Discussiones Mathematicae Graph Theory 36 (2016) 867–876 doi:10.7151/dmgt.1900

THE GUTMAN INDEX AND THE EDGE-WIENER INDEX OF GRAPHS WITH GIVEN VERTEX-CONNECTIVITY

JAYA PERCIVAL MAZORODZE

Department of Mathematics University of Zimbabwe, Harare, Zimbabwe e-mail: mazorodzejaya@gmail.com

SIMON MUKWEMBI

Department of Mathematics University of Zimbabwe, Harare, Zimbabwe and School of Mathematics, Statistics and Computer Science University of KwaZulu-Natal Durban, South Africa

e-mail: mukwembi@ukzn.ac.za

AND

Tomáš Vetrík¹

Department of Mathematics and Applied Mathematics University of the Free State, Bloemfontein, South Africa

e-mail: vetrikt@ufs.ac.za

Abstract

The Gutman index and the edge-Wiener index have been extensively investigated particularly in the last decade. An important stream of research on graph indices is to bound indices in terms of the order and other parameters of given graph. In this paper we present asymptotically sharp upper bounds on the Gutman index and the edge-Wiener index for graphs of given order and vertex-connectivity κ , where κ is a constant. Our results substantially generalize and extend known results in the area.

Keywords: Gutman index, edge-Wiener index, vertex-connectivity.2010 Mathematics Subject Classification: 05C35, 05C12.

¹The work of T. Vetrík has been supported by the National Research Foundation of South Africa; Grant numbers: 91499, 90793.

1. INTRODUCTION

We consider finite connected graphs G with the vertex set V(G) and the edge set E(G). The degree of a vertex $v \in V(G)$, $\deg(v)$, is the number of edges incident with v. The distance d(u, v) between two vertices u and v in G is the number of edges in a shortest path connecting them. The eccentricity of v is the greatest distance between v and any other vertex of G. The diameter of G is the maximum eccentricity among the vertices of G. The *i*-th neighborhood $N_i(v)$ of a vertex v is the set of vertices at distance *i* from v. $N_0(v) = \{v\}$, $N_1(v)$ is often denoted by N(v), and $N[v] = N(v) \cup \{v\}$. The vertex-connectivity κ of G is the minimum number of vertices, whose removal from G results in a disconnected graph.

The edge-Wiener index $W_e(G)$ of a connected graph G is equal to the sum of distances between all pairs of edges in G, where the distance between the edges e and f in G is defined as the distance between the vertices e and f in the line graph of G. The edge-Wiener index was first defined in [11] in terms of the distance between edges. Several interesting results related to the edge-Wiener index originally presented in [2, 8] and [10] are summarized in [3]. Gutman [8] studied graphs of given order and size, and Gutman and Pavlović [10] considered unicyclic and bicyclic graphs. The edge-Wiener index has been studied in the last decade; see for example [1, 5] and [14].

Another graph index, which has been recently considered in a number of research papers is the Gutman index. The Gutman index of a connected graph G is defined as

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

The Gutman index of acyclic structures was considered in [9]. Feng [6] studied this index for unicyclic graphs, and Feng and Liu [7] considered bicyclic graphs in their research. Upper bounds on the Gutman index of graphs of given order were considered in [3] and [13]. In [3] Dankelmann *et al.* showed that for connected graphs G of order n, $\text{Gut}(G) \leq \frac{2^4}{5^5}n^5 + O(n^{\frac{9}{2}})$, and Mukwembi [13] proved that

(1)
$$\operatorname{Gut}(G) \le \frac{2^4}{5^5} n^5 + O(n^4).$$

In [12] the authors showed that for any connected graph G of order n and minimum degree δ ,

(2)
$$\operatorname{Gut}(G) \le \frac{2^4 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4).$$

This bound is asymptotically sharp for a fixed δ ; the extremal graph being of

vertex-connectivity 1. It is therefore natural to ask if the bound

(3)
$$\operatorname{Gut}(G) \le \frac{2^4 \cdot 3}{5^5(\kappa+1)} n^5 + O(n^4),$$

which follows from (2) by applying the well-known inequality $\kappa \leq \delta$ (see [15]), can be improved.

