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Subtree Number versus Wiener Index

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Abstract

The subtree number $N(G)$ of a graph G is defined as the number of non-empty subtrees of G. The Wiener index $W(G)$ of a graph G is defined as the sum of distances over all pairs of vertices in G. It has been noted that, for many families of trees and graphs, the graphs that achieve the largest number of subtrees are exactly those that attain the smallest Wiener index, and vice versa. Consequently, it is often said that the subtree number and the Wiener index have a "negative" correlation. In this paper, we show that, except for extremal graphs, this "negative" correlation does not generally hold. In particular, for every $n \geq 14$, we construct a pair of unicyclic graphs G and H, each having n vertices and identical degree sequences, such that $W(G) < W(H)$ and $N(G) < N(H)$. Furthermore, our construction shows that both differences, $N(H) - N(G)$ and $W(H) - W(G)$, grow unbounded as n increases.

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1 Introduction

The subtree number $N(G)$ of a graph G is the number of non-empty subtrees of G. This quantity has been extensively studied for trees [7,13,14,19] and recently even for general graphs [17]. The inverse problem for the number of subtrees was studied in [2]. The problems related to the subtree number were recently the motivation for the research on the number of subpaths also [8, 9].

An interesting relation of the subtree number with the Wiener index was observed in the literature. First, let us say that the Wiener index $W(G)$ of a graph G is obtained by summing the distances over all pairs of vertices in G. This quantity was first introduced by Wiener [15] who established the correlation of the Wiener index $W(G)$ with some chemical properties of the molecule represented by G. This opened the door into the research of topological indices of graphs, and the Wiener index became one of the most intensively studied topological indices. A nice overview of the research of mathematical properties of the Wiener index is given in the surveys [10, 11].

The observed relation of the subtree number and the Wiener index involves the extremal graphs. Namely, it was observed that in many classes of trees and graphs it holds that the graphs which maximize the subtree number are the same ones which minimize the Wiener index, and vice versa. Due to this, it is usually said that the subtree number and the Wiener index have a "negative" correlation [1, 3, 16, 18]. The classes of graphs for which this "negative" correlation is observed include binary trees with n leaves [4,6,13,14], unicyclic graphs and unicyclic graphs with a given girth [1], graphs with given number of cut edges [17], all cacti of order n with k cycles and all block graphs of order n with k blocks [5,12]. These observations motivate the research of the relation of $N(G)$ and $W(G)$ in [16].

In this paper, we show that, except for extremal graphs, the Wiener index and the subtree number are not always negatively correlated. Namely, for any $n \geq 14$ we provide a pair of unicyclic graphs G and H both on n vertices and with the same degree sequences, such that $W(G) < W(H)$

and $N(G) < N(H)$. Moreover, both differences $W(H) - W(G)$ and $N(H) - N(G)$ tend to infinity as the number of vertices increases. On the other hand, by a slight change in our construction, one easily obtains graphs G and H with $W(G) > W(H)$ and $N(G) < N(H)$, where the differences again tend to infinity.

2 Main results

Let us introduce some basic notation that will be used in this section. First, let $G = (V, E)$ be a graph with the set of vertices $V = V(G)$ and the set of edges $E = E(G)$. Throughout the paper we tacitly assume that G is simple and connected. For a pair of vertices $x, y \in V(G)$, the *distance* $d_G(x, y)$ is the length of a shortest path in G between x and y. Further, for two sets $X, Y \subseteq V(G)$ we define $d_G(X, Y) = \sum_{x \in X, y \in Y} d_G(x, y)$. For a graph G, the Wiener index $W(G)$ is defined to be the sum of distances over all pairs of vertices in G, i.e. $W(G) = \sum_{\{x,y\} \subseteq V(G)} d_G(x, y)$.

A *subtree* of a graph G is any subgraph of G which is also a tree. The subtree number $N(G)$ of a graph G is defined as the number of non-empty subtrees of G. As we stated in the introduction, there are many papers in literature which report a "negative" correlation between the Wiener index and the subtree number, i.e. that in many graph classes graphs which maximize the Wiener index minimize the subtree number. In the next theorem, we provide graphs which show that this "negative" correlation is not always the case.

