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The edge-Wiener index of a graph

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ABSTRACT

If G is a connected graph, then the distance between two edges is, by definition, the distance between the corresponding vertices of the line graph of G. The edge-Wiener index W_e of G is then equal to the sum of distances between all pairs of edges of G. We give bounds on W_e in terms of order and size. In particular we prove the asymptotically sharp upper bound $W_e(G) \leq \frac{2^5}{5^5}n^5 + O(n^{9/2})$ for graphs of order n.

1. Introduction

The Wiener index, the sum of distances between all pairs of vertices in a connected graph, is a graph invariant much studied in both mathematical and chemical literature; for details see the reviews [6,7,10,16] and the references cited therein. In this paper we are concerned with a quantity closely analogous to the Wiener index, namely the sum of all distances between all pairs of edges in a connected graph. Whereas the Wiener index was conceived (by chemists) as early as in 1947, and its mathematical investigation started already in the 1970s [11], it is remarkable that until now, its edge-version eluded the attention of both "pure" and applied graph theoreticians.

The aim of the present paper is to contribute towards filling this gap.

Definition 1. Let G be a connected graph. Then the edge-Wiener index of G is defined as the sum of the distances (in the line graph) between all pairs of edges of G, i.e.,

$$W_e(G) = \sum_{\{e,f\}\subseteq E(G)} d(e,f),$$

where the distance between two edges is the distance between the corresponding vertices in the line graph of G.

In view of the above definition, the edge-Wiener index of a graph equals the ordinary Wiener index of its line graph. Only a few results on this latter quantity are known. These can now be re-stated in terms of the edge-Wiener index.

The following result is due to Buckley [2]. We rephrase his result, originally stated in terms of average distance of the line graph of a tree, as:

Theorem 1 (*Buckley [2]*). *Let T be a tree of order n. Then*

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

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As a corollary we obtain that there exists no tree whose Wiener index equals its edge-Wiener index.

Buckley's equality was extended to graphs containing cycles [13,15]. In terms of edge-Wiener indices the respective results read:

Theorem 2 (*Gutman [13]*). *If G is a connected graph of order n and size q, then*

$$W_e(G) \geq W(G) - n(n-1) + \frac{1}{2}\, q(q+1).$$

Theorem 3 (*Gutman & Pavlović [15]*). *If G is a connected unicyclic graph of order n, then $W_e(G) \leq W(G)$, with equality if and only if $G \cong C_n$.*

In connected bicyclic graphs all the three cases $W_e < W$, $W_e = W$, and $W_e > W$ may occur [15]. The smallest bicyclic graph with the property $W_e = W$ has 9 vertices and is unique. There are already 26 ten-vertex bicyclic graphs with the same property [14]. For further work along these lines see [5,8,9].

Two graph parameters that are closely related to the Wiener index also feature in this paper. The *average distance* is defined as the average (or arithmetic mean) of the distances between all pairs of vertices of a graph. It is denoted by $\mu(G)$. Clearly, $W(G) = \binom{n}{2}\,\mu(G)$. We also consider a variant of the Wiener index, put forward in [12] and called there the *Schultz index of the second kind*, but for which the name *Gutman index* has also sometimes been used [19]. It is defined as

$$\mathrm{Gut}(G) := \sum_{\{x,y\}\subseteq V(G)} \deg(x)\deg(y)\, d(x,y).$$

As observed in [3], the average distance of a regular graph does not differ significantly from the average distance of its line graph.

Theorem 4 (*[3]*). *Let G be a connected δ-regular graph of order n. Then*

$$\frac{\delta n - \delta}{\delta n - 2}\,\mu(G) - 1 \leq \mu(L(G)) \leq \frac{\delta n - \delta}{\delta n - 2}\,\mu(G) + 1.$$

Corollary 1. *Let G be a connected δ-regular graph. Then*

$$\frac{1}{4}\,\delta^2\, W(G) - \binom{\delta n/2}{2} \leq W_e(G) \leq \frac{1}{4}\,\delta^2\, W(G) + \binom{\delta n/2}{2}.$$

2. Results

Proposition 1. *Let G be a connected graph of order n. Then*

$$W_e(G) \geq \binom{n-1}{2},$$

with equality if and only if G is a star.

