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Differences between detour and Wiener indices

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Abstract

Let G be a connected graph and let $\mu(G) = DD(G) - W(G)$, where $DD(G)$ and $W(G)$ stand for the detour and Wiener numbers of G, respectively. Nadjafi-Arani et al. [Math. Comput. Model. 55 (2012), 1644–1648] classified connected graphs whose difference between Szeged and Wiener numbers are n, for $n = 4, 5$. In this paper, we continue their work to prove that for any positive integer $n \neq 1, 2, 4, 6$ there is a graph with $\mu(G) = n$.

1 Introduction

It is well-known that an important domain in chemical graph theory is distance properties of molecular graphs. A topological invariant is a numeric quantity from the molecular graph of a molecule based on distances between any pair of vertices, degrees of vertices, combination of distance and degree etc. Hosoya was the first scientist who proposed the term topological index for characterizing the topological nature of a graph [11]. The Wiener number or Wiener index is one of distance-based topological invariants. It has been researched from the purely mathematical viewpoint, giving rise to a vast corpus of literature over the last decades. We refer the reader to a comprehensive survey of results for trees by Dobrynin, Entringer and Gutman as an illustration of that effort [5]. For some of the numerous results obtained for the Wiener index, see for example [4, 6, 7, 8, 9, 12, 13, 14, 16, 21, 22, 23, 24].

The detour index, in contrast to the Wiener index that considers the length of the shortest path between vertices, considers the length of the longest distance between each pair of vertices. This topological index has recently received some attention in the chemical literature; see [1, 2, 3, 15, 18, 19, 20]. The detour index certainly carries some interesting structural information for cyclic compounds. For acyclic structures the Wiener and the detour indices are equal, since there is only a

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single possible path connecting any pair of vertices. Many methods and algorithms for computing the Wiener index of a graph have been proposed in the chemical literature. In recent years some mathematicians considered the relationship between Wiener index and other topological indices. For instance, Nadjafi-Arani et al. [17] computed the difference between Szeged and Wiener indices. They also constructed graphs whose difference between Szeged and Wiener indices is n, for a given integer n. In other words, they determined which numbers can be considered as the difference between these topological indices. We continue the mentioned work to compute the difference between detour and Wiener indices. In the next section, we give the necessary definitions and some preliminary results. Our last section contains the main results explicit formulas for the difference between Wiener and detour indices of connected graphs. Here, our notation is standard and mainly taken from standard books of graph theory such as [10].

2 Definitions and preliminaries

All graphs considered in this paper are simple and connected. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The distance $d_G(x, y)$ between two vertices x and y of $V(G)$ is defined as the length of any shortest path in G connecting x and y and the distance matrix $D = [d_{ij}]$ can be defined with entries $d_{ii} = 0$ and $d_{ij}, i \neq j$, as the distance between vertices v_i and v_j. By this notation the Wiener index is

$$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d_G(u, v).$$

The detour matrix was introduced in graph theory some time ago by F. Harary [6] for describing the connectivity in directed graphs. The detour matrix, in contrast to the distance matrix that records the length of the shortest path between vertices, records the length of the longest distance between each pair of vertices. The detour distance $dd_G(x, y)$ between two vertices x and y is defined as the length of a longest path in G connecting x and y. Then the detour index $DD(G)$ of a graph G is defined as

$$DD(G) = \frac{1}{2} \sum_{u,v \in V(G)} dd_G(u, v).$$

3 Main Results

In this section, at first we compute the differences between detour and Wiener indices of unicyclic graphs. The difference number of a graph G is denoted by $\mu(G)$ and it is defined as $\mu(G) = DD(G) - W(G)$. It is clear that $\mu(G) = 0$ if and only if G is a tree. So, in the whole of this section by a graph we mean a connected graph with at least one cycle. The detour and Wiener indices are integers and always detour index is greater than or equal to the Wiener index. This implies that for a given non acyclic connected graph G, $\mu(G) \geq 0$. We also prove that for every integer $n \neq 1, 2, 4, 6,$

there is a graph with $\mu(G) = n$. Suppose U_n is a unicyclic graph composed of a cycle on n vertices where any vertex of its cycle is the root of a tree with t_i vertices $t_i \geq 1$, see Figure 1. In the following theorem let $d^{'}(x, y) = dd(x, x) - d(x, x)$, T_i be a tree and $k_{T_i} - 1$ be the number of pendant vertices of T_i, $1 \leq i \leq n$.

