An inequality between the edge-Wiener index and the Wiener index of a graph

Martin Knor [a,b], **Riste Škrekovski** [b,c,d],
Aleksandra Tepeh [b,e]

[a] *Slovak University of Technology in Bratislava, Faculty of Civil Engineering, Department of Mathematics, Radlinského 11, 813 68, Bratislava, Slovakia,*
`knor@math.sk`

[b] *Faculty of Information Studies, 8000 Novo Mesto, Slovenia,*
[c] *FAMNIT, University of Primorska, 6000 Koper, Slovenia,*
[d] *Faculty of Mathematics and Physics, University of Ljubljana, 1000 Ljubljana,*
`skrekovski@gmail.com`

[e] *Faculty of Electrical Engineering and Computer Science, University of Maribor, Smetanova ulica 17, 2000 Maribor, Slovenia,*
`aleksandra.tepeh@gmail.com`

Abstract

The Wiener index $W(G)$ of a connected graph G is defined to be the sum $\sum_{u,v} d(u,v)$ of distances between all unordered pairs of vertices in G. Similarly, the edge-Wiener index $W_e(G)$ of G is defined to be the sum $\sum_{e,f} d(e,f)$ of distances between all unordered pairs of edges in G, or equivalently, the Wiener index of the line graph $L(G)$. Wu [37] showed that $W_e(G) \geq W(G)$ for graphs of minimum degree 2, where equality holds only when G is a cycle. Similarly, in [24] it was shown that $W_e(G) \geq \frac{\delta^2-1}{4} W(G)$ where δ denotes the minimum degree in G. In this paper, we extend/improve these two results by showing that $W_e(G) \geq \frac{\delta^2}{4} W(G)$ with equality satisfied only if G is a path on 3 vertices or a cycle. Besides this, we also consider the upper bound for $W_e(G)$ as well as the ratio $\frac{W_e(G)}{W(G)}$. We show that among graphs G on n vertices $\frac{W_e(G)}{W(G)}$ attains its minimum for the star.

Keywords: Wiener index, Gutman Index, Line graph

1 Introduction

For a graph G, let $\deg(u)$ and $d(u,v)$ denote the degree of a vertex $u \in V(G)$ and the distance between vertices $u, v \in V(G)$, respectively. Let $L(G)$ denote the line graph of

G, that is, the graph with vertex set $E(G)$ and two distinct edges $e, f \in E(G)$ adjacent in $L(G)$ whenever they share an end-vertex in G. Furthermore, for $e, f \in E(G)$, we let $d(e, f)$ denote the distance between e and f in the line graph $L(G)$.

In this paper we consider three important graph invariants, called *Wiener index* (denoted by $W(G)$ and introduced in [36]), *edge-Wiener index* (denoted by $W_e(G)$ and introduced in [21]) and *Gutman index* (denoted by $\mathrm{Gut}(G)$ and introduced in [12]), which are defined as follows:

$$\begin{aligned} W(G) &= \sum_{\{u,v\} \subseteq V(G)} d(u, v), \\ W_e(G) &= \sum_{\{e,f\} \subseteq E(G)} d(e, f), \\ \mathrm{Gut}(G) &= \sum_{\{u,v\} \subseteq V(G)} \deg(u) \deg(v)\, d(u, v). \end{aligned}$$

Observe that the edge-Wiener index of G is nothing but the Wiener index of the line graph $L(G)$ of G. Note also that in the literature a slightly different definition of the edge-Wiener index is sometimes used; for example, in [20] edge-Wiener index is defined to be $W_e(G) + \binom{n}{2}$ where $W_e(G)$ is defined as above and n is the order of G.

The Wiener index and related distance-based graph invariants have found extensive application in chemistry, see for example [14, 15, 34], and [2, 8, 16, 17, 18, 30, 31] for some recent studies. The Wiener index of a graph was investigated also from a purely graph-theoretical point of view (for early results, see for example [9, 33], and [4, 25, 26, 38] for some surveys). Generalizations of Wiener index and relationships between these were studied in a number of papers (see for example [3, 5, 6, 20]), and relationships between generalized graph entropies and the Wiener index (among other related topological indices) were established in [28]. New results on the Wiener index are constantly being reported, see for instance [10, 19, 23, 29, 35] for recent research trends.

Wu [37] showed that $W_e(G) \geq W(G)$ for graphs of minimum degree 2 where equality holds only when G is a cycle. Similarly, in [24] it was shown that $W_e(G) \geq \frac{\delta^2 - 1}{4} W(G)$ where δ denotes the minimum degree in G. In this paper, we improve these two results by showing that $W_e(G) \geq \frac{\delta^2}{4} W(G)$ with equality satisfied only if G is a path on 3 vertices or a cycle. One of the closely related distance-based graph invariant is the Szeged index [11], and a relation between the Szeged index and its edge version was recently established in [27].