Proof. G has at least $n-1$ edges, and the distance between any two edges is at least 1. Hence

$$W_e(G) = \sum_{\{e,f\}\subseteq E(G)} d(e,f) \geq \binom{|E(G)|}{2} \geq \binom{n-1}{2}.$$

If we have equality above, then G must have $n-1$ edges, so G is a tree. Moreover, the line graph of G is complete since the distance between any two edges is 1. Hence G is a star. □

We note that deletion of an edge can increase or decrease the edge-Wiener index but always increases the ordinary Wiener index. Similarly, addition of an edge can decrease or increase the edge-Wiener index. To see this, consider the star $K_{1,n}$. It follows directly from Proposition 1 that $W_e(K_{1,n}+e) > W_e(K_{1,n})$ for any edge e not in $K_{1,n}$. As an example of a graph where addition of an edge decreases the edge-Wiener index consider the path P_n, and the cycle C_n, obtained by adding an edge between the end vertices of the path. We have $W_e(P_n) = n(n-1)(n-2)/6 > \frac{n^3}{8} \geq W_e(C_n)$ if $n > 11$.

Definition 2. Let $G = (V, E)$ be a connected graph and c be a real valued weight function on the vertices of G. Then the Wiener index of G with respect to c is

$$W(G, c) = \sum_{\{x,y\}\subseteq V} c(x)\, c(y)\, d(x,y).$$

We note that for $c \equiv 1$ this yields the usual Wiener index, while for $c(x) = \deg(x)$ we obtain the Gutman index. The edge-Wiener index of a graph is connected to its Gutman index by the following inequality.

Theorem 5. *Let G be a connected graph of order n. Then*

$$\left| W_e(G) - \frac{1}{4}\,\mathrm{Gut}(G) \right| \le \frac{n^4}{8}.$$

Proof. Consider the graph H obtained from G by subdividing each edge once. Consider the following functions a and b on $V(H)$ defined as follows.

$$a(v) = \begin{cases} \deg(v) & \text{if } v \in V(G), \\ 0 & \text{if } v \in V(H) - V(G), \end{cases} \qquad b(v) = \begin{cases} 0 & \text{if } v \in V(G), \\ 2 & \text{if } v \in V(H) - V(G). \end{cases}$$

Since for any two vertices u, v of G we have $d_H(u, v) = 2d_G(u, v)$, it follows that

$$\begin{aligned} W(H, a) &= \sum_{\{x,y\} \subseteq V(H)} a(x)\, a(y)\, d_H(x, y) \\ &= \sum_{\{x,y\} \subseteq V(G)} 2\, \deg(x) \deg(y) d_G(x, y) \\ &= 2\,\mathrm{Gut}(G). \end{aligned} \tag{1}$$

Denote the vertex of degree 2 in $V(H) - V(G)$ that subdivides the edge $e \in E(G)$ by v_e. Then $b(x) \neq 0$ only if $x = v_e$ for some edge e of G. For any two edges e, f of G we have $d_H(v_e, v_f) = 2\, d_G(e, f)$, and so

$$\begin{aligned} W(H, b) &= \sum_{\{x,y\} \subseteq V(H)-V(G)} b(x)\, b(y)\, d_H(x, y) \\ &= \sum_{\{e,f\} \subseteq E(G)} 8\, d_G(e, f) \\ &= 8\, W_e(G). \end{aligned} \tag{2}$$

We now compare $W(H, a)$ and $W(H, b)$. Clearly, the weight function a is obtained from the weight function b by moving one weight unit of a vertex v_{uw} to vertex u and the other weight unit to vertex w for all $uw \in E(G)$. Hence no weight has been moved over a distance of more than one, so no distance between two weights has been changed by more than 2. Since we have $2|E(G)|$ weight units in total, the sum of the distances between the weight units has changed by at most $2\binom{2|E(G)|}{2}$. Hence

$$|W(H, a) - W(H, b)| \le 2 \binom{2|E(G)|}{2} \le n^4,$$

which, with (1) and (2), completes the proof. $\square$

We now consider the problem of finding a lower bound on the edge-Wiener index of a graph of given order and size. We make use of the following well-known lower bound on the regular Wiener index.