Theorem 1 *Let U_n be a unicyclic graph. Then*

$$\mu(U_n) = A + B + C + D,$$

where

$$\begin{aligned}
A &= \frac{1}{2}\sum_{i=1}^{k}[\sum_{x_{T_i}\neq x, y\in(T_i,C)} d^{'}(x,y) + \sum_{x_{T_i}\neq x, y\in(k_{T_i},C)} d^{'}(x,y)],\\
B &= \frac{1}{2}\sum_{i,j=1, i\neq j}^{k}\ \sum_{x_{T_i}, x_{T_j}\neq x, y\in(T_i,k_{T_j})} d^{'}(x,y),\\
C &= \frac{n^2(n-1)}{2}\begin{cases}\frac{n^3}{4} & 2|n\\ \frac{n(n^2-1)}{4} & 2\nmid n\end{cases},\\
D &= \frac{1}{2}\sum_{i,j=1, i\neq j}^{k}[\sum_{x_{T_i}, x_{T_j}\neq x, y\in(T_i,T_j), i\neq j} d^{'}(x,y) + \sum_{x_{T_i}, x_{T_j}\neq x, y\in(k_{T_i},k_{T_j}), i\neq j} d^{'}(x,y)].
\end{aligned}$$

Proof. It is clear that $d'(x, y) = 0$ if and only if $dd(x, y) = d(x, y)$, if and only if x and y belong to the same trees. Then

$$\begin{aligned}
A &= \sum_{i=1}^{k}[(|T_i|-1)\sum_{x_{T_i}\neq y\in C}(n-2d(x_{T_i},y)) + (|K_{T_i}|-1)\sum_{x_{T_i}\neq y\in C}(n-2d(x_{T_i},y))],\\
B &= \sum_{i=1}^{k}[(|T_i|-1)(|k_{T_j}|-1)(n-2d(x_{T_i},x_{T_j})),\\
D &= \frac{1}{2}\sum_{i,j=1, i\neq j}^{k}[(|T_i|-1)(|T_j|-1) + (|k_{T_i}|-1)(|k_{T_j}|-1)](n-2d(x_{T_i},x_{T_j})).
\end{aligned}$$

This completes the proof.

Theorem 2 *Let G be a connected graph; then $\mu(G) \neq 1, 2, 4, 6$.*

Proof. It is clear that the cycle graph C_3 has the minimum non zero value of $\mu(G)$, namely 3. This implies that $\mu(G) \geq 3$. Clearly, the second minimum value of $\mu(G)$ holds in a unicyclic graph and this graph should have the shortest possible girth, namely 3. On the other hand, this graph must have the minimum possible number of vertices. Hence, if we add a new vertex in the middle of an edge, then the resulting graph is a square and so $\mu(G) = 8$. By adding a pendant edge to C_3, one can see that

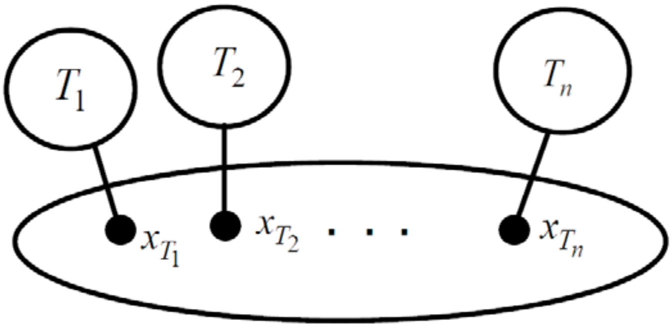

Figure 1: The general form of a unicyclic graph.

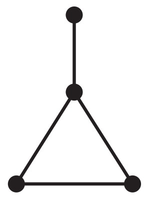

Figure 2: Graph $C_3 + e$.