In [3] it was proved that $W_e(G) \leq \frac{2^2}{5^5} + O(n^{9/2})$ for graphs of order n. Using the result of [32] we improve this bound to $W_e(G) \leq \frac{2^2}{5^5} + O(n^4)$. We also consider the ratio $\frac{W_e(G)}{W(G)}$ and show that this ratio is minimum if G is the star S_n on n vertices. Consequently, if G is a graph on n vertices, then $\frac{W_e(G)}{W(G)} \geq \frac{n-2}{2(n-1)}$.

2 Distances, average distance and D_α relations

Note that for any two distinct edges $e = u_1u_2$ and $f = v_1v_2$ in $E(G)$, the distance between e and f equals

$$d(e, f) = \min\{d(u_i, v_j) : i, j \in \{1, 2\}\} + 1. \tag{1}$$

In the case when e and f coincide, we have $d(e, f) = 0$. In addition to the distance between two edges we will also consider the *average distance* between the endpoints of two edges, defined by

$$s(u_1u_2, v_1v_2) = \frac{1}{4}\big(d(u_1, v_1) + d(u_1, v_2) + d(u_2, v_1) + d(u_2, v_2)\big).$$

Notice that $s(e,f) = \frac{1}{2}$ when e and f coincide. The average distance of endpoints is in an interesting relationship with the Gutman index of a graph. Namely, if one likes to consider the version of edge-Wiener index where the distances between edges are replaced by the average distances of their endpoints, then what one gets is essentially the Gutman index, see Lemma 1.

A variation to the following result was mentioned in [24, 37], where the sum in (2) is taken over all ordered pairs of edges. In our case the sum runs over all 2-element subsets of $E(G)$.

Lemma 1. *Let G be a connected graph. Then*

$$\sum_{\{e,f\}\subseteq E(G)} s(e,f) = \frac{1}{4}\Big(\mathrm{Gut}(G) - |E(G)|\Big). \tag{2}$$

Proof. Consider the sum on the left-hand side of (2). We can rewrite it as

$$\frac{1}{4}\sum_{\{uw,vz\}\subseteq E(G)} \Big(d(u,v) + d(u,z) + d(w,v) + d(w,z)\Big)\,.$$

Now, for any two non-adjacent vertices of G, say u and v, the distance $d(u,v)$ appears in the above sum precisely once for each pair of edges, where one of these edges is incident with u and the other is incident with v. Thus, $d(u,v)$ appears in total precisely $\deg(u)\cdot\deg(v)$ times. And, if u and v are two adjacent vertices of G, then the distance $d(u,v) = 1$ appears in that sum precisely $\deg(u)\cdot\deg(v) - 1$ times. Thus, the above sum equals

$$\frac{1}{4}\Big[\sum_{uv\notin E(G)} \deg(u)\deg(v)d(u,v) + \sum_{uv\in E(G)} \Big(\deg(u)\deg(v) - 1\Big)d(u,v)\Big],$$

which is the right-hand side of (2). □

Now we define the following notions. Let G be a graph. For a pair of edges e and f of G we define the *difference*

$$D(e,f) = d(e,f) - s(e,f).$$

Moreover, if $D(e,f) = \alpha$, we say that e, f form a pair of type D_α or that the pair e, f *belongs to the set* D_α. Note that if $e = f$, then $D(e,f) = -\frac{1}{2}$. Denote by $\mathcal{I}$ the set $\{0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1\}$. Note that $\sum_{\alpha\in\mathcal{I}} |D_\alpha| = \binom{|E(G)|}{2}$. Next easy lemma shows that $D(e,f) \in \mathcal{I}$ whenever $e \neq f$.

Lemma 2. *In a connected graph, every pair of distinct edges belongs to D_α for some $\alpha \in \mathcal{I}$.*

Proof. Let $e = u_1u_2$ and $f = v_1v_2$ be two distinct edges. We may assume that

$$d(u_1, v_1) = \min_{i,j\in\{1,2\}} \{d(u_i, v_j)\}\,.$$

Let $k = d(u_1, v_1)$. Notice that

$$d(u_1, v_2), d(u_2, v_1) \in \{k, k+1\} \qquad \text{and} \qquad d(u_2, v_2) \in \{k, k+1, k+2\}.$$

If $d(u_2, v_2) = k + 2$, then it must hold $d(u_1, v_2) = d(u_2, v_1) = k + 1$, and hence $D(e, f) = 0$, which means that the pair e, f belongs to D_0. So, in the sequel, we assume that $d(u_2, v_2) = k$ or $k + 1$. Suppose $d(u_1, v_2) = d(u_2, v_1) = k$. If $d(u_2, v_2) = k$, then the pair e, f belongs to D_1. And, if $d(u_2, v_2) = k + 1$ then the pair e, f belongs to $D_{\frac{3}{4}}$. Suppose now that $d(u_1, v_2) = k + 1$ and $d(u_2, v_1) = k$. If $d(u_2, v_2) = k$, then again the pair e, f belongs to $D_{\frac{3}{4}}$. On the other hand, if $d(u_2, v_2) = k + 1$, then the pair e, f belongs to $D_{\frac{1}{2}}$. We argue similarly if $d(u_1, v_2) = k$ and $d(u_2, v_1) = k+1$. Finally, suppose that $d(u_1, v_2) = d(u_2, v_1) = k + 1$. If $d(u_2, v_2) = k$, the pair e, f belongs to $D_{\frac{1}{2}}$. If $d(u_2, v_2) = k + 1$, the pair e, f belongs to $D_{\frac{1}{4}}$. □

To prove our main result we will have to distinguish two possibilities for $\alpha = \frac{1}{2}$. If (according to the notation in the proof of Lemma 2) $d(u_1, v_1) = d(u_2, v_2) = k$ and $d(u_1, v_2) = d(u_2, v_1) = k + 1$ then we say that the pair belongs to $D'_{\frac{1}{2}}$, and if $d(u_1, v_1) = d(u_2, v_1) = k$ and $d(u_1, v_2) = d(u_2, v_2) = k + 1$, we say that the pair belongs to $D''_{\frac{1}{2}}$. In Figure 1, where all different configurations of pairs of edges are presented, full lines represent the edges u_1u_2 and v_1v_2.

Proposition 3. *Let G be a connected graph. Then*

$$W_e(G) = \frac{\mathrm{Gut}(G)}{4} - \frac{|E(G)|}{4} + |D_1| + \frac{1}{4}|D_{\frac{1}{4}}| + \frac{1}{2}|D_{\frac{1}{2}}| + \frac{3}{4}|D_{\frac{3}{4}}|. \tag{3}$$

Proof. By Lemma 1, we have

$$\begin{aligned} W_e(G) &= \sum_{\{e,f\}\subseteq E(G)} d(e, f) \\ &= \sum_{\{e,f\}\subseteq E(G)} s(e, f) + \sum_{\{e,f\}\subseteq E(G)} D(e, f) \\ &= \frac{\mathrm{Gut}(G)}{4} - \frac{|E(G)|}{4} + \sum_{\{e,f\}\subseteq E(G)} D(e, f)\,. \end{aligned}$$

Now, as every pair e, f belongs to precisely one of D_α for some $\alpha \in \mathcal{I}$, we have

$$\sum_{\{e,f\}\in E(G)} D(e, f) = 0 \cdot |D_0| + \frac{1}{4} \cdot |D_{\frac{1}{4}}| + \frac{1}{2} \cdot |D_{\frac{1}{2}}| + \frac{3}{4} \cdot |D_{\frac{3}{4}}| + 1 \cdot |D_1|,$$

and the proof follows. □

3 Bounds for $W_e(G)$

Klavžar and Lipovec [22] proved the following result.

Lemma 4. *Let G be a 2-connected graph that is not a cycle. Then G contains two isometric cycles $C_1 = u_1u_2 \dots u_ku_{k+1} \dots u_ru_1$ and $C_2 = u_1u_2 \dots u_kv_{k+1} \dots v_su_1$, where $r \geq s > k \geq 2$ and $v_i \neq u_j$ for $i, j \geq k+1$.*

Note that the path $S = u_1u_2 \dots u_k$ cannot contain more than half of the edges of one of the cycles C_1 and C_2, otherwise the other cycle would not be isometric. Thus S is a shortest path among the three paths between u_1 and u_k in $C_1 \cup C_2$, and as such it is isometric (otherwise again a contradiction is obtained with C_1 and C_2 being isometric). This fact will be of use in the proof of the next lemma.

Lemma 5. *In a 2-connected graph G, we have*

$$2|D'_{\frac{1}{2}}| + |D_{\frac{1}{4}}| \geq |E(G)|. \tag{4}$$

Moreover, equality holds if and only if G is a cycle.

Proof. Let G be a 2-connected graph. It is well-known that if an edge $e = xy$ belongs to a cycle, then it must belong to an isometric cycle. (In order to obtain such a cycle just take the edge e and a shortest path distinct from the path e connecting x and y, which must exist since xy lies on a cycle.) Let E_0 (resp. E_1) be the set of edges that belong to some isometric cycle in G of even (resp. odd) length. Since $|E(G)| = |E_0| + |E_1| - |E_0 \cap E_1|$, we have $|E(G)| \leq |E_0| + |E_1|$.

Notice that if e is an edge of an even isometric cycle C, and e' is its antipodal edge on C, then the pair e, e' belongs to $D'_{\frac{1}{2}}$. Let G_0 be a graph such that $V(G_0) = E_0$ and two vertices are adjacent in G_0 if the corresponding edges in G belong to a pair in $D'_{\frac{1}{2}}$. This gives us

$$|E_0| = |V(G_0)| \leq \sum_{v \in V(G_0)} \deg(v) = 2|E(G_0)| = 2|D'_{\frac{1}{2}}|, \tag{5}$$

as every vertex in $V(G_0)$ is of degree at least 1, since every edge of E_0 is at least in some pair of $D'_{\frac{1}{2}}$.

Similarly, if e is an edge of an odd isometric cycle C, and e_1, e_2 are antipodal edges of e, then the pairs e, e_1 and e, e_2 belong to $D_{\frac{1}{4}}$. Defining a graph G_1 with $V(G_1) = E_1$ and two vertices being adjacent in G_1 if the corresponding edges in G belong to a pair in $D_{\frac{1}{4}}$, we get

$$2|E_1| = 2|V(G_1)| \leq \sum_{v \in V(G_1)} \deg(v) = 2|E(G_1)| = 2|D_{\frac{1}{4}}|, \tag{6}$$

since every vertex in $V(G_1)$ is of degree at least 2, as every edge of E_1 is at least in two pairs of $D_{\frac{1}{4}}$. Thus $|E_1| \leq |D_{\frac{1}{4}}|$ and $2|D'_{\frac{1}{2}}| + |D_{\frac{1}{4}}| \geq |E_0| + |E_1| \geq |E(G)|$.

If G is an even cycle, we clearly have $|E_0| = 2|D'_{\frac{1}{2}}|$ and $|E_1| = 0$, and if G is an odd cycle, then $|E_1| = |D_{\frac{1}{4}}|$ and $|E_0| = 0$. Thus, if G is a cycle, we have equality in (4). Now, we show that as soon as G is not a cycle, strict inequality holds in (4). By Lemma 4, there exist two different isometric cycles C and C' such that $C \cap C'$ is a path of length at least one. Denote this path by S and let u_1u_2 be the first edge on this path.

If one of the cycles C and C' is even and the other is odd, we have $u_1u_2 \in E_0 \cap E_1$, thus $|E(G)| < |E_0| + |E_1|$, which readily implies $|E(G)| < 2|D'_{\frac{1}{2}}| + |D_{\frac{1}{4}}|$.

Now assume that both C and C' are even. Observe that every pair of edges that lie on an isometric path belongs to D_0. Thus, since S is isometric, the edge that is antipodal to the edge u_1u_2 on C (C', respectively) belongs to $C \setminus S$ ($C' \setminus S$, respectively). This means that the degree of the vertex in G_0 that corresponds to u_1u_2 is at least 2, which implies strict inequality in (5), i.e $|E_0| < 2|D'_{\frac{1}{2}}|$ and thus $|E(G)| \leq |E_0| + |E_1| < 2|D'_{\frac{1}{2}}| + |D_{\frac{1}{4}}|$.

Similarly, if both C and C' are odd, we observe that the two antipodal edges of u_1u_2 in C are different from the antipodal edges of u_1u_2 in C'. This yields a strict inequality in (6) (since the vertex corresponding to u_1u_2 is of degree at least 4 in G_1) and the result follows. □

To prove the main theorem in case of regular graphs the following observation will be needed.

Lemma 6. *Suppose that $G \neq K_2$ is a regular graph containing bridges. Then every end-block of G contains an edge e such that for every bridge b the pair e, b is in $D''_{\frac{1}{2}}$.*

Proof. Let G be a regular graph of degree k. Since $G \neq K_2$, we have $k \geq 2$. Let B be an end-block, and let v be the cut-vertex incident with B. Since $k \geq 2$, B contains at least 3 vertices. Moreover, all vertices of B are of degrees k in B except v.

We claim that B is a non-bipartite graph. Suppose to the contrary that B is bipartite with bipartition L, R of $V(B)$. Assume that $v \in R$. Then $k|L| = |E(B)| = k(|R| - 1) + \deg_B(v)$, which implies that k divides $\deg_B(v)$, a contradiction.

For each $i \geq 0$, denote by L_i the vertices of B at the distance i from v. As B is non-bipartite, some L_i will contain adjacent vertices. Hence, there is an edge $e = u_1u_2$ of B with $d(u_1, v) = d(u_2, v)$.

Now we will show that e is the required edge. For any bridge $b = v_1v_2$ notice that $d(v_1, v) \neq d(v_2, v)$, otherwise we obtain that b lies on a cycle. So, we may assume that $d(v_1, v) = d(v_2, v) + 1$. As B is an end-block attached to the rest of the graph at v, every shortest path from a vertex of B to a vertex in $G - B$ must contain the vertex v. Hence

$$d(u_1, v_2) = d(u_1, v) + d(v, v_2) = d(u_2, v) + d(v, v_2) = d(u_2, v_2),$$

and similarly, $d(u_1, v_1) = d(u_2, v_1)$. Thus,

$$d(u_1, v_2) = d(u_2, v_2) = d(u_1, v_1) - 1 = d(u_2, v_1) - 1,$$

and hence the pair e, b is in $D''_{\frac{1}{2}}$. □

Now we are ready to prove the main result.

Theorem 7. *Let G be a connected graph of minimum degree δ. Then,*

$$W_e(G) \geq \frac{\delta^2}{4} W(G) \tag{7}$$

with equality holding if and only if G is isomorphic to a path on three vertices or a cycle.

Proof. We distinguish two cases.

Case 1: *G is non-regular.*

Then G has a vertex $w \in V(G)$ of degree at least $\delta+1$. By Proposition 3, we have

$$\begin{aligned}
4W_e(G) &= \operatorname{Gut}(G) - |E(G)| + 4|D_1| + |D_{\frac{1}{4}}| + 2|D_{\frac{1}{2}}| + 3|D_{\frac{3}{4}}| \\
&\geq \operatorname{Gut}(G) - |E(G)| \\
&\geq \delta^2 \sum_{\{u,v\}\in V(G)\setminus\{w\}} d(u,v) + (\delta+1) \sum_{u\in V(G)\setminus\{w\}} \deg(u) d(u,w) - |E(G)| \\
&\geq \delta^2 W(G) + \sum_{u\in V(G)\setminus\{w\}} \deg(u) - |E(G)| \\
&\geq \delta^2 W(G).
\end{aligned}$$

Note that in order to obtain equality in (7), no edge lies on a cycle by Lemma 5, otherwise we have $|D_{\frac{1}{4}}| > 0$ or $|D'_{\frac{1}{2}}| > 0$. This implies that G is a tree, and so $\delta = 1$. Moreover, each edge is incident with w, as we need that $\sum_{u\in V(G)\setminus\{w\}} \deg(u) = |E(G)|$, which implies that G is a star. And finally, we need $\deg(w) = \delta + 1 = 2$, which implies that G is isomorphic to P_3. This establishes the case.

Case 2: *G is regular.*

Let B be the set of bridges of G and let E_c be the set of edges of G that lie on at least one cycle. Then $E(G) = B \cup E_c$ and $B \cap E_c = \emptyset$. One can check that if a pair of edges belongs to $D'_{\frac{1}{2}}$ or $D_{\frac{1}{4}}$, then this pair belongs to the same block. Now, applying Lemma 5 to every nontrivial block of G, i.e. to every block containing a cycle, we obtain cumulatively that

$$2|D'_{\frac{1}{2}}| + |D_{\frac{1}{4}}| \geq |E_c|.$$

If G has bridges, i.e. if $B \neq \emptyset$, then G has at least two end-blocks. Now, Lemma 6 assures the existence of two distinct edges e' and e'' such that for every bridge b each of the pairs b, e' and b, e'' belongs to $D''_{\frac{1}{2}}$. So we have

$$|D''_{\frac{1}{2}}| \geq 2|B|.$$

Now, starting with the equality (3) and using the fact that $\operatorname{Gut}(G) = \delta^2 W(G)$ for regular graphs, we obtain

$$\begin{aligned}
4W_e(G) &= \operatorname{Gut}(G) - |E(G)| + 4|D_1| + |D_{\frac{1}{4}}| + 2|D_{\frac{1}{2}}| + 3|D_{\frac{3}{4}}| \\
&= \delta^2 W(G) - |E_c| - |B| + 4|D_1| + |D_{\frac{1}{4}}| + 2|D'_{\frac{1}{2}}| + 2|D''_{\frac{1}{2}}| + 3|D_{\frac{3}{4}}| \\
&\geq \delta^2 W(G) - |E_c| - |B| + 4|D_1| + |E_c| + 4|B| + 3|D_{\frac{3}{4}}| \\
&= \delta^2 W(G) + 4|D_1| + 3|B| + 3|D_{\frac{3}{4}}| \\
&\geq \delta^2 W(G)\,.
\end{aligned}$$

Note that in order to obtain equality in (7), $B = \emptyset$, i.e., G must have no bridges. So there are no trivial blocks in G. Next, in order to have the equality, by Lemma 5 every nontrivial block must be a cycle. This means that all blocks of G are cycles. Consequently, since G is regular, we conclude that G is a cycle. □

Now we consider the upper bound for $W_e(G)$. In [32] we have the following theorem:

Theorem 8. *Let G be a connected graph on n vertices. Then*

$$\mathrm{Gut}(G) \leq \frac{2^4}{5^5}n^5 + O(n^4).$$

Using this theorem we prove the following statement.

Theorem 9. *Let G be a connected graph on n vertices. Then*

$$W_e(G) \leq \frac{2^2}{5^5}n^5 + O(n^4).$$

Proof. For all pairs of edges $e, f \in E(G)$ and for all u_i, v_j, where $e = u_1u_2$, $f = v_1v_2$ and $i, j \in \{1, 2\}$, we sum the distances $d_{L(G)}(e, f)$. In this way we get $4W_e(G)$. Now we group these distances according to the pairs u_i, v_j. That is, for all pairs of vertices $u, v \in V(G)$ (including the pairs of identical vertices) we take all edges e incident to u, all edges f incident to v, and we sum $d_{L(G)}(e, f)$. Let e be an edge incident to u and let f be an edge incident to v. Then

$$d_{L(G)}(e, f) \leq d_G(u, v) + 1.$$

By $c(u, v)$ we denote the sum $\sum_{e,f} d_{L(G)}(e, f)$ taken over all edges e, f such that e is incident with u and f is incident with v. Then

$$c(u, v) = \sum_{e,f} d_{L(G)}(e, f) \leq \deg(u)\deg(v)\Big(d_G(u, v) + 1\Big).$$

By Theorem 8, we have

$$\begin{aligned}
4W_e(G) &= \sum_{u \neq v} c(u, v) + \sum_{u} c(u, u) \\
&\leq \sum_{u \neq v} \deg(u)\deg(v)\Big(d_G(u, v) + 1\Big) + \sum_{u} (\deg(u))^2 \cdot 1 \\
&\leq \mathrm{Gut}(G) + \sum_{u \neq v} \deg(u)\deg(v) + \sum_{u} (\deg(u))^2 \\
&\leq \frac{2^4}{5^5}n^5 + O(n^4) + O(n^4) + O(n^3) \\
&= \frac{2^4}{5^5}n^5 + O(n^4).
\end{aligned}$$

□

4 A lower bound for $W_e(G)/W(G)$

The problem of finding the graphs on n vertices, whose line graph has maximal Wiener index (i.e. whose edge-Wiener index is maximal) was given by Gutman [13] (see also [7]). Moreover, Dobrynin and Mel'nikov [7] proposed to estimate the ratio $W(L^i(G))/W(G)$, where $L^i(G)$ stands for an *iterated line graph*, defined inductively as

$$L^i(G) = \begin{cases} G & \text{if } i = 0, \\ L(L^{i-1}(G)) & \text{if } i > 0. \end{cases}$$

In this section we consider the case $i = 1$ and give a tight lower bound for $\frac{W_e(G)}{W(G)}$.

We need two well-known results. While the first one is already a folklore (and follows from a result in [9]), the second was proved by Buckley in [1].

Theorem 10. *Among all trees on n vertices, the star S_n has the smallest Wiener index.*

Theorem 11. *If T is a tree on n vertices, $n \geq 2$, then $W_e(T) = W(T) - \binom{n}{2}$.*

Now we are able to prove our lower bound.

Theorem 12. *Among all connected graphs on n vertices, the fraction $\frac{W_e(G)}{W(G)}$ is minimum for the star S_n, in which case $\frac{W_e(G)}{W(G)} = \frac{n-2}{2(n-1)}$.*

Proof. First we prove that if G is not a tree, then $\frac{W_e(G)}{W(G)} \geq \frac{1}{2}$. Thus, assume that G is not a tree. We start with the following claim.

Claim 1. *There is $f : V(G) \to E(G)$ such that for every $v \in V(G)$ the edge $f(v)$ is incident with v and $f(u) \neq f(v)$ whenever $u \neq v$.*

By Claim 1, G has a collection of n edges that can be considered as a system of distinct representatives for the vertices in such a way, that a vertex and an edge representing the vertex must be incident.

Proof of Claim 1. We start with trees. Since trees have only $n-1$ edges, they cannot satisfy Claim 1. However, for every tree T and for every vertex $v_0 \in V(T)$, one can find $f : V(T) \setminus \{v_0\} \to E(T)$ satisfying Claim 1. To see this, it suffices to set $f(v)$ to be the first edge of the unique v, v_0-path in T.