Proposition 2 (*Entringer, Jackson, and Snyder [11]*). *Let G be a connected graph of order n and size q. Then*

$$W(G) \ge n(n-1) - q,$$

with equality if and only if $\mathrm{diam}(G) \le 2$.

For the edge-Wiener index we obtain

$$W_e(G) = W(L(G)) \ge q(q-1) - |E(L(G))|,$$

with equality if and only if $\mathrm{diam}(L(G)) \le 2$. Since

$$|E(L(G))| = \sum_{v \in V(G)} \binom{\deg(v)}{2} = \frac{1}{2} \sum_{v \in V(G)} (\deg(v))^2 - q,$$

the problem essentially reduces to finding the graphs of given order n and size q that maximise the sum of the squares of the vertex degrees. A good, but not sharp, upper bound,

$$\sum_{v \in V(G)} (\deg(v))^2 \le \frac{2\,q^2}{n-1} + q(n-2),$$

was given by de Caen [4]. This yields

$$W_e(G) \geq q^2 \frac{n-2}{n-1} - \frac{1}{2} q(n-2).$$

In [1], it was shown that for each value of n there exists an extremal graph which is either of the form $K_a + (bK_1 \cup K_{1,c})$ or of the form $bK_1 \cup (K_a + \overline{K_{1,c}})$. (All extremal graphs were determined in [18].) These extremal graphs maximise the edge-Wiener index among all graphs of given order and size. An exact expression for the edge-Wiener index of these graphs would be rather unpleasant. But if $q \gg n$, then their edge-Wiener index is approximately

$$W_e(G) = (1 + o(1)) \left(q^2 \frac{n-3}{n-1} - q(n-1) \right).$$

In order to determine an asymptotically sharp upper bound on the edge-Wiener index of a graph of given order, we first find a bound on the Gutman index. We will make use of the following Lemma. The ith distance layer of a vertex v is the set of vertices at distances i from v.

Lemma 1. *Let v be a vertex of eccentricity d, and let $k > 2$ be a positive real. Let A_k be the number of distance layers of v that contain only vertices of degree less than k. Then*

$$A_k \geq (d+1) \frac{k+1}{k-2} - \frac{3n}{k-2}.$$

Proof. Let V_i be the ith distance layer of v, and let $n_i = |V_i|$. Then, with $n_{-1} = n_{d+1} = 0$,

$$\sum_{i=0}^{d} (n_{i-1} + n_i + n_{i+1} - 1) = 3n - d - 2 - n_d. \tag{3}$$

A vertex in V_i has degree at most $n_{i-1} + n_i + n_{i+1} - 1$. So each of the $d + 1 - A_k$ distance layers V_i containing a vertex of degree at least k satisfies $n_{i-1} + n_i + n_{i+1} - 1 \geq k$. Each of the remaining A_k distance layers V_i satisfies $n_{i-1} + n_i + n_{i+1} - 1 \geq 2$, unless $i \in \{0, d\}$, in which case $n_{i-1} + n_i + n_{i+1} - 1 \geq 1$. Hence, by $n_d \geq 1$,

$$2A_k - 2 + (d + 1 - A_k)k \leq 3n - d - 3,$$

and the statement of the lemma follows after simplification. □

Theorem 6. *Let G be a connected graph of order n. Then*

$$\mathrm{Gut}(G) \leq \frac{2^4}{5^5} n^5 + O(n^{9/2}),$$

and the coefficient of n^5 is best possible.

Proof. Let $d = \mathrm{diam}(G)$. Fix a vertex v of eccentricity d. Let u_1, u_2 be two vertices that, among all pairs of vertices at distance at least 3, have maximum degree sum, say B.

By Lemma 1, vertex v has at least $(d+1)(k+1)/(k-2) - (3n)/(k-2)$ distance layers that contain only vertices of degree less than k. Since $N[u_1] \cup N[u_2]$ has vertices in at most 6 distance layers of v, there exists a set R of $\lfloor (d+1)\frac{k+1}{k-2} - \frac{3n}{k-2} - 6 \rfloor$ vertices of degree less than k, that is disjoint from $N[u_1] \cup N[u_2]$. Let $k = \sqrt{n}$. Then R is a set containing $d - O(\sqrt{n})$ vertices, all of degree less than $\sqrt{n}$. Let $\mathcal{R}$ be the set of all unordered pairs of vertices that have at least one vertex in R. Then $|\mathcal{R}| = \binom{n}{2} - \binom{n-|R|}{2}$ and

$$\sum_{\{x,y\} \in \mathcal{R}} \deg(x)\ \deg(y)\, d(x, y) \leq |\mathcal{R}| k(n-1)d \leq \binom{n}{2} \sqrt{n}(n-1)^2 = O(n^{9/2}). \tag{4}$$

Let $\mathcal{U}$ be the set of pairs of vertices that are either both in $N[u_1]$ or both in $N[u_2]$. Then the distance between any two such vertices is at most 2, hence

$$\sum_{\{x,y\} \in \mathcal{U}} \deg(x)\ \deg(y)\, d(x, y) \leq |\mathcal{U}|\, 2(n-1)^2 \leq \binom{n}{2} 2(n-1)^2 = O(n^4). \tag{5}$$

From the above it follows that the pairs in $\mathcal{U} \cup \mathcal{R}$ do not contribute any term of order greater than $n^{9/2}$. If $\mathcal{V}$ denotes the set of all unordered pairs of vertices of G then

$$\mathrm{Gut}(G) = \left(\sum_{\{x,y\} \in \mathcal{V} - (\mathcal{U} \cup \mathcal{R})} \deg(x)\ \deg(y)\, d(x, y) \right) + O(n^{9/2}).$$

Let $\{x, y\} \in \mathcal{V} - (\mathcal{U} \cup \mathcal{R})$. If x, y are at distance at least 3, then we have

$$\deg(x)\ \deg(y) \le \frac{1}{4}(\deg(x) + \deg(y))^2 \le \frac{1}{4}B^2.$$

Hence $\deg(x)\ \deg(y)\, d(x, y) \le \frac{1}{4}B^2 d$. If $d(x, y) \le 2$, then we have $\deg(x)\ \deg(y)\, d(x, y) \le 2(n-1)^2$. We distinguish two cases, depending on which of the two upper bounds is greater.

Case 1: $\frac{1}{4}B^2 d \le 2(n-1)^2$.

Then $\deg(x)\ \deg(y)\, d(x, y) \le 2(n-1)^2$ for all $\{x, y\} \in \mathcal{V} - (\mathcal{R} \cup \mathcal{U})$. So

$$\begin{aligned}\mathrm{Gut}(G) &= \left(\sum_{\{x,y\}\in\mathcal{V}-(\mathcal{U}\cup\mathcal{R})} \deg(x)\ \deg(y)\, d(x, y)\right) + O(n^{9/2})\\ &\le \binom{n}{2} 2(n-1)^2 + O(n^{9/2}) = O(n^{9/2}),\end{aligned}$$

as desired.

Case 2: $\frac{1}{4}B^2 d > 2(n-1)^2$.

$$\begin{aligned}\mathrm{Gut}(G) &= \left(\sum_{\{x,y\}\in\mathcal{V}-(\mathcal{R}\cup\mathcal{U})} \deg(x)\ \deg(y)\, d(x, y)\right) + O(n^{9/2})\\ &\le (|\mathcal{V}| - |\mathcal{R}| - |\mathcal{U}|)\,\frac{B^2 d}{4} + O(n^{9/2}). \qquad (6)\end{aligned}$$

Now, $|\mathcal{R}| = \binom{n}{2} - \binom{n-|R|}{2}$, where $|R| = d - O(\sqrt{n})$, and so $(|\mathcal{V}| - |\mathcal{R}|) = \binom{n-|R|}{2} = \binom{n-d+O(\sqrt{n})}{2} = \frac{1}{2}(n-d)^2 + O(n^{3/2})$. We now find a lower bound on $|\mathcal{U}|$. It follows from $|\mathcal{U}| = \binom{\deg(u_1)+1}{2} + \binom{\deg(u_2)+1}{2}$ and $\deg(u_1) + \deg(u_2) = B$ that $|\mathcal{U}|$ attains its minimum value if $\deg(u_1) = \deg(u_2) = \frac{B}{2}$. Hence $|\mathcal{U}| \ge \frac{B^2}{4} + \frac{B}{2} > \frac{B^2}{4}$. Therefore,

$$|\mathcal{V}| - |\mathcal{R}| - |\mathcal{U}| \le \frac{1}{2}(n-d)^2 - \frac{B^2}{4} + O(n^{3/2}).$$

This, in conjunction with (6) yields

$$\begin{aligned}\mathrm{Gut}(G) &\le \left(\frac{1}{2}(n-d)^2 - \frac{B^2}{4} + O(n^{3/2})\right)\frac{B^2 d}{4} + O(n^{9/2})\\ &= d\left(\frac{1}{2}(n-d)^2 - \frac{B^2}{4}\right)\frac{B^2}{4} + O(n^{9/2}).\end{aligned}$$

Since $N(u_i)$ has at most 3 vertices on any geodesic, in particular a geodesic of length d, we have that $d + B \le n + 5$, so that $B \le n - d + O(1)$. A simple differentiation shows that the term $d\left(\frac{1}{2}(n-d)^2 - \frac{B^2}{4}\right)\frac{B^2}{4}$ is maximised for $B = n - d$. Substituting back yields

$$\mathrm{Gut}(G) \le \frac{1}{16}d(n-d)^4 + O(n^{9/2}).$$

A simple differentiation now shows that $d(n-d)^4$ is maximised for $d = \frac{1}{5}n$. Substituting back yields the upper bound in the theorem.

To see that the upper bound is sharp consider the graph G_n, where n is a multiple of 5, obtained from a path with $\frac{n}{5}$ vertices and two vertex disjoint cliques of order $\frac{2n}{5}$ by adding two edges, each joining an end vertex of the path to a vertex in a clique. A simple calculation shows that

$$\mathrm{Gut}(G_n) = \frac{2^4}{5^5}\, n^5 + O(n^4),$$

as desired. □

Corollary 2. *Let G be a connected graph of order n. Then*

$$W_e(G) \le \frac{2^2}{5^5}\, n^5 + O(n^{9/2}),$$

and the coefficient of n^5 is best possible.

In conclusion we remark that, in [17] a measure of distance $D(f, g)$ between edges f and g of a graph G is defined to be the length of a shortest path between a vertex of f and a vertex of g (clearly not a metric). For the corresponding edge-Wiener index, $W'_e(G) = \sum_{\{f,g\}\subset E(G)} D(f, g)$, the inequality $W'_e(G) \leq \frac{n^5}{8}$ is established in [17] and the problem is posed to find the maximum value of $W'_e(G)$, given the order of G. As $D(f, g) = d(f, g) - 1$, it follows from the definitions of $W_e(G)$ and $W'_e(G)$ that $W'_e(G) \leq W_e(G) \leq \frac{2^2}{5^5} n^5 + O(n^{9/2})$ and the extremal graph in Theorem 6 shows that this bound on $W'_e(G)$ is sharp.

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