t-2), \tag{12}$$

and

$$f(\lceil \hat{p} \rceil) = 4t(t^2-t-2)^2 \frac{1}{t+2} > f(\lfloor \hat{p} \rfloor),$$

for $t > 2$.

We can note that by the formula (6) we get extremal 2-trees for the case

$$W_6(G) = \frac{1}{2} f(\lfloor \hat{p} \rfloor).$$

Now we compare this value with $W_k(G)$ for $p > 2$. By the formula (3) for $p = 2$ we get

$$W_6(G) \le (t^2+1)^2 - 5(2t^2+2) + 25 = t^4 - 8t^2 + 16.$$

So we get the following inequality

$$\frac{1}{2} f(\lfloor \hat{p} \rfloor) > t^4 - 8t^2 + 16.$$

By the formula (12) we get

$$2t(t-2)(t-1)^2 > t^4 - 8t^2 + 16. \quad (13)$$

The inequality (13) is equivalent to the following one

$$2t(t-1)^2 > (t-2)^2(t+2). \quad (14)$$

Suppose now that $t = 6$, then by (10) we have $n = 2 \cdot 6^2 + 2 = 74$ and by (9) we have $\lfloor \hat{p} \rfloor = 3$. The inequality (14) holds in this case. So we obtained the maximum $W_6(G) = 3 \cdot 20^2$ for the 2-tree G with parameters $n = 74,\ k = 6,\ p = 3$ and $|A_i| = (n-14)/3 = 20$.

An extremal 2-tree is presented below in Fig. 2.

Example 2:

By the formula (9) for $k = 4$ we get

$$f(\hat{p}) = \left((n-2)^2 - (n-2)\left(1+\sqrt{4n-7}\right) + \frac{1}{4}\left(1+\sqrt{4n-7}\right)^2\right) \cdot \left(1 - \frac{\sqrt{4n-7}-1}{n-2}\right).$$

We have:

$$n = t^2 + 2 \ge 15k - 28 = 15 \cdot 4 - 28 = 32. \quad (15)$$

By (8) for even t we have

$$\lfloor \hat{p} \rfloor = \left\lfloor \frac{1}{4} + \frac{1}{4}\sqrt{4t^2+1} \right\rfloor = \left\lfloor \frac{1}{4} + \frac{t}{2} \right\rfloor = \frac{t}{2}. \quad (16)$$

and then by (7)

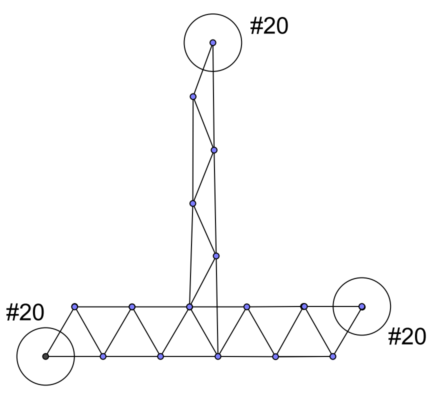

Fig. 2. An extremal graph of order $n = 74$ with $k = 6$ and three groups $|A_i| = 20,\ i = 1, 2, 3$.

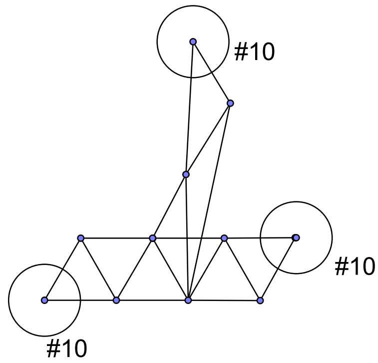

Fig. 3. An example of extremal graph for $k = 4$.

$$f(\lfloor \hat{p} \rfloor) = t(t-2)(t-1)^2,$$

and

$$f(\lceil \hat{p} \rceil) = t(t^2-t-2)^2 \frac{1}{t+2},$$

We can note that by the formula (6) we get

$$W_4(G) = \frac{1}{2} f(\lfloor \hat{p} \rfloor).$$

By the formula (3) for $p = 2$ and $k = 4$ we get $W_4(G) = \frac{1}{4}t^4 - 2t^2 + 4$.

