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1

## RELATIONSHIP BETWEEN EDGE-WIENER INDEX AND GUTMAN INDEX OF A GRAPH

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ABSTRACT. The Wiener index W(G) of a connected graph G is defined to be the sum  $\sum_{u,v} d(u,v)$  of the distances between the 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 the distances between the pairs of edges in G, or equivalently, the Wiener index of the line graph L(G). Finally, the Gutman index  $\operatorname{Gut}(G)$  is defined to be the sum  $\sum_{u,v} \deg(u) \deg(v) d(u,v)$ , where  $\deg(u)$  denotes the degree of a vertex u in G. In this paper we prove an inequality involving the edge-Wiener index and the Gutman index of a connected graph. In particular, we prove that  $W_e(G) \geq \frac{1}{4}\operatorname{Gut}(G) - \frac{1}{4}|E(G)| + \frac{3}{4}\kappa_3(G) + 3\kappa_4(G)$  where  $\kappa_m(G)$  denotes the number of all m-cliques in G. Moreover, equality holds if and only if G is a tree or a complete graph. Using this result we show that  $W_e(G) \geq \frac{\delta^2 - 1}{4}W(G)$  where  $\delta$  denotes the minimum degree in G.

## 1. INTRODUCTION

For a graph G with vertex set V = V(G) and edge set E = E(G), let deg(u)and d(u, v) denote the degree of a vertex  $u \in V$  and the distance between vertices  $u, v \in V$ , respectively. Let L(G) denote the line graph of G, that is, the graph with vertex set E and two distinct edges  $e, f \in E$  adjacent in L(G) whenever they share an endpoint in G. Furthermore, for  $e, f \in E$ , we let d(e, f) denote the distance between e and f in the line graph L(G). For adjacent vertices x and y, we write  $x \sim y$ .

In this paper we consider three important graph invariants, called *Wiener index* (denoted by W(G) and introduced in [10]), *edge-Wiener index* (denoted by  $W_e(G)$ ) and *Gutman index* (denoted by Gut(G)), which are defined as follows:

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

$$W_e(G) = \sum_{\{e,f\} \subseteq E} d(e,f) = \frac{1}{2} \sum_{(e,f) \in E^2} d(e,f),$$
  

$$Gut(G) = \sum_{\{u,v\} \subseteq V} \deg(u) \deg(v) d(u,v) = \frac{1}{2} \sum_{(u,v) \in V^2} \deg(u) \deg(v) d(u,v).$$

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Note that 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 [8] edge-Wiener index is defined to be  $W_e(G) + \binom{n}{2}$  where  $W_e(G)$  is as defined above and n is the order of G.

Besides applications in chemistry (see for example [7]), Wiener index of a graph was studied also from a purely graph-theoretical point of view (for early results, see for example [6, 9], and [3] for a nice survey). Generalizations of Wiener index and relationship between these were studied in a number of papers (see for example [2, 4, 5, 8]).

The main result of this paper is the following inequality, involving the edge-Wiener index and the Gutman index of a connected graph:

$$W_e(G) \ge \frac{1}{4} \operatorname{Gut}(G) - \frac{1}{4} |E(G)| + \frac{3}{4} \kappa_3(G) + 3\kappa_4(G),$$
 (\*)

where by  $\kappa_m(G)$  we denote the number of *m*-cliques in *G*. In addition, we show that equality holds in (\*) if and only if *G* is a tree or a complete graph.

As a consequence of (\*), we prove the following inequality involving the Wiener index and the edge-Wiener index of a connected graph G:

$$W_e(G) \ge \frac{\delta^2 - 1}{4} W(G),$$

where  $\delta = \delta(G)$  denotes the minimum degree in G. Notice that Wu [11] proved that for any graph G of minumum degree at least 2,  $W_e(G) \ge W(G)$  with equality holding for cycles; see also [1] for the case when the minimum degree equals 2.