In this paper, we study the Gutman index of graphs of given order and vertex-connectivity. We show that

$$\operatorname{Gut}(G) \le \frac{2^4}{5^5 \kappa} n^5 + O(n^4)$$

for connected graphs G of order n and vertex-connectivity $\kappa \geq 1$, where κ is a constant. Our bound is best possible for every $\kappa \geq 1$ and it substantially generalizes the bound (1), and improves on the bound (3). We also obtain, as a corollary, a similar result for the edge-Wiener index of connected graphs of given order and vertex-connectivity.

2. Results

First we bound degrees of vertices of a graph G in terms of the order, diameter and vertex-connectivity of G. This result will be used in the proof of Theorem 2, which bounds the Gutman index of a graph.

Lemma 1. Let G be a connected graph of order n, diameter d and vertexconnectivity κ , where κ is a constant. Let v, v' be any vertices of G.

- (i) Then $\deg(v) \le n \kappa d + 4\kappa 3$.
- (ii) If $d(v, v') \ge 3$, then $\deg(v) + \deg(v') \le n \kappa d + 7\kappa 4$.

Proof. Let G be a connected graph of order n, diameter d and vertex-connectivity κ . Let v_0 be any vertex of G of eccentricity d and let N_i be the *i*-th neighborhood of v_0 , $i = 0, 1, 2, \ldots, d$.

Let $v \in V(G)$. Then $v \in N_i$ for some *i*. Note that $N(v) \subset N_{i-1} \cup N_i \cup N_{i+1}$, which implies that $\deg(v) \leq |N_{i-1}| + |N_i| + |N_{i+1}| - 1$. It is also easy to see that removal of all vertices in N_j , j = 1, 2, ..., d-1, disconnects *G*, thus $|N_j| \geq \kappa$ for j = 1, 2, ..., d-1. It follows that

(4)
$$n = \left| \bigcup_{j=0}^{d} N_{j} \right| \geq \left| \bigcup_{j=0}^{i-2} N_{j} \right| + \deg(v) + |\{v\}| + \left| \bigcup_{j=i+2}^{d} N_{j} \right|$$
$$\geq \deg(v) + 1 + \kappa(d-4) + 2.$$

Note that the inequalities hold also if $v \in N_i$, where $i \in \{0, 1, d-1, d\}$. For example, if i = d, we obtain $n \ge |\bigcup_{j=0}^{d-2} N_j| + \deg(v) + |\{v\}| \ge 1 + \kappa(d-2) + \deg(v) + 1$.

Rearranging the terms of (4), we obtain $\deg(v) \leq n - \kappa d + 4\kappa - 3$, which completes the proof of (i).

Now we prove the statement (ii). Let $v, v' \in V(G)$ such that $d(v, v') \geq 3$. Then $N(v) \cap N(v') = \emptyset$. Since $|N_i| \geq \kappa$ for $i = 1, 2, \ldots, d-1$ and $\deg(v) \leq |N_{i-1}| + |N_i| + |N_{i+1}| - 1$ (similarly for v'), we obtain

$$n \ge (\deg(v) + 1) + (\deg(v') + 1) + (d - 7)\kappa + 2.$$

Rearranging the terms, we get $\deg(v) + \deg(v') \le n - \kappa d + 7\kappa - 4$, which completes the proof of (ii).

In the following theorem we present an upper bound on the Gutman index of a graph G in terms of its order, diameter and vertex-connectivity.

Theorem 2. Let G be a connected graph of order n, diameter d and vertexconnectivity κ , where κ is a constant. Then

$$\operatorname{Gut}(G) \le \frac{1}{16}d\left(n - \kappa d\right)^4 + O(n^4),$$

and the bound is asymptotically sharp.

Proof. Let v_0 be a vertex of G of eccentricity d and let N_i be the *i*-th neighborhood of v_0 , i = 0, 1, 2, ..., d. Since $|N_i| \ge \kappa$ for all i = 1, 2, ..., d - 1, we can choose κ vertices $u_{i1}, u_{i2}, ..., u_{i\kappa}$ of N_i . Then for each $j = 1, 2, ..., \kappa$, let $P_j = \{u_{1j}, u_{2j}, u_{3j}, ..., u_{d-1j}\}$ and $P = \bigcup_{j=1}^{\kappa} P_j$. We have

$$(5) |P| = (d-1)\kappa$$

We partition the 2-subsets of V(G), $Z = \{\{x, y\} : x, y \in V(G)\}$, as follows

$$Z = C \cup A \cup B,$$

where

$$C = \{\{x, y\} : x \in P \text{ and } y \in V(G)\},\$$

$$A = \{\{x, y\} \in Z \setminus C : d(x, y) \ge 3\},\$$

$$B = \{\{x, y\} \in Z \setminus C : d(x, y) \le 2\}.$$

We set |A| = a, |B| = b, which implies $\binom{n}{2} = |C| + a + b$, and consequently from (5) we obtain

(6)
$$a+b = \binom{n-|P|}{2} = \frac{1}{2} \Big[n-(d-1)\kappa \Big] \Big[n-(d-1)\kappa - 1 \Big].$$

Note that

$$\operatorname{Gut}(G) = \sum_{\{x,y\}\in A} \operatorname{deg}(x)\operatorname{deg}(y)d(x,y) + \sum_{\{x,y\}\in B} \operatorname{deg}(x)\operatorname{deg}(y)d(x,y) + \sum_{\{x,y\}\in C} \operatorname{deg}(x)\operatorname{deg}(y)d(x,y).$$

We bound these three terms in the following claims.

Claim 1. Assume the previous notation. Then

$$\sum_{\{x,y\}\in C} \deg(x) \deg(y) d(x,y) \le O(n^4).$$

Proof. For $j = 1, 2, ..., \kappa$, let $P_j = U_{1j} \cup U_{2j} \cup U_{3j}$, where U_{1j}, U_{2j} and U_{3j} are defined as follows:

$$U_{1j} = \{u_{1j}, u_{4j}, u_{7j}, \dots \},\$$

$$U_{2j} = \{u_{2j}, u_{5j}, u_{8j}, \dots \},\$$

$$U_{3j} = \{u_{3j}, u_{6j}, u_{9j}, \dots \}.$$

Note that for any two different vertices x, y in the same set U_{ij} , i = 1, 2, 3, we have $N(x) \cap N(y) = \emptyset$, since $d(x, y) \ge 3$. Therefore $\sum_{x \in U_{ij}} \deg(x) < n$ for i = 1, 2, 3 and $j = 1, 2, \ldots, \kappa$.

For each vertex x in P, we define the score s(x) as

(7)
$$s(x) = \sum_{y \in V(G)} \deg(x) \deg(y) d(x, y) = \deg(x) \left(\sum_{y \in V(G)} \deg(y) d(x, y) \right).$$

Then from Lemma 1 we have

$$\begin{split} s(x) &\leq \deg(x) \left(\sum_{y \in V(G)} (n - \kappa d + O(1)) d(x, y) \right) \\ &= \deg(x) (n - \kappa d + O(1)) \left(\sum_{y \in V(G)} d(x, y) \right) < \deg(x) (n - \kappa d + O(1)) (nd). \end{split}$$

Then for $j = 1, 2, \ldots, \kappa$,

$$\begin{split} \sum_{x \in P_j} s(x) &= \sum_{x \in U_{1j}} s(x) + \sum_{x \in U_{2j}} s(x) + \sum_{x \in U_{3j}} s(x) < \sum_{x \in U_{1j}} \deg(x)(n - \kappa d + O(1))(nd) \\ &+ \sum_{x \in U_{2j}} \deg(x)(n - \kappa d + O(1))(nd) + \sum_{x \in U_{3j}} \deg(x)(n - \kappa d + O(1))(nd) \\ &= (n - \kappa d + O(1))(nd) \left(\sum_{x \in U_{1j}} \deg(x) + \sum_{x \in U_{2j}} \deg(x) + \sum_{x \in U_{3j} \deg(x)}\right) \\ &< (n - \kappa d + O(1))(nd)(3n). \end{split}$$

Hence from (7), we have

$$\sum_{\{x,y\}\in C} \deg(x) \deg(y) d(x,y) \le \sum_{x\in P} s(x) = \sum_{x\in P_1} s(x) + \sum_{x\in P_2} s(x) + \dots + \sum_{x\in P_{\kappa}} s(x) \\ < \kappa (n - \kappa d + O(1)) (nd) (3n),$$

which implies Claim 1.