$\mu(C_3 + e) = 5$ and this shows that for any graph G with $G \not\cong C_3$, we have $\mu(G) \geq 5$; see Figure 2.

We can also add a new pendant edge to the graph $C_3 + e$ depicted in Figure 2 and thus we achieve three graphs depicted in Figure 3.

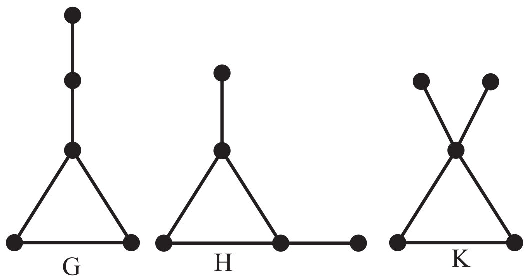

Figure 3: Three graphs obtained from $C_3 + e$.

The computation of $\mu(G)$ for all these graphs shows that $\mu(G) = \mu(H) = \mu(K) = 7$. By adding a new vertex to the middle of an edge of $C_3 + e$, we also construct a graph with $\mu(G) \geq 7$. Hence, for any unicyclic graph $G \not\cong C_3, C_3 + e$, we have $\mu(G) \geq 7$. Amongst all bicyclic graphs, it is sufficient to compute $\mu(G)$ for the graphs depicted in Figure 4.

For all graphs in Figure 4, $\mu(G)$ is greater than or equal to 7. If a graph has more than three cycles, clearly $\mu(G) \geq 7$ and this completes the proof.

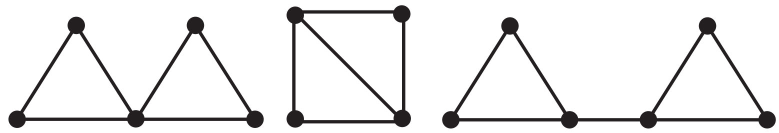

Figure 4: Three main bicyclic graphs in Theorem 2.

For $r, s \geq 0$, we denote by $U_n^{r,s}$ a complete graph on n vertices with r and s pendant vertices added to vertices u and v, respectively; see Figure 5.

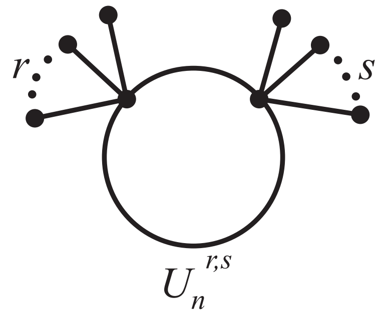

Figure 5: Graph $U_n^{r,s}$.

The proof of the following theorem is straightforward:

Theorem 3 *Let $r, s \geq 1$; then*

$$\mu(U_n^{r,s}) = (n-2)[n(n-1))/2 + (n-1)(r+s) + rs].$$

Corollary 1 *Let $s \geq 1$; then*

$$\mu(U_3^{r,s}) = 2(r+s) + rs + 3.$$

The general form of the graph $U_3^{r,s}$ in Corollary 1 is depicted in Figure 6. As a result of Corollary 1, one can prove that $\mu(U_3^{0,s}) = 2s + 3$. This implies that for any odd integer $n = 2k + 1$, $\mu(U_3^{0,k-1}) = n$.

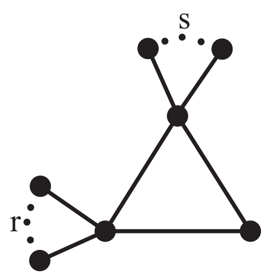

Figure 6: Graph $U_3^{r,s}$.

Theorem 4 *For any integer $n \geq 7$, there is a graph G where $\mu(G) = n$.*

Proof. Clearly, n mod 6 is one of the integers 0, 1, 2, 3, 4 and 5. If $n \equiv 1, 3, 5 \pmod 6$, then n is an odd number and by the last discussion, the proof is complete. In continuing, let n be an even integer; hence to complete the proof, we should consider the three following cases:

- **Case 1**. $n \equiv 0 \pmod 6$, $n \geq 8$. In this case $n = 6k$ for $k = 2, 3, \ldots$ and for the graph $G = U_4^{0,s}$ as depicted in Figure 8 with respect to Theorem 3, we have $\mu(G) = n$.