## 2. The proof

Throughout this section, let G be a connected graph with vertex set V and edge set E. Further, we let  $A = \{(u, v) : uv \in E\}$  stand for the *arc set* of G. Recall that for any two edges  $e = u_1u_2$  and  $f = v_1v_2$  in E, the distance between e and f is defined as the distance  $d_{L(G)}(e, f)$  between e and f in the line graph L(G), and observe that if  $e \neq f$ , then

(1) 
$$d(u_1u_2, v_1v_2) = \min\{d(u_i, v_j) : i, j \in \{1, 2\}\} + 1.$$

In addition to the distance between two edges, we will also consider the *average* distance between the endpoints of two edges, defined by

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

The average distance of endpoints has an interesting relationship with the Gutman index of a graph. Namely, if one wants to consider the version of edge-Wiener index where the distances of edges in the sum are substituted by average distances of endpoints, then what one gets is essentially the Gutman index. More precisely, the following holds (which was also observed by Wu [11]): **Lemma 2.1.** Let G be a connected graph with vertex set V and edge set E. Then

$$\frac{1}{2}\sum_{(e,f)\in E^2}s(e,f)=\frac{1}{4}\mathrm{Gut}(G).$$

*Proof.* Let A be the arc set of G. Then:

$$\frac{1}{2} \sum_{(e,f)\in E^2} s(e,f) = \frac{1}{8} \sum_{(u_1,u_2)\in A} \sum_{(v_1,v_2)\in A} \frac{1}{4} \left( d(u_1,v_1) + d(u_2,v_1) + d(u_1,v_2) + d(u_2,v_2) \right).$$
(+)

Now for each pair  $i, j \in \{1, 2\}$ , we see that

$$\sum_{(u_1, u_2) \in A} \sum_{(v_1, v_2) \in A} d(u_i, v_j) = \sum_{u \in V} \sum_{u' \in N(u)} \sum_{v \in V} \sum_{v' \in N(v)} d(u, v) =$$
$$= \sum_{u \in V} \sum_{v \in V} \deg(u) \deg(v) d(u, v) = 2 \operatorname{Gut}(G).$$

By plugging this into (+), we get

 $\frac{1}{2} \sum_{(e,f)\in E^2} s(e,f) = \frac{1}{8} \cdot \frac{1}{4} \cdot 4 \cdot 2 \cdot \operatorname{Gut}(G) = \frac{1}{4} \operatorname{Gut}(G),$ 

as required.

Lemma 2.3 below will be needed in the proof of the main theorem. Since it might be of independent graph-theoretical interest, we state it separately. But first we define the following notions.

**Definition 2.2.** Let G be a graph with vertex set V and edge set E. For a pair of distinct edges  $e = u_1u_2$ ,  $f = v_1v_2$  of G we say that they form a triangle whenever the graph induced on the set  $\{u_1, u_2, v_1, v_2\}$  of the endvertices is  $K_3$ . Similarly, we say that e and f form a  $K_4$  provided that the graph induced on  $\{u_1, u_2, v_1, v_2\}$  is the complete graph  $K_4$ . Finally, we will say that edges  $u_1u_2$  and  $v_1v_2$  are on a straight line provided that the difference between the maximum and minimum value of  $d(u_i, v_j)$ ,  $i, j \in \{1, 2\}$ , is 2.

**Lemma 2.3.** Let G be a connected graph such that every pair of distinct edges of G either lies on a straight line or forms a triangle or a  $K_4$ . Then G is a tree or a complete graph.

Proof. Suppose that G is not a tree. We will first show that for every cycle C in G the subgraph G[V(C)], induced by the vertices of C, is a complete graph. Suppose that this is not the case and let  $C = v_0v_1 \dots v_{m-1}v_0$  be a shortest cycle in G for which G[V(C)] is not a complete graph. Clearly  $m \ge 4$ . Let k be the integer part of  $\frac{m}{2}$ . If C is isometrically embedded into G (that is, if  $d_G(v_i, v_j) = d_C(v_i, v_j)$  for all  $i, j \in \{0, 1, \dots, m-1\}$ ), then the pair of "opposite" edges  $v_0v_1$  and  $v_kv_{k+1}$  does not lie on a straight line and thus forms a  $K_4$ . But this contradicts the assumption that