Now we get the following inequality

$$f(\lfloor \hat{p} \rfloor) = t(t-2)(t-1)^2 > t(t^2-t-2)^2 \frac{1}{t+2} = f(\lceil \hat{p} \rceil).$$

The above inequality is equivalent to the following one

$$(t+2)(t-2)(t-1)^2 > (t^2-t-2)^2. \quad (17)$$

Suppose now that $t = 6$, then by (15) we have $n = 6^2 + 2 = 38 > 32$ and $\lfloor \hat{p} \rfloor = 3$. So the inequality (17) holds in this case and we have the maximum $W_4(G) = 3 \cdot 10^2$ for the 2-tree G with parameters $n = 38,\ k = 4,\ \hat{p} = 3$ and $|A_i| = (n-8)/3 = 10, i = 1, 2, 3$.

An extremal 2-tree is presented in Fig. 3.

In general case we have the following result.

Let $p_- = \lfloor \hat{p} \rfloor$ and $p_+ = \lceil \hat{p} \rceil$ where $\hat{p}$ is defined in (8) . We present a theorem for 2-trees of order n equal to $g(k)$, where $g(k)$ is some function defined in the proof.

Theorem 1. *Let n and k be integers. For each even integer $k \ge 4$ there exists a 2-tree G of order n with extremal generalized Wiener polarity index $W_k(G)$ and with $p_- \ge 3$ or $p_+ \ge 3$ groups of pendant vertices for $n = g(k)$ where $g(k)$ is some function in variable k. Then we have an infinite family of such 2-trees.*

Proof: By (7) and (8) we have $p_- \le \hat{p} \le p_+$ and $W_k(G) = \frac{1}{2}\max\{f(p_+), f(p_-)\}$, where

$$f(p_-) = \left((n-2)^2 + p_-^2(k-2)^2\right)\left(1 - \frac{1}{p_-}\right) - 2(k-2)(n-2)(p_- - 1).$$

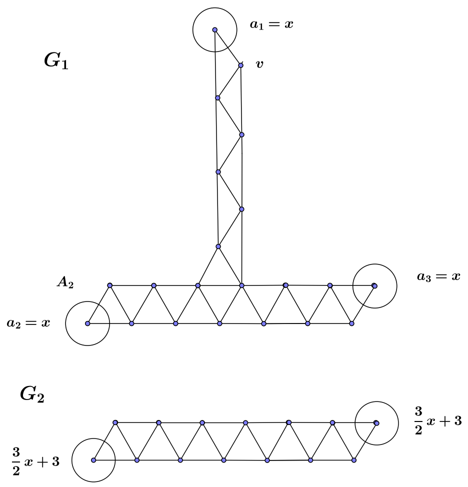

Fig. 4. Examples of 2-trees of the same order with diameter $k = 7$, where $W_7(G_1) > W_7(G_2)$ for even $x \geq 12$.

We get the inequality

$$\frac{1}{2}f(p_-) > \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil - (k-1)(n-(k-1)).$$

Hence

$$p_-^3(k-2)^2 - p_-^2(k-2)(2n+k-6)$$
$$+ p_- \left((n-2)^2 - 2\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil + 4kn - 6n - 2k^2 + 6 \right)$$
$$- (n-2)^2 > 0.$$

Similarly we can compare

$$\frac{1}{2}f(p_+) > \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil - (k-1)(n-(k-1)).$$

This two above inequalities are equivalent to the following one:

$$n^2 - n(12((p-2)k - 2p) + 52) + 52 - 12k^2$$
$$+ 6p((p-2)(k-2)^2 + (k-2)(k+2)) > 0$$

where $p = p_+$ or $p = p_-$.

By solving this inequality we can construct 2-trees G with $p_- \geq 3$ or $p_+ \geq 3$ groups of pendant vertices with extremal generalized Wiener polarity index $W_k(G)$. It is enough to take $g(k) = 2 + p(k - 2 + a)$, where $a = |A_i|$ for each integer $a \geq (k-2)\max\{11, 2(p-1)\}$ and $i = 1, ..., p$ with $p = p_-$ or $p = p_+$. It follows by formula (8). This is the end of the proof.

In the theorem we are presenting the results for even k. Note that for odd k the generalized Wiener polarity index $W_k(G)$ for 2-trees of order n with two groups of pendant vertices in general case is not greater than such index for 2-trees of order n with $p = 3$ groups of pendant vertices.
An infinite number of such examples of 2-trees is presented in Fig. 4.

In this paper we proved Theorem 1 for 2-trees of order n with an extremal $W_k(G)$ for given n and k. In the future work we wish to find an efficient algorithm for counting $W_k(G)$ for the considered family of graphs.

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