Theorem 1. *Let $a \geq 2$, $b \geq 1$ and $c \geq 1$ be three integers. For $n = 2a + 2b + 2c + 4$, there exist unicyclic graphs G and H, both on n vertices and with the same degree sequences, such that*

$$W(H) - W(G) = (b - c)^2$$
$$N(H) - N(G) = 2(a - 1)\left(2^c - 1\right)\left(2^b - 1\right)\left(2^{b+c} + 1\right) - 3(2^b - 2^c)^2.$$

Similarly, for $n = 2a + 2b + 2c + 5$, there exist unicyclic graphs G' and H',

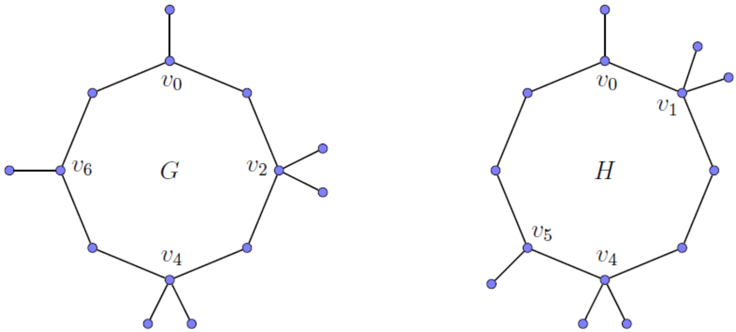

Figure 1. The graph G and H for $a = 2$, $b = 1$ and $c = 2$.

both on n vertices and with the same degree sequences, such that

$$\begin{aligned} W(H') - W(G') &= (b-c)^2 - (b-c), \\ N(H') - N(G') &= 9 \cdot 2^{b+c} - 3 \cdot 2^{2b} - 6 \cdot 2^{2c} \\ &\quad - (a-1)(3 \cdot 2^{2b+c} + 4 \cdot 2^{b+2c} - 4 \cdot 2^{2b+2c} - 6 \cdot 2^{b+c} \\ &\quad + 2 \cdot 2^b + 3 \cdot 2^c - 2). \end{aligned}$$

Proof. We will consider separately the case of $n = 2a + 2b + 2c + 4$ and $n = 2a + 2b + 2c + 5$.

Case 1. $n = 2a + 2b + 2c + 4$. In order to construct a graph G on n vertices, let a and b be positive integers. We denote $k = a + 2$ and let C_{2k} be a cycle on $2k$ vertices labeled $v_0, v_1, \ldots, v_{2k-1}$. To each of the vertices v_0 and v_{k+2} precisely b pendant vertices are attached. Also, to each of the vertices v_2 and v_k precisely c pendant vertices are attached. The resulting graph is the graph G, illustrated by Figure 1.

In order to arrive at the graph H, we again start with the cycle C_{2k} whose vertices are labeled the same way as above. In the case of graph H, precisely b pendant vertices are attached to each of v_0 and v_{k+1}. Also, precisely c pendant vertices are attached to each of v_1 and v_k. This yields a graph denoted by H. The graph H is also illustrated by Figure 1.

Obviously, the number of vertices in each of the graphs G and H is

$n = 2a+2b+2c+4$. Also, both G and H have the same degree sequences. Next, we will establish that graphs G and H satisfy the requirements of the theorem. Let us first establish the claim regarding the Wiener index of these two graphs.

Claim A. *It holds that* $W(H) - W(G) = (b-c)^2$.

Let us partition the vertices of G (resp. H) into five sets. Namely, the set of vertices which belong to C_{2k} is denoted by O. Further, the set of pendant vertices of G (resp. H) attached to v_0, v_2, v_k and v_{k+2} (resp. v_0, v_1, v_k and v_{k+1}) is denoted by A, B, C and D, respectively. The following table gives the difference $d_G(X,Y)-d_H(X,Y)$ for $X, Y \in \{A,B,C,D,O\}$, with the omission of the symmetric cases.

X \ Y	A	B	C	D	O
A	0	bc	0	$-b^2$	0
B		0	$-c^2$	0	0
C			0	bc	0
D				0	0
O					0

Notice that the value of $W(G) - W(H)$ is obtained by summing all the entries in the above table, so we have

$$W(G) - W(H) = -b^2 + 2bc - c^2 = -(b-c)^2$$

as claimed.

Claim B. *It holds that*

$$N(H) - N(G) = 2(a-1)\,(2^c-1)\left(2^b-1\right)\left(2^{b+c}+1\right) - 3(2^b-2^c)^2.$$

A vertex of G (resp. H) is a *big* vertex, if its degree is greater than two, otherwise it is a *small* vertex. Since the set of big vertices of C_{2k} is not the same for G and H, the big vertices of G (resp. H) will also be called

G-big (resp. *H-big*) vertices. There are precisely four G-big (resp. H-big) vertices, and they are v_0, v_2, v_k and v_{k+2} (resp. v_0, v_1, v_k and v_{k+1}).

Let B_G (resp. B_H) denote the set of big vertices in G (resp. H). We will count subtrees of G (resp. H) by counting the subpaths of the cycle C_{2k} contained in it. If a subpath of C_{2k} contains one or more big vertices, then for such a path there are many corresponding subtrees of G (resp. H) which are obtained by attaching all possible combinations of pendant vertices hanging at this big vertex in G (resp. H). We have to precisely count all these subtrees.

Let P be a subpath of C_{2k} and let T be a subtree of G (resp. H). We say that T *reduces* to P if $V(T) \cap V(C_{2k}) = V(P)$. If P contains a big vertex x with b (resp. c) pendant vertices hanging at x, then there are 2^b (resp. 2^c) choices for which pendant vertices hanging at x will be included in T. If P contains more than one big vertex, the choices of pendant vertices hanging at them which will be included in T are independent. Since each big vertex x of G and its corresponding big vertex $f(x)$ of H have the same number of pendant vertices, we may characterize paths with the same number of subtrees of both G and H reducing to them.

Namely, denote by $N(G, P)$ (resp. $N(H, P)$) the number of subtrees of G (resp. H) which reduce to P. Notice that

$$N(G) = \sum_{P \subseteq C_{2k}} N(G, P) + 2b + 2c$$

since there are $2b + 2c$ trees in G which contain no vertex of C_{2k}, namely the 1-vertex trees consisting of pendant vertices. The same holds for H.

Let us first establish $N(G)$. We partition subpaths of C_{2k} into five classes $\mathcal{P}_i$ for $i = 0, \ldots, 4$ so that $\mathcal{P}_i$ contains precisely i big vertices. Notice that if P and P' belong to a same class $\mathcal{P}_i$, then $N(G, P) = N(G, P')$.

Assume first that $i = 0$. Notice that in $\mathcal{P}_0$ there are $2(k-2)$ paths of zero length and $2\binom{k-3}{2}$ paths of non-zero length. Also, for each path $P \in \mathcal{P}_0$ it holds that $N(G, P) = 1$. Hence,

$$\sum_{P \in \mathcal{P}_0} N(G, P) = 2\left(k - 2 + \binom{k-3}{2}\right).$$

Assume next that $i = 1$. In this case, for each of the four big vertices there are $2(k-2)$ subpaths of C_{2k} which contain this precise big vertex. If $P \in \mathcal{P}_1$ contains v_0 or v_{k+2}, then $N(G,P) = 2^b$. Otherwise, if $P \in \mathcal{P}_1$ contains v_2 or v_k, then $N(G,P) = 2^c$. Hence,

$$\sum_{P \in \mathcal{P}_1} N(G,P) = 4(k-2)(2^b + 2^c).$$

Assume next that $i = 2$. If a subpath of C_{2k} contains precisely two big vertices, these two vertices must be consecutive on C_{2k}. For each pair of vertices $\{v_0, v_2\}$ and $\{v_k, v_{k+2}\}$, there are $(k-2)^2$ subpaths of C_{2k} that contain it, and for each such subpath P we have $N(G,P) = 2^{b+c}$. On the other hand, for each pair of vertices $\{v_0, v_{k+2}\}$ and $\{v_2, v_k\}$ there are 4 subpaths of C_{2k} which contain it. If subpath P of C_{2k} contains $\{v_0, v_{k+2}\}$, then $N(G,P) = 2^{2b}$. For P which contains $\{v_2, v_k\}$, it holds that $N(G,P) = 2^{2c}$. Hence,

$$\sum_{P \in \mathcal{P}_2} N(G,P) = 2(k-2)^2 2^{b+c} + 4(2^{2b} + 2^{2c}).$$

Assume next that $i = 3$. If a subpath of C_{2k} contains precisely three big vertices, then it does not contain precisely one big vertex. Let us first consider the case when P does not contain v_0 or v_{k+2}. For each of those two vertices, there are $2(k-2)$ subpaths of C_{2k} which do not contain it. And for each such path P, we have $N(G,P) = 2^{b+2c}$. If we consider vertices v_2 and v_k, then for each of them there are again $2(k-2)$ subpaths of C_{2k} which do not contain it. Yet, in this case $N(G,P) = 2^{2b+c}$. Hence,

$$\sum_{P \in \mathcal{P}_3} N(G,P) = 4(k-2)(2^{b+2c} + 2^{2b+c}).$$

Assume finally that $i = 4$. For each subpath P of C_{2k} which contains all four big vertices we have $N(G,P) = 2^{2b+2c}$. There are $2\left(3 + \binom{k-1}{2}\right)$ such paths, so

$$\sum_{P \in \mathcal{P}_4} N(G,P) = 2\left(3 + \binom{k-1}{2}\right) 2^{2b+2c}.$$

A similar analysis for graph H yields

$$\sum_{P\in\mathcal{P}_0} N(H,P) = 2\left(k-2+\binom{k-2}{2}\right),$$
$$\sum_{P\in\mathcal{P}_1} N(H,P) = 2(k-1)(2^b+2^c),$$
$$\sum_{P\in\mathcal{P}_2} N(H,P) = 2(k-1)^2 2^{b+c} + (2^{2b}+2^{2c}),$$
$$\sum_{P\in\mathcal{P}_3} N(H,P) = 2(k-1)(2^{b+2c}+2^{2b+c}),$$
$$\sum_{P\in\mathcal{P}_4} N(H,P) = 2\left(1+\binom{k}{2}\right)2^{2b+2c}.$$

After we have considered all possible cases where a path P belongs with respect to the partition $\mathcal{P}_i$ for $i = 0,\ldots,4$, we can summarize the results. It follows that

$$N(G) - N(H) = \sum_{i=0}^{4}\sum_{P\in\mathcal{P}_i}(N(G,P) - N(H,P)) =$$
$$= 3(2^b-2^c)^2 - 2(a-1)\left(2^c-1\right)\left(2^b-1\right)\left(2^{b+c}+1\right),$$

so multiplying this equality with -1 establishes Claim B.

Case 2. $n = 2a+2b+2c+5$. Notice that $n-1 = 2a+2b+2c+4$, so for $n-1$ let G and H be the graphs as we defined them in Case 1. Now, let G' be the graph obtained from G by attaching one additional pendant vertex at v_2. Also, let H' be the graph obtained from H by attaching one additional pendant vertex at v_1. Obviously, both G' and H' have precisely $n = 2a+2b+2c+5$ vertices.

Claim C. *It holds that* $W(H') - W(G') = (b-c)^2 - (b-c)$.

Denote by z the additional vertex of G' (resp. H'). Also, let V_G (resp. V_H) denote the set of vertices of G (resp. H) which is a subset of $V(G')$ (resp. $V(H')$). Notice that $W(G') = W(G) + d_G(z,V_G)$ and $W(H') = W(H) + d_H(z,V_H)$. By Claim A we know that $W(H) - W(G) = (b-c)^2$. Next, we wish to establish the relation between $d_G(z,V_G)$ and $d_H(z,V_H)$.

Recall that V_G (resp. V_H) is partitioned into sets A, B, C, D and O. It holds that

$$\begin{aligned}
d_G(z,A) - d_H(z,A) &= b,\\
d_G(z,B) - d_H(z,B) &= 0,\\
d_G(z,C) - d_H(z,C) &= -c,\\
d_G(z,D) - d_H(z,D) &= 0,\\
d_G(z,O) - d_H(z,O) &= 0.
\end{aligned}$$

We conclude that $d_G(z,V_G) - d_H(z,V_H) = b - c$. Now, we obtain

$$W(G')-W(H') = W(G)-W(H)+d_G(z,V_G)-d_H(z,V_H) = -(b-c)^2+b-c,$$

so Claim C is established.

Claim D. *It holds that*

$$\begin{aligned}
N(H') - N(G') = 9 \cdot 2^{b+c} - 3 \cdot 2^{2b} - 6 \cdot 2^{2c}\\
&- (a-1)(3 \cdot 2^{2b+c} + 4 \cdot 2^{b+2c} - 4 \cdot 2^{2b+2c}\\
&- 6 \cdot 2^{b+c} + 2 \cdot 2^b + 3 \cdot 2^c - 2).
\end{aligned}$$

We use the same approach and notation as in Claim B. For graph G' we obtain

$$\begin{aligned}
\sum_{P\in\mathcal{P}_0} N(G',P) &= 2\left(k-2+\binom{k-3}{2}\right),\\
\sum_{P\in\mathcal{P}_1} N(G',P) &= 2(k-2)(2^b+2^b+2^c+2^{c+1}),\\
\sum_{P\in\mathcal{P}_2} N(G',P) &= (k-2)^2(2^{b+c}+2^{b+c+1}) + 4(2^{2b}+2^{2c+1}),\\
\sum_{P\in\mathcal{P}_3} N(G',P) &= 4(k-2)(2^{b+2c+1}) + 2(k-2)(2^{2b+c+1}+2^{2b+c}),\\
\sum_{P\in\mathcal{P}_4} N(G',P) &= 2\left(3+\binom{k-1}{2}\right)2^{2b+2c+1}.
\end{aligned}$$

Similarly, for graph H' it holds that

$$\sum_{P\in\mathcal{P}_0} N(H',P) = 2\left(k-2+\binom{k-2}{2}\right),$$
$$\sum_{P\in\mathcal{P}_1} N(H',P) = (k-1)(2\cdot 2^b + 2^c + 2^{c+1}),$$
$$\sum_{P\in\mathcal{P}_2} N(H',P) = (k-1)^2(2^{b+c} + 2^{b+c+1}) + (2^{2b} + 2^{2c+1}),$$
$$\sum_{P\in\mathcal{P}_3} N(H',P) = (k-1)(2^{b+2c+1} + 2^{2b+c} + 2^{2b+c+1}),$$
$$\sum_{P\in\mathcal{P}_4} N(H',P) = 2\left(1+\binom{k}{2}\right)2^{2b+2c+1}.$$

After finishing considerations on $N(G',P)$ and $N(H',P)$ for all possible cases of P, we conclude that

$$\begin{aligned} N(G') - N(H') &= \sum_{i=0}^{4}\sum_{P\in\mathcal{P}_i}(N(G,P)-N(H,P)) \\ &= 3\cdot 2^{2b} + 6\cdot 2^{2c} - 9\cdot 2^{b+c} + (a-1)(3\cdot 2^{2b+c} \\ &\quad + 4\cdot 2^{b+2c} - 4\cdot 2^{2b+2c} - 6\cdot 2^{b+c} + 2\cdot 2^b + 3\cdot 2^c - 2), \end{aligned}$$

so Claim D is established. ■

After we have established the existence of graphs with precise values of the differences $W(H) - W(G)$ and $N(H) - N(G)$, this easily yields the following corollary which is the main result of this paper.

Corollary. *For every $n \geq 14$, there exist unicyclic graphs G and H, both on n vertices and with the same degree sequences, such that $W(G) < W(H)$ and $N(G) < N(H)$. Moreover, the differences $W(H)-W(G)$ and $N(H)-N(G)$ can be arbitrarily large given sufficiently large n.*

Proof. We distinguish two cases with respect to the parity of n.

Case 1. *n is even.* Let $a = 2$ and $b = 1$. Since $n \geq 14$, there exists $c \geq 2$ such that $n = 2a+2b+2c+4$. Theorem 1 implies that there exist unicyclic graphs G and H, each on n vertices and with the same degree sequence, such that

$$
\begin{aligned}
W(H) - W(G) &= (1-c)^2 \\
N(H) - N(G) &= 2\left(2^c - 1\right)\left(2^{1+c}+1\right) - 3(2-2^c)^2 = 2^{2c} + 10\cdot 2^c - 14.
\end{aligned}
$$

Since $c \geq 2$, we have $W(H) - W(G) > 0$, i.e. $W(G) < W(H)$. Moreover, if $n \to \infty$, then $c \to \infty$, from which we conclude that $W(H) - W(G)$ grows unbounded.

As for the difference of the subtree number, the expression $2^{2c} + 10\cdot 2^c - 14$ is increasing in c and for $c = 2$ it is equal to 42 which is positive. Hence, we conclude that $N(H) - N(G) > 0$ for every $c \geq 2$, i.e. $N(G) < N(H)$. Moreover, it obviously holds that $N(H) - N(G)$ tends to infinity as n tends to infinity, which proves the claim in this case.

Case 2. *n is odd.* Again, let $a = 2$ and $b = 1$. Since n is odd, we know that $n \geq 15$. Hence, there exists $c \geq 2$ such that $n = 2a + 2b + 2c + 5$. Theorem 1 implies that there exist unicyclic graphs G' and H', both on n vertices and with the same degree sequences, such that

$$
\begin{aligned}
W(H') - W(G') &= c\,(c-1)\,, \\
N(H') - N(G') &= 2\cdot 2^{2c} + 15\cdot 2^c - 14.
\end{aligned}
$$

Since $c \geq 2$, it is easily seen that both $W(H') - W(G') > 0$ and $N(H') - N(G')$. Moreover, both expressions $c\,(c-1)$ and $2\cdot 2^{2c} + 15\cdot 2^c - 14$ grow unbounded as c tends to infinity. Since $n \to \infty$ implies $c \to \infty$, we conclude that both differences $W(H) - W(G)$ and $N(H) - N(G)$ grow unbounded as the number of vertices n increases and we are finished. ■

In the above corollary we used the values $a = 2$ and $c \geq 2$. It is easily seen that the same conclusion holds for any fixed $a \geq 2$. Further, a graph G is *chemical* if the degrees of all vertices are at most 4. If we set $b = 1$ and $c = 2$, then Theorem 1 easily yields the following theorem.

Corollary. *Let $n \geq 16$. There exist chemical graphs G and H, both on n vertices and with the same degree sequence, such that $1 \leq W(H) - W(G) \leq 2$ and $N(H) - N(G)$ can be arbitrarily large given sufficiently large n.*

Another observation is that, from an asymptotic point of view (i.e., when the parameters a and b are "big") the key term for the subtree number is $8(a-1)\cdot 2^{4b}$ in the even case and $16(a-1)\cdot 2^{4b}$ in the odd case. Hence, it is straightforward to construct classes of unicyclic graphs G and H for which the indices W and N have different orderings. Specifically, if we attach pendent vertices to v_{k+2} instead of v_2 in G, and to v_{k+1} instead of v_1 in H, we obtain $W(G) = W(H) + 1$ in the even case and $W(G) = W(H) + 2$ in the odd case. Thus, we have $W(G) > W(H)$. However, because of the largest term in N, we get $N(G) < N(H)$.

To conclude, the graphs G and H we constructed belong to the family of unicyclic graphs. It would be interesting to investigate whether a similar construction can be developed for graphs with a prescribed number of cycles. More broadly, one might consider the case of graphs with a given cyclomatic number. A particularly natural case is that of acyclic graphs, i.e., trees.

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