Now we study pairs of vertices, which are in B.

Claim 2. Assume the notation above. Then

$$\sum_{\{x,y\}\in B} \deg(x)\deg(y)d(x,y) \le O(n^4).$$

Proof. We know that if $\{x, y\} \in B$, then $d(x, y) \leq 2$ and $b = O(n^2)$. Using these facts and Lemma 1, we obtain

$$\sum_{\{x,y\}\in B} \deg(x)\deg(y)d(x,y) \le \sum_{\{x,y\}\in B} 2(n-\kappa d+O(1))^2$$

= $2b(n-\kappa d+O(1))^2 = O(n^4),$

as claimed.

Finally, we bound those pairs of vertices, which are in A.

Claim 3. Assume the notation above. Then

$$\sum_{\{x,y\}\in A} \deg(x) \deg(y) d(x,y) \le \frac{d}{16} \left(n - \kappa d\right)^4 + O(n^4).$$

Proof. Let $\{w, z\}$ be any pair in A, such that $\deg(w) + \deg(z)$ is maximum. Let $\deg(w) + \deg(z) = s$. Since $\deg(w)\deg(z) \le \frac{1}{4}(\deg(w) + \deg(z))^2$, we get

(8)
$$\deg(w)\deg(z) \le \frac{1}{4}s^2.$$

Now we find an upper bound on the cardinality of A. From (6) it follows that

(9)
$$a = \frac{1}{2} \Big[n - (d-1)\kappa \Big] \Big[n - (d-1)\kappa - 1 \Big] - b.$$

Note that all pairs $\{x, y\}, x, y \in N[w] - P$ and all pairs $\{x, y\}, x, y \in N[z] - P$ are in *B*. Clearly, $w \in N_i$ for some $i = 0, 1, \ldots, d$, and consequently we have $N[w] \subseteq N_{i-1} \cup N_i \cup N_{i+1}$. Since $|N_i| \ge \kappa$ for any $i = 1, 2, \ldots, d-1$, we obtain $|N[w] \cap P| \le 3\kappa$. Similarly, $|N[z] \cap P| \le 3\kappa$, which implies

$$b \ge \begin{pmatrix} \deg(w) + 1 - 3\kappa \\ 2 \end{pmatrix} + \begin{pmatrix} \deg(z) + 1 - 3\kappa \\ 2 \end{pmatrix}$$
$$= \frac{1}{2} \Big[(\deg(w))^2 + (\deg(z))^2 \Big] - \frac{6\kappa - 1}{2} \Big(\deg(w) + \deg(z) \Big) + 9\kappa^2 - 3\kappa$$
$$\ge \frac{1}{4}s^2 - \frac{6\kappa - 1}{2}s + 9\kappa^2 - 3\kappa.$$

Then from (9), we get

$$a \le \frac{1}{2} \Big[n - (d-1)\kappa \Big] \Big[n - (d-1)\kappa - 1 \Big] - \frac{1}{4}s^2 + \frac{6\kappa - 1}{2}s - 9\kappa^2 + 3\kappa,$$

and consequently from (8), we have

$$\begin{split} &\sum_{\{x,y\}\in A} \deg(x) \deg(y) d(x,y) \le \sum_{\{x,y\}\in A} \frac{s^2 d}{4} \\ &\le \frac{s^2 d}{4} \bigg[\frac{1}{2} \Big[n - (d-1)\kappa \Big] \Big[n - (d-1)\kappa - 1 \Big] - \frac{1}{4}s^2 + \frac{6\kappa - 1}{2}s - 9\kappa^2 + 3\kappa \bigg] \\ &= \frac{s^2 d}{4} \bigg[\frac{1}{2} \Big[(n - \kappa d)^2 + O(n) \Big] - \frac{1}{4}s^2 + O(n) \bigg] = \frac{s^2 d}{4} \bigg[\frac{1}{2} (n - \kappa d)^2 - \frac{1}{4}s^2 \bigg] + O(n^4) \end{split}$$

By Lemma 1, $s \le n - \kappa d + 7\kappa - 4$. Subject to this condition, $\frac{s^2 d}{4} [\frac{1}{2}(n - \kappa d)^2 - \frac{1}{4}s^2]$ is maximized for $s = n - \kappa d + O(1)$ to give

$$\sum_{\{x,y\}\in A} \deg(x)\deg(y)d(x,y)$$

$$\leq \frac{d}{4}\Big((n-\kappa d)^2 + O(n)\Big)\Big[\frac{1}{2}\Big(n-\kappa d\Big)^2 - \frac{1}{4}\Big(n-\kappa d\Big)^2 + O(n)\Big] + O(n^4)$$

$$= \frac{d}{16}\Big(n-\kappa d\Big)^4 + O(n^4),$$

which completes the proof of Claim 3.

Now we complete the proof of the theorem. From Claims 1, 2 and 3, we obtain

$$\begin{aligned} \operatorname{Gut}(G) &= \sum_{\{x,y\} \in A} \operatorname{deg}(x) \operatorname{deg}(y) d(x,y) + \sum_{\{x,y\} \in B} \operatorname{deg}(x) \operatorname{deg}(y) d(x,y) \\ &+ \sum_{\{x,y\} \in C} \operatorname{deg}(x) \operatorname{deg}(y) d(x,y) \leq \frac{1}{16} d\left(n - \kappa d\right)^4 + O(n^4) + O(n^4) + O(n^4) \\ &= \frac{1}{16} d\left(n - \kappa d\right)^4 + O(n^4). \end{aligned}$$

Finally we show that our bound is asymptotically sharp. We construct a graph $G_{n,d,\kappa}$ such that

$$\operatorname{Gut}(G_{n,d,\kappa}) = \frac{1}{16}d\left(n-\kappa d\right)^4 + O(n^4).$$

Let $G_{n,d,\kappa}$ be a graph join defined as follows:

$$G_{n,d,\kappa} = K_{\lceil \frac{1}{2}(n-\kappa(d-1))\rceil} + G_1 + G_2 + \dots + G_{d-1} + K_{\lfloor \frac{1}{2}(n-\kappa(d-1))\rfloor},$$

where $G_1 = G_2 = \cdots = G_{d-1} = K_{\kappa}$. Note that every vertex of G_i is adjacent to every vertex of G_{i+1} , $i = 1, 2, \ldots, d-2$. It can be checked that $G_{n,d,\kappa}$ has order n, diameter d, vertex-connectivity κ and $\operatorname{Gut}(G_{n,d,\kappa}) = \frac{1}{16}d(n-\kappa d)^4 + O(n^4)$.

Now we present an upper bound on the Gutman index of a graph in terms of its order and vertex-connectivity.

Corollary 3. Let G be a connected graph of order n and vertex-connectivity κ , where κ is a constant. Then

$$Gut(G) \le \frac{2^4}{5^5 \kappa} n^5 + O(n^4),$$

and the bound is asymptotically sharp.

Proof. By Theorem 2, we have $\operatorname{Gut}(G) \leq \frac{1}{16}d(n-\kappa d)^4 + O(n^4)$ for connected graphs G of order n, diameter d and vertex-connectivity κ . Since

$$\frac{1}{16}d\Big(n-\kappa d\Big)^4$$

is maximized, with respect to d, for $d = \frac{n}{5\kappa}$, we obtain $\operatorname{Gut}(G) \leq \frac{2^4}{5^5\kappa}n^5 + O(n^4)$ for connected graphs G of order n and vertex-connectivity κ .

Consider the graph $G_{n,d,\kappa}$ described in the proof of Theorem 2. Let $\frac{n}{5\kappa}$ be an integer. Then the graph $G_{n,\frac{n}{5\kappa},\kappa}$ has the Gutman index $\frac{2^4}{5^5\kappa}n^5 + O(n^4)$.

The following lemma proved in [3] can be used to obtain a bound on the edge-Wiener index of a graph G.

Lemma 4. Let G be a connected graph of order n. Then

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

Corollary 5. Let G be a connected graph of order n and vertex-connectivity κ , where κ is a constant. Then

$$W_e(G) \le \frac{2^2}{5^5 \kappa} n^5 + O(n^4),$$

and the bound is asymptotically sharp.

Proof. From Corollary 3 and Lemma 4, we obtain $W_e(G) \leq \frac{2^2}{5^5\kappa}n^5 + O(n^4)$. The graph $G_{n,\frac{n}{5\kappa},\kappa}$ is the extremal graph also for the edge-Wiener index (we have $W_e(G_{n,\frac{n}{5\kappa},\kappa}) = \frac{2^2}{5^5\kappa}n^5 + O(n^4)$), therefore the bound is best possible.

References

- M. Azari and A. Iranmanesh, Computation of the edge Wiener indices of the sum of graphs, Ars Combin. 100 (2011) 113–128.
- [2] F. Buckley, Mean distance in line graphs, Congr. Numer. 32 (1981) 153-162.
- [3] P. Dankelmann, I. Gutman, S. Mukwembi and H.C. Swart, The edge-Wiener index of a graph, Discrete Math. 309 (2009) 3452–3457. doi:10.1016/j.disc.2008.09.040
- [4] A.A. Dobrynin and A.A. Kochetova, Degree distance of a graph: a degree analogue of the Wiener index, J. Chem. Inf. Comput. Sci. 34 (1994) 1082–1086. doi:10.1021/ci00021a008
- [5] A.A. Dobrynin and L.S. Mel'nikov, Wiener index, line graphs and the cyclomatic number, MATCH Commun. Math. Comput. Chem. 53 (2005) 209–214.
- [6] L. Feng, *The Gutman index of unicyclic graphs*, Discrete Math. Algorithms Appl. 4 (2012) 669–708. doi:10.1142/S1793830912500310
- [7] L. Feng and W. Liu, The maximal Gutman index of bicyclic graphs, MATCH Commun. Math. Comput. Chem. 66 (2011) 699–708.
- [8] I. Gutman, Distance of line graphs, Graph Theory Notes N. Y. 31 (1996) 49-52.
- [9] I. Gutman, Selected properties of the Schultz molecular topological index, J. Chem. Inf. Comput. Sci. 34 (1994) 1087–1089. doi:/10.1021/ci00021a009

- [10] I. Gutman and L. Pavlović, More on distance of line graphs, Graph Theory Notes N. Y. 33 (1997) 14–18.
- [11] M.H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi and S.G. Wagner, Some new results on distance-based graph invariants, European J. Combin. **30** (2009) 1149–1163. doi:10.1016/j.ejc.2008.09.019
- [12] J.P. Mazorodze, S. Mukwembi and T. Vetrík, On the Gutman index and minimum degree, Discrete Appl. Math. 173 (2014) 77–82. doi:10.1016/j.dam.2014.04.004
- [13] S. Mukwembi, On the upper bound of Gutman index of graphs, MATCH Commun. Math. Comput. Chem. 68 (2012) 343–348.
- [14] M.J. Nadjafi-Arani, H. Khodashenas and A.R. Ashrafi, Relationship between edge Szeged and edge Wiener indices of graphs, Glas. Mat. Ser. III 47 (2012) 21–29. doi:10.3336/gm.47.1.02
- [15] H. Whitney, Congruent graphs and the connectivity of graphs, Amer. J. Math. 54 (1932) 150–168. doi:10.2307/2371086
- [16] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947) 17–20. doi:10.1021/ja01193a005

Received 1 April 2015 Revised 30 December 2015 Accepted 30 December 2015