C is isometrically embedded into G. Therefore there exists a path  $P = u_0 u_1 \ldots u_t$ in G between some vertices  $u_0 = v_\alpha$  and  $u_t = v_\beta$  on C of length  $t < d_C(v_\alpha, v_\beta)$ . We may assume without loss of generality that no interior vertex of P intersects C, for otherwise we can substitute P with the part of P between two consecutive intersections of P with C. The path P, together with the two parts of C between  $v_\alpha$  and  $v_\beta$ , then forms two cycles, say  $C_1$  and  $C_2$ , which are shorter than C. It follows from the minimality of C that both  $G[V(C_1)]$  and  $G[V(C_2)]$  are complete graphs. In particular, any two vertices of C which both lie in  $C_1$  or both in  $C_2$ are adjacent. Now take two vertices  $x, y \in V(C)$  such that  $x \in V(C_1) \setminus V(P)$  and  $y \in V(C_2) \setminus V(P)$ . Since both x and y are adjacent to  $v_\alpha$  and  $v_\beta$  and since also  $v_\alpha \sim v_\beta$ , the edges  $xv_\alpha$  and  $yv_\beta$  do not lie on a straight line. But then they form a  $K_4$ , implying that also x is adjacent to y. This finally shows that any two vertices of C are adjacent in G, which contradicts our assumptions on C. We have thus proved that any cycle in G induces a complete graph.

Now let C be the longest cycle in G. If C contains all the vertices of G, then G = G[V(C)] is a complete graph, as required. We may thus assume that there exists a vertex  $v \in V(G) \setminus V(C)$  which is adjacent to a vertex  $u \in V(C)$ . By considering any edge e of C not incident with u we see that e and uv do not lie on a straight line, implying that they form a  $K_4$ . But then we can find a cycle with vertex set  $V(C) \cup \{v\}$  of length larger than that of C. This contradiction finally shows that G is a complete graph.

The following lemma describes the relationship between the distance d(e, f) and the average distance of endpoints s(e, f) in more detail.

**Lemma 2.4.** Let  $u_1u_2, v_1v_2$  be a pair of edges of a connected graph G. Then

(2) 
$$d(u_1u_2, v_1v_2) \ge s(u_1u_2, v_1v_2) + D(u_1u_2, v_1v_2)$$

where

(3) 
$$D(u_1u_2, v_1v_2) = \begin{cases} -\frac{1}{2} & \text{if } u_1u_2 = v_1v_2; \\ \frac{1}{4} & \text{if the pair } u_1u_2, v_1v_2 \text{ forms a triangle;} \\ 1 & \text{if the pair } u_1u_2, v_1v_2 \text{ forms a } K_4; \\ 0 & \text{otherwise.} \end{cases}$$

Moreover, equality holds in (2) if and only if

- (*i*)  $u_1u_2 = v_1v_2$ , or
- (ii) the pair  $u_1u_2$ ,  $v_1v_2$  forms a triangle or  $K_4$ , or
- (iii) if  $u_1u_2$  and  $v_1v_2$  lie on a straight line.

In particular, equality in (2) holds for every pair of distinct edges of G if and only if G is a tree or a complete graph.

*Proof.* If  $u_1u_2 = v_1v_2$ , then  $d(u_1u_2, v_1v_2) = 0$  and  $s(u_1u_2, v_1v_2) = \frac{1}{2}$ . Hence  $d(u_1u_2, v_1v_2) = s(u_1u_2, v_1v_2) + D(u_1u_2, v_1v_2)$  in this case. We may thus assume that  $u_1u_2 \neq v_1v_2$ .

Suppose that the minimum value of  $d(u_i, v_j)$  is attained for i = s and j = t, i.e.

$$\min\{d(u_i, v_j) : i, j \in \{1, 2\}\} = d(u_s, v_t).$$

If  $u_1u_2$  and  $v_1v_2$  form a triangle, then  $d(u_s, v_t) = 0$  while  $d(u_s, v_{3-t}) = d(u_{3-s}, v_t) = d(u_{3-s}, v_{3-t}) = 1$ . Therefore

$$s(u_1u_2, v_1v_2) = \frac{1}{4}(d(u_s, u_t) + d(u_s, v_{3-t}) + d(u_{3-s}, v_t) + d(u_{3-s}, v_{3-t})) = \frac{3}{4} = 1 - D(u_1u_2, v_1v_2) + d(u_3v_1v_2) + d(u_3v_1v_2) = \frac{1}{4}(d(u_3v_1v_1) + d(u_3v_1v_2) + d(u_3v_1v_2) + d(u_3v_1v_1) + d(u_3v_1v_1$$

On the other hand  $d(u_1u_2, v_1v_2) = 1$ , and thus (3) holds with equality, as claimed.

If  $u_1u_2$  and  $v_1v_2$  form a  $K_4$ , then  $d(u_s, v_t) = d(u_s, v_{3-t}) = d(u_{3-s}, v_t) = d(u_{3-s}, v_{3-t}) = 1$ , and so  $s(u_1u_2, v_1v_2) = 1 = 2 - D(u_1u_2, v_1v_2)$ . On the other hand  $d(u_1u_2, v_1v_2) = 2$ , and again equality in (3) holds.

Finally, suppose that  $u_1u_2$  and  $v_1v_2$  do not form a triangle or a  $K_4$ . Then

(4) 
$$d(u_{3-s}, v_{3-t}) - d(u_s, v_t) \leq 2$$

(5) 
$$d(u_s, v_{3-t}) - d(u_s, v_t) \leq 1,$$

(6)  $d(u_{3-s}, v_t) - d(u_s, v_t) \leq 1.$ 

By summing up these inequalities (together with the equality  $d(v_s, v_t) - d(v_s, v_t) = 0$ ) and dividing by 4 one obtains

 $s(u_1v_1, u_2v_2) - d(u_s, v_t) \le 1.$ 

Using formula (1) we may thus conclude that

$$d(u_1v_1, u_2v_2) = d(u_s, v_t) + 1 \ge s(u_1u_2, v_1v_2).$$

Since  $D(u_1u_2, v_1v_2) = 0$  in this case, this proves that the inequality in (2) holds. Observe also that, in this case, equality holds in (2) if and only if we have equality in (4), which happens if and only if  $u_1u_2$  and  $v_1v_2$  lie on a straight line.

We have thus proved that (2) holds in all cases, and that we have equality in (2) if and only if  $u_1u_2$  and  $v_1v_2$  lie on a straight line or form a triangle or a  $K_4$ . The second part of the claim now follows directly from Lemma 2.3.

Recall that  $\kappa_m(G)$  denotes the number of all *m*-cliques in *G*. Similarly, for an edge uv of *G*, we let  $\kappa_m(uv)$  denote the number of *m*-cliques of *G* that contain uv. Note that

(7) 
$$\sum_{uv\in E(G)}\kappa_m(uv) = \binom{m}{2}\kappa_m(G).$$

In particular, for m = 2 we obtain  $\kappa_2(G) = |E(G)|$ . We are now ready to prove the main result of the paper.

**Theorem 2.5.** Let G be a connected graph. Then

(8) 
$$W_e(G) \ge \frac{1}{4} \operatorname{Gut}(G) - \frac{1}{4} |E(G)| + \frac{3}{4} \kappa_3(G) + 3\kappa_4(G)$$

with equality in (8) if and only if G is a tree or a complete graph.

*Proof.* Let V and E denote the vertex set and the edge set of G respectively, and let A be the arc set of G, that is, the set of all ordered pairs of adjacent vertices in G. Then it follows directly from the definition of the edge-Wiener index that

(9) 
$$W_e(G) = \frac{1}{2} \sum_{(e,f)\in E^2} d(u_1u_2, v_1v_2) = \frac{1}{8} \sum_{(u_1,u_2)\in A} \sum_{(v_1,v_2)\in A} d(u_1u_2, v_1v_2).$$

By Lemma 2.4, for a fixed  $(u_1, u_2) \in A$ , we have that  $d(u_1u_2, v_1v_2) \ge s(u_1u_2, v_1v_2) + D(u_1u_2, v_1v_2)$ . Hence, by (9), we see that

(10) 
$$W_e(G) \ge \frac{1}{8} \sum_{(u_1, u_2)} \sum_{(v_1, v_2)} s(u_1 u_2, v_1 v_2) + \frac{1}{8} \sum_{(u_1, u_2)} \sum_{(v_1, v_2)} D(u_1 u_2, v_1 v_2),$$

Let us now compute the two sums in (10). Observe first that in view of Lemma 2.1, for the first sum we have

$$\frac{1}{8} \sum_{(u_1, u_2)} \sum_{(v_1, v_2)} s(u_1 u_2, v_1 v_2) = \frac{1}{2} \sum_{(e, f) \in E^2} s(e, f) = \frac{1}{4} \operatorname{Gut}(G).$$

To determine the second sum in (10), note that  $D(u_1u_2, v_1v_2)$  equals 0 unless one of the following holds:

- (i)  $v_1v_2 = u_1u_2$  (note that there are precisely 2 arcs  $(v_1, v_2)$  for which this holds);
- (*ii*)  $v_1v_2$  shares an endpoint with  $u_1u_2$  and forms a triangle with it (note that there are precisely  $4\kappa_3(u_1u_2)$  such arcs  $(v_1, v_2)$ );
- (*iii*)  $v_1v_2$  forms a  $K_4$  with  $u_1u_2$  (note that there are precisely  $2\kappa_4(u_1u_2)$  such arcs  $(v_1, v_2)$ ).

Hence

$$\sum_{(u_1,u_2)} \sum_{(v_1,v_2)} D(u_1u_2,v_1v_2) = -\frac{1}{2} \sum_{(u_1,u_2)} 2 + \frac{1}{4} \sum_{(u_1,u_2)} 4\kappa_3(u_1u_2) + \sum_{(u_1,u_2)} 2\kappa_4(u_1u_2).$$

In view of (7), we see that the above sum equals:

$$-2|E(G)| + 6\kappa_3(G) + 24\kappa_4(u_1u_2).$$

Therefore, by (10), it follows that

$$W_e(G) \ge \frac{1}{8} (2\operatorname{Gut}(G) - 2|E(G)| + 6\kappa_3(G) + 24\kappa_4(u_1u_2)),$$

as required. Moreover, in view of Lemma 2.4, equality holds if and only if G is a tree or a complete graph.  $\hfill \Box$ 

**Corollary 2.6.** Let G be a connected graph of minimal degree  $\delta \geq 2$ . Then

$$W(L(G)) > \frac{\delta^2}{4}W(G) - \frac{1}{4}|E(G)| \ge \frac{\delta^2 - 1}{4}W(G).$$

*Proof.* Note that

$$\operatorname{Gut}(G) = \sum_{\{u,v\} \subseteq V(G)} \operatorname{deg}(u) \operatorname{deg}(v) d(u,v) \ge \sum_{\{u,v\} \subseteq V(G)} \delta^2 d(u,v) = \delta^2 W(G).$$

Now, since  $\delta \geq 2$ , the graph G is not a tree, and so Theorem 2.5 implies the first inequality in the corollary. The second inequality then follows, if one observes that, since every pair of adjacent vertices contributes exactly 1 to the Wiener index of the graph (while the non-adjacent ones contribute even more), we have that  $|E(G)| \leq W(G)$ .

We expect that Corollary 2.6 can be improved to  $W(L(G)) \geq \frac{\delta^2}{4}W(G)$ , with equality holding for cycles, which would correspond to the result of Wu [11].

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RELATIONSHIP BETWEEN EDGE-WIENER INDEX AND GUTMAN INDEX OF A GRAPH 9

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