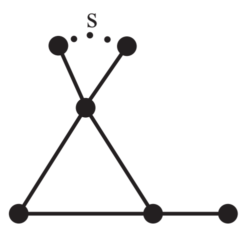

Figure 7: Graph $U_3^{1,s}$.

- **Case 2**. $n \equiv 2 \pmod 6$, $n \geq 8$. In this case $n = 6k + 2$ for $k = 1, 2, \ldots$ and by using Corollary 1, for the graph $U_3^{1,s}$ depicted in Figure 7, we have:

$$\mu(U_3^{1,2k-1}) = 6k + 2 = n$$

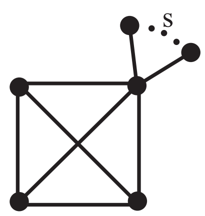

Figure 8: Graph $U_4^{0,s}$.

- **Case 3**. $n \equiv 4 \pmod 6$, $n \geq 28$. In this case $n = 6k + 4$ for $k = 4, 5, \ldots$ and for the graph E depicted in Figure 9, we have $\mu(E) = n$.

To complete the proof, it remains to obtain graphs G with $\mu(G) = 10, 16, 22$. One can see that $\mu(K_4/e) = 10$ and for graphs H and K depicted in Figure 10, we have $\mu(H) = 16, \mu(K) = 22$. This completes the proof.

Theorem 4 implies that for a given integer $n \neq 1, 2, 4, 6$, there is a graph G with $\mu(G) = n$. It should be noted that these graphs are not unique. In other words, there are many graphs, except the graphs mentioned in Figures 1–10, with $\mu(G) = n$. For example, for $n = 23$, there are two non isomorphic graphs $C_5 + e$, $U_3^{0,10}$ such that $\mu(C_5 + e) = \mu(U_3^{0,10}) = 23$.

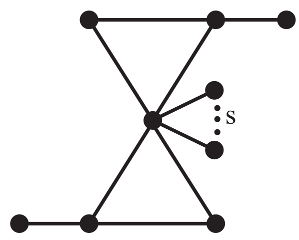

Figure 9: Graph E.

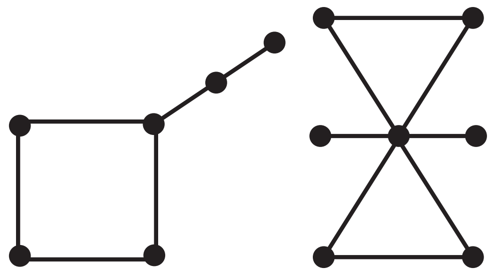

Figure 10: Graphs H and K in Theorem 4.

Lemma 1 *Let G be a graph with k blocks, all of them being complete graphs and intersecting in a common vertex, as depicted in Figure 11. Then*

$$\mu(G) = \sum_{i=1}^{k} \binom{n_i}{2}(n_i - 2) + \sum_{i,j=1, i \neq j}^{k} (n_j - 1)(n_i - 2),$$

where every block has n_i vertices, $i = 1, 2, \ldots, k$.

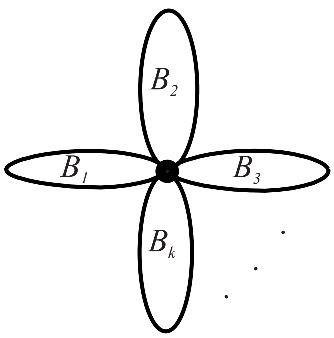

Figure 11: A graph with k blocks intersects in a common vertex.

4 Conclusion

Let $\mu(G)$ be the difference between detour and Wiener indices. In this paper, we have proved that for any integer $n \notin \{1, 2, 4, 6\}$ there is a graph with $\mu(G) = n$. We have also shown that for a given integer n, the graph G with $\mu(G) = n$ cannot be determined uniquely.

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