Now let e_0 be an edge of G such that deleting e_0 results in a connected graph. Further, let T be a spanning tree of G which does not contain e_0. Denote by v_0 a vertex incident with e_0 in G and construct $f : V(T) \setminus \{v_0\} \to E(T)$ as described above. Then the extension of f to $V(T) = V(G)$ by setting $f(v_0) = e_0$ satisfies Claim 1.

Now we proceed with the proof of Theorem 12. Consider a function f satisfying Claim 1. We have

$$W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d_{L(G)}(e, f) \geq \sum_{\{u,v\} \subseteq V(G)} d_{L(G)}(f(u), f(v)),$$

where the sums are taken over all pairs of distinct elements of $E(G)$ and $V(G)$, respectively. Hence,

$$\frac{W_e(G)}{W(G)} \geq \frac{\sum\limits_{\{u,v\} \subseteq V(G)} d_{L(G)}(f(u), f(v))}{\sum\limits_{\{u,v\} \subseteq V(G)} d_G(u, v)}.$$

The fraction on the right-hand side is the smallest when the denominator is as big as possible compared with the numerator. Since $d_{L(G)}(f(u), f(v)) \geq d_G(u, v) - 1$, that is $d_G(u, v) \leq d_{L(G)}(f(u), f(v)) + 1$, we get

$$\frac{W_e(G)}{W(G)} \geq \frac{\sum\limits_{\{u,v\} \subseteq V(G)} d_{L(G)}(f(u), f(v))}{\sum\limits_{\{u,v\} \subseteq V(G)} (d_{L(G)}(f(u), f(v)) + 1)}.$$

Since $f(u) \neq f(v)$ whenever $u \neq v$, we have $d_{L(G)}(f(u), f(v)) \geq 1$, which gives $\frac{W_e(G)}{W(G)} \geq \frac{1}{2}$.

Thus, assume that G is a tree. By Theorem 11, we have

$$\frac{W_e(G)}{W(G)} = \frac{W(G) - \binom{n}{2}}{W(G)}.$$

Hence, $\frac{W_e(G)}{W(G)}$ achieves its minimum for a tree with the minimum Wiener index. Since $W(S_n) = 2\binom{n-1}{2} + (n-1) = (n-1)^2$, Theorem 10 completes the proof. $\square$

Acknowledgment. The first author acknowledges partial support by Slovak research grants VEGA 1/0781/11, VEGA 1/0065/13 and APVV 9223-10. All authors are partially supported by Slovenian research agency ARRS, program no. P1–00383, project no. L1–4292, and Creative Core–FISNM–3330-13-500033.

References

[1] F. Buckley, Mean distance in line graphs, *Congr. Numer.* **32** (1981) 153–162.

[2] A. S. Çevik, A. D. Maden, New distance-based graph invariants and relations among them, *Appl. Math. Comput.* **219** (2013) 11171–11177.

[3] P. Dankelmann, I. Gutman, S. Mukwembi, H. C. Swart, The edge-Wiener index of a graph, *Discrete Math.* **309** (2009) 3452–3457.

[4] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[5] A. A. Dobrynin, L. S. Mel'nikov, Some results on the Wiener index of iterated line graphs, *Electronic Notes in Discrete Math.* **22** (2005) 469–475.

[6] A. A. Dobrynin, L. S. Mel'nikov, Wiener index for graphs and their line graphs with arbitrary large cyclomatic numbers, *Appl. Math. Lett.* **18** (2005) 307–312.

[7] A. A. Dobrynin, L. S. Mel'nikov, Wiener index of line graphs, in I. Gutman, B. Furtula (Eds.) *Distance in Molecular Graphs-Theory*, Univ. Kragujevac, Kragujevac (2012) 85–121.

[8] W. Du, X. Li, Y. Shi, Algorithms and extremal problem on Wiener polarity index, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 235–244.

[9] R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, *Czechoslovak Math. J.* **26** (1976) 283–296.

[10] C. M. da Fonseca, M. Ghebleh, A. Kanso, D. Stevanović, Counterexamples to a conjecture on Wiener index of common neighborhood graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 333–338.

[11] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes New York* **27** (1994) 9–15.

[12] I. Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1087–1089.

[13] I. Gutman, Distance of line graphs, *Graph Theory Notes N. Y.* **31** (1996) 49–52.

[14] I. Gutman, Y. N. Yeh, S. L. Lee, Y. L. Luo, Some recent results in the theory of the Wiener number, *Indian J. Chem.* **32 A** (1993) 651–661.

[15] I. Gutman, I. G. Zenkevich, Wiener index and vibrational energy, *Z. Naturforsch.* **57 A** (2002 824–828.

[16] I. Gutman, Y. Zhang, M. Dehmer, A. Ilič, Altenburg, Wiener, and Hosoya polynomials, in I. Gutman, B. Furtula (Eds.) *Distance in Molecular Graphs-Theory*, Univ. Kragujevac, Kragujevac (2012).

[17] A. Hamzeh, A. Iranmanesh, T. Réti, I. Gutman, Chemical graphs constructed of composite graphs and their q-Wiener index, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 807–823.

[18] H. Hou, B. Liu, Y. Huang, The maximum Wiener polarity index of unicyclic graphs, *Appl. Math. Comput.* **218** (2012) 10149–10157.

[19] K. Hriňáková, M. Knor, R. Škrekovski, A. Tepeh, A congruence relation for the Wiener index of graphs with a tree-like structure, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 791–806.

[20] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, S. G. Wagner, Some new results on distance-based graph invariant, *European J. Combin.* **30** (2009) 1149–1163.

[21] A. Iranmanesh, I. Gutman, O. Khormali, A. Mahmiani, The edge versions of the Wiener index, *MATCH Commun. Math. Computer Chem.* **61** (2009) 663–672.

[22] S. Klavžar, A. Lipovec, Partial cubes as subdivision graphs and as generalized Petersen graphs, *Discrete Math.* **263** (2003) 157–165.

[23] M. Knor, B. Lužar, R. Škrekovski, I. Gutman, On Wiener index of common neighborhood graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 321–332.

[24] M. Knor, P. Potočnik, R. Škrekovski, Relationship between the edge-Wiener index and the Gutman index of a graph, *Discrete Appl. Math.* **167** (2014) 197–201.

[25] M. Knor, R. Škrekovski, Wiener index of line graphs, in M. Dehmer and F. Emmert-Streib (Eds.), *Quantitative Graph Theory: Mathematical Foundations and Applications)*, CRC Press (2014) 279–301.

[26] M. Knor, R. Škrekovski, A. Tepeh, *Mathematical aspects of Wiener index*, manuscript, 2015.

[27] J. Li, A relation between the edge Szeged index and the ordinary Szeged index *MATCH Commun. Math. Comput. Chem.* **70** (2013) 621–625.

[28] X. Li, Z. Qin, M. Wei, I. Gutman, M. Dehmer, Novel inequalities for generalized graph entropies Graph energies and topological indices, *Appl. Math. Comput.* **259** (2015) 470–479.

[29] H. Lin, On the Wiener index of trees with given number of branching vertices, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 301–310.

[30] J. Liu, I. Gutman, Z. Mu, Y. Zhang, q-Wiener index of some compound trees, *Appl. Math. Comput.* **218** (2012) 9528–9535.

[31] J. Ma, Y. Shi, J. Yue, The Wiener polarity index of graph products, *Ars Combin.* **116** (2014) 235–244.

[32] S. Mukwembi, On the upper bound of Gutman index of graphs, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 343–348.

[33] J. Plesník, On the sum of all distances in a graph or digraph, *J. Graph Theory* **8** (1984) 1–21.

[34] B. E. Segan, Y. N. Yeh, P. Zhang, The Wiener polynomial of a graph, *Int. J. Quantum Chem.* **60** (1996) 959–969.

[35] R. Škrekovski, I. Gutman, Vertex version of the Wiener theorem, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 295–300.

[36] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.

[37] B. Wu, Wiener index of line graphs, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 699–706.

[38] K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula, A survey on graphs extremal with respect to distance-based topological indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 461–508.

Figures

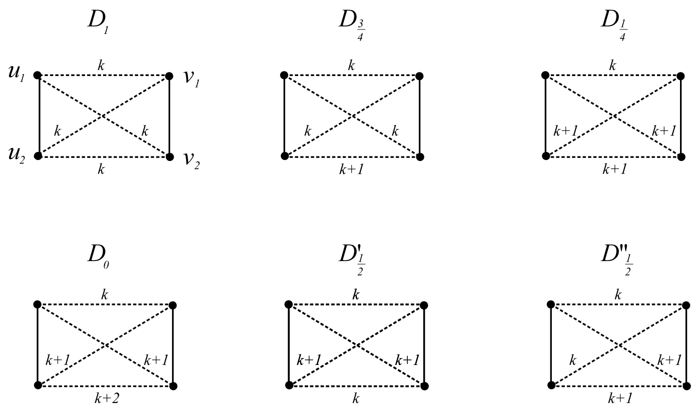

Figure 1: Different configurations of pairs of edges.