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On the Gutman Index and Minimum Degree of a Triangle–Free Graph

Jaya Percival Mazorodze, Phillip Mafuta*, Sheunesu Munyira

Department of Mathematics, University of Zimbabwe
Harare, Zimbabwe
mazorodzejaya@gmail.com,
phillipmafuta@gmail.com, munyirask@gmail.com

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Abstract

Gutman index $\mathrm{Gut}(G)$ of a graph G is defined as $\sum_{\{x,y\}\subseteq V(G)} \deg(x)\deg(y)d(x,y)$, where $V(G)$ is the vertex set of G, $\deg(x), \deg(y)$ are the degrees of vertices x and y in G, and $d(x,y)$ is the distance between vertices x and y in G. We show that for finite connected triangle−free graphs of order n and minimum degree δ, where δ is a constant, $\mathrm{Gut}(G) \leq \frac{2^5}{5^5\delta}n^5 + O(n^4)$. Our bound is asymptotically sharp for every $\delta \geq 2$ and it extends results of Mazorodze, Mukwembi and Vetrík [On the Gutman index and minimum degree, Discrete Math. **173** (2014) 77–82].

1 Introduction

Let $G = (V, E)$ be a finite simple connected graph. We denote the order of G by n. The degree of a vertex $v \in V(G)$ is denoted by $deg(v)$. The distance, $d_G(u, v)$, is defined as the length of a shortest $u - v$ path in G.

A real number related to structural graph of a molecule is called a *topological index*. For instance, the *first Zagreb index* and the *second Zagreb index* [9], the *Wiener index* [16], the weighted version of the *Wiener index* known as *Schultz index* or *degree distance* [5,8] and the *Schultz index* of the second kind known as the Gutman index [8]. A topological index related to distance is known as “distance-based topological index”, for instance, the

*Corresponding author.

Wiener index and its invariant, the Gutman index. Topological indices have received a lot of attention, partly because of their numerous applications in chemistry, see for instance, [8, 10, 12, 16]. The topological and graph invariants based on distances between vertices of a graph are widely used for characterizing molecular graphs, establishing relationships between structures and properties of molecules, predicting biological activities of chemical compounds and making their chemical applications, see [13–16].

The Gutman index, $\mathrm{Gut}(G)$, of a graph G was introduced in [8] and is defined as $\sum_{\{x,y\}\subseteq V(G)} \deg(x)\deg(y)d(x,y)$. A question on whether theoretical investigations on the Schultz index of the second kind, focusing on the more difficult case of polycyclic molecules can be done, was posed. Afterwards, a number of authors [2–4, 6, 7, 11, 12] researched on the Gutman index. The following upper bound on the Gutman index was presented in [4];

Theorem 1 *[4] Let G be a connected graph of order n. Then*

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

and the coefficient of n^5 is best possible.

Mukwembi [12] improved the bound in Theorem 1 by replacing $O(n^{\frac{9}{2}})$ by $O(n^4)$. His result in [12] is best possible. In 2014, Mazorodze, Mukwembi and Vetrík [11] investigated on the upper bound of Gutman index based on order and minimum degree. Precisely, they proved the following theorem;

Theorem 2 *[11] Let G be a finite simple connected graph with minimum degree δ and order n. Then*

$$\mathrm{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\delta+1)}n^5 + O\left(n^4\right)$$

and the bound is asymptotically sharp.

The purpose of this paper is to improve Theorem 2 for triangle$-$free graphs for $\delta > 2$. Moreover, our bound is asymptotically tight.

No doubt that research on the Gutman index is an on going process. Attracted by applications of topological indices, Chen and Liu [2, 3] studied the maximal and minimal Gutman index of unicyclic graphs as well as minimal Gutman index of bicyclic graphs. In [1], it was shown that the star graph has a minimal Gutman index, apart from other results presented. Pauraja and Sheeba [13] concentrated on the Gutman indices of the

Cartesian product and wreath product of graphs. Recently, Kazemi and Meimondari [10], were motivated by structural properties of many molecule which are tree like, to work on the expected value and variance of the Gutman index and degree distance in random trees. In this paper, we continue to investigate upper bounds on the Gutman index in triangle−free graphs.

2 Results

First we present Lemma 1, which will be used in the proof of our main result.

Lemma 1 *Let G be a connected triangle-free graph of order n, diameter d and minimum degree δ. Let v, v' be any vertices of G.*

(1) Then $\deg(v) \leq n - \frac{\delta d}{2} + 2\delta$.

(2) If $d(v, v') \geq 3$, *then* $\deg(v) + \deg(v') \leq n - \frac{\delta d}{2} + 4\delta$.

Proof. Let $P : v_0, v_1, \ldots, v_d$ be a diametric path of G. Let $S \subset V(P)$ be the set

$$S := \Big\{v_i : i \equiv 1 \text{ or } 2 \text{ (mode 4) } 1 \leq i \leq d\Big\}.$$

For each $u \in S$, choose any δ neighbors $u_1, u_2, \ldots, u_\delta$ of u and denote the set $\{u_1, u_2, \ldots, u_\delta\}$ by $M(u)$. Let $\mathbf{A} = \cup_{u \in S} M(u)$. Then

$$|\mathbf{A}| \geq \frac{\delta d}{2} .$$

Let v be any vertex of G. We denote by $N(v)$ the open neighbourhood of v, which is the set that consists of neighbours of v. Note that if $v \notin \mathbf{A}$, then v can be adjacent to at most one vertex in S and to neighbours of at most 2 vertices of S. Hence v is adjacent to at most 2δ vertices in $\mathbf{A}$ since G is triangle-free. If $v \in \mathbf{A}$, then it can be checked that v can be adjacent to at most 2δ vertices in $\mathbf{A}$. In both cases we obtain $|\mathbf{A} \cap N(v)| \leq 2\delta$ which implies

$$n \geq |\mathbf{A}| + |N(v)]| - |\mathbf{A} \cap N(v)| \geq +\frac{\delta d}{2} + \deg(v) - 2\delta.$$

Rearranging the terms, we have $\deg(v) \leq n - \frac{\delta d}{2} + 2\delta$, which completes the proof of (1).

Now we prove the statement (2). If v, v' are any two vertices of G, such that $d(v, v') \geq 3$, then $N(v) \cap N(v') = \emptyset$. It follows that

$$n \;\; \geq \;\; |\mathbf{A}| + |N(v)| + |N(v')| - |\mathbf{A} \cap N(v)| - |\mathbf{A} \cap N(v')|$$

$$\geq \frac{\delta d}{2} + \deg(v) + \deg(v') - 2(2\delta).$$

Therefore $\deg(v) + \deg(v') \leq n - \frac{\delta d}{2} + 4\delta$. ■

Now we present our main result.

Theorem 3 *Let G be a connected triangle-free graph of order n and minimum degree δ, where δ is a constant. Then*

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

and this bound is asymptotically sharp.

Proof. We denote the diameter of G by d. Let $P : v_0, v_1, \ldots, v_d$ be a diametric path of G and let $S \subset V(P)$ be the set

$$S := \Big\{v_i : i \equiv 1 \text{ or } 2 \text{ (mode 4) } 1 \leq i \leq d\Big\}.$$

For each $v_i \in S$, choose any δ neighbours $u_1, u_2, \ldots, u_\delta$ of v_i and denote the set $\{u_1, u_2, \ldots, u_\delta\}$ by $M(v_i)$. Let $\mathbf{A} = \cup_{v_i \in S} M(v_i)$. Since G is triangle-free, $M(v_i) \cap M(v_j) = \emptyset$ for any $v_i, v_j \in S$. Since S contains about $\frac{d}{2}$ vertices, we write $|S| = \frac{d}{2} + O(1)$. Then

$$|\mathbf{A}| = \frac{\delta d}{2} + O(1). \tag{1}$$

Now let $\mathcal{V} = \{\{x, y\} : x, y \in V\}$. We partition $\mathcal{V}$ as follows:

$$\mathcal{V} = \mathcal{P} \cup \mathcal{A} \cup \mathcal{B},$$

where

$$\mathcal{P} := \{\{x, y\} \ : \ x \in \mathbf{A} \text{ and } y \in V(G)\},\ \mathcal{A} := \{\{x, y\} \in \mathcal{V} - \mathcal{P} \ : \ d(x, y) \geq 3\}$$

and

$$\mathcal{B} := \{\{x, y\} \in \mathcal{V} - \mathcal{P} \ : \ d(x, y) \leq 2\}.$$

Setting $|\mathcal{A}| = a$, $|\mathcal{B}| = b$, we have $\binom{n}{2} = |\mathcal{P}| + a + b$, and so from (1), $a + b =$

$$\begin{aligned}
\binom{n - |\mathbf{A}|}{2} &= \frac{1}{2}\Big[(n - |\mathbf{A}|)(n - |\mathbf{A}| - 1)\Big] \\
&= \frac{1}{2}\Big[\Big(n - \frac{\delta d}{2}\Big) + O(1)\Big]\Big[\Big(n - \frac{\delta d}{2}\Big) + O(1)\Big] \\
&= \frac{1}{2}\Big(n - \frac{\delta d}{2}\Big)^2 + O(n). \qquad (2)
\end{aligned}$$

Note that

$$\begin{aligned}\mathrm{Gut}(G) &= \sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y) + \sum_{\{x,y\}\in\mathcal{B}} \deg(x)\deg(y)d(x,y)\\ &+ \sum_{\{x,y\}\in\mathcal{P}} \deg(x)\deg(y)d(x,y).\end{aligned}$$

We bound each term separately.

Claim 1 *Assume the notation as above. Then*

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

Proof of Claim 1: We partition S as $S = S_1 \cup S_2 \cup S_3 \cup S_4$ since G is triangle-free, where

$$\begin{aligned} S_1 &= \{v_i \mid i \equiv 1 \pmod 8, 1 \le i \le d\},\\ S_2 &= \{v_i \mid i \equiv 2 \pmod 8, 2 \le i \le d\},\\ S_3 &= \{v_i \mid i \equiv 5 \pmod 8, 5 \le i \le d\},\\ S_4 &= \{v_i \mid i \equiv 6 \pmod 8, 6 \le i \le d\}.\end{aligned}$$

It follows that

$$\mathbf{A} = (\cup_{v\in S_1} M(v)) \cup (\cup_{v\in S_2} M(v)) \cup (\cup_{v\in S_3} M(v)) \cup (\cup_{v\in S_4} M(v)).$$

For each vertex x in $\mathbf{A}$, define the score $s(x)$ of x as

$$s(x) := \sum_{y\in V} \deg(x)\deg(y)d(x,y).$$

Then

$$\begin{aligned}\sum_{\{x,y\}\in\mathcal{P}} \deg(x)\deg(y)d(x,y) \le \sum_{x\in\mathbf{A}} s(x) &= \sum_{x\in(\cup_{v\in S_1} M(v))} s(x)\\ + \sum_{x\in(\cup_{v\in S_2} M(v))} s(x) + \sum_{x\in(\cup_{v\in S_3} M(v))} s(x) &+ \sum_{x\in(\cup_{v\in S_4} M(v))} s(x).\end{aligned}$$

We now consider $\cup_{v\in S_1} M(v)$. For each $u, v \in S_1$, $u \neq v$, we have $M(u) \cap M(v) = \emptyset$ and the neighbourhoods of $M(u)$ and $M(v)$ are also disjoint.

Write the elements of S_1 as $S_1 = \{w_1, w_2, \ldots, w_{|S_1|}\}$. For each $w_j \in S_1$, let $M(w_j) = \{w_1^j, w_2^j, \ldots, w_\delta^j\}$, where $w_1^j, w_2^j, \ldots, w_\delta^j$ are neighbours of w_j. Since $d_G(w, w') \ge 8$ for any $w, w' \in S_1$, then

$$n \ge \deg(w_1) + \deg(w_2) + \cdots + \deg(w_{|S_1|})$$

and for $t = 1, 2, \ldots, \delta$,

$$n \geq \deg(w_t^1) + \deg(w_t^2 + \cdots + \deg(w_t^{|S_1|}.$$

Summing we get

$$\delta n \geq \sum_{x \in (\cup_{u \in S_1} M(u))} \deg(x) + \delta |S_1|.$$

That is,

$$\sum_{x \in (\cup_{u \in S_1} M(u))} \deg(x) \leq \delta n - \delta |S_1|. \tag{3}$$

Similarly,

$$\sum_{x \in (\cup_{u \in S_2} M(u))} \deg(x) \leq \delta n - \delta |S_2|, \tag{4}$$

$$\sum_{x \in (\cup_{u \in S_3} M(u))} \deg(x) \leq \delta n - \delta |S_3| \tag{5}$$

and

$$\sum_{x \in (\cup_{u \in S_4} M(u))} \deg(x) \leq \delta n - \delta |S_4|. \tag{6}$$

Now from Lemma 1, for every $x \in \mathbf{A}$, we have

$$\begin{aligned} s(x) &= \deg(x)\left(\sum_{y \in V} \deg(y) d(x,y)\right) \leq \deg(x)\left(\sum_{y \in V}\Big(n - \frac{\delta d}{2} + 2\delta\Big) d\right) \\ &\leq \deg(x)\left(nd\Big(n - \frac{\delta d}{2} + 2\delta\Big)\right). \end{aligned}$$

This, in conjunction with (3), (4), (5), (6) and the fact that δ is a constant, yields

$$\begin{aligned} \sum_{\{x,y\} \in \mathcal{P}} \deg(x)\deg(y) d_G(x,y) &\leq \sum_{x \in (\cup_{v \in S_1} M(v))} \Big[\deg(x)\Big[nd\Big(n - \frac{\delta d}{2} + 2\delta\Big)\Big]\Big] \\ &+ \sum_{x \in (\cup_{v \in S_2} M(v))} \Big[\deg(x)\Big[nd\Big(n - \frac{\delta d}{2} + 2\delta\Big)\Big]\Big] \\ &+ \sum_{x \in (\cup_{v \in S_3} M(v))} \Big[\deg(x)\Big[nd\Big(n - \frac{\delta d}{2} + 2\delta\Big)\Big]\Big] \\ &+ \sum_{x \in (\cup_{v \in S_4} M(v))} \Big[\deg(x)\Big[nd\Big(n - \frac{\delta d}{2} + 2\delta\Big)\Big]\Big] \\ &= nd\Big(n - \frac{\delta d}{2} + 2\delta\Big)\left(\sum_{x \in (\cup_{v \in S_1} M(v))} \deg(x) + \sum_{x \in (\cup_{v \in S_2} M(v))} \deg(x)\right. \\ &+ \left.\sum_{x \in (\cup_{v \in S_3} M(v))} \deg(x) + \sum_{x \in (\cup_{v \in S_4} M(v))} \deg(x)\right) \end{aligned}$$

$$\begin{aligned} &\leq nd\Big(n - \frac{\delta d}{2} + 2\delta\Big)\Big[\delta n - \delta|S_1| + \delta n - \delta|S_2| + \delta n - \delta|S_3| + \delta n - \delta|S_4|\Big] \\ &= nd\Big(n - \frac{\delta d}{2} + 2\delta\Big)\Big[4\delta n - \delta(|S_1| + |S_2| + |S_3| + |S_4|)\Big] = O(n^4), \end{aligned}$$

as claimed.

Now we bound those pairs of vertices, which are in $\mathcal{B}$.

Claim 2 *Assume the notation as above. Then*

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

Proof of Claim 2: Note that if $\{x,y\} \in \mathcal{B}$, then $d(x,y) \leq 2$. This, together with Lemma 1 and the fact that $b = O(n^2)$, gives

$$\begin{aligned} \sum_{\{x,y\}\in\mathcal{B}} \deg(x)\deg(y)d(x,y) &\leq \sum_{\{x,y\}\in\mathcal{B}} 2\Big(n - \frac{\delta d}{2} + 2\delta\Big)^2 \\ &= 2b\Big(n - \frac{\delta d}{2} + 2\delta\Big)^2 = O(n^4), \end{aligned}$$

so Claim 2 is proven.

Finally, we study pairs of vertices, which are in $\mathcal{A}$.

Claim 3 *Assume the notation above. Then*

$$\sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y) \leq \frac{d}{16}\Big(n - \frac{\delta d}{2}\Big)^4 + O(n^4).$$

Proof of Claim 3: Let $\{w,z\}$ be a pair in $\mathcal{A}$, such that $\deg(w) + \deg(z)$ is maximum. Let $\deg(w) + \deg(z) = t$. Since $\deg(w)\deg(z) \leq \frac{1}{4}(\deg(w) + \deg(z))^2$, we have

$$\deg(w)\deg(z) \leq \frac{1}{4}t^2. \tag{7}$$

Now we find an upper bound on $a = |\mathcal{A}|$. From (2) we have

$$a = \frac{(n - |\mathbf{A}|)(n - |\mathbf{A}| - 1)}{2} - b.$$

Since $|\mathbf{A}| \geq \frac{\delta d}{2}$, then

$$a \leq \frac{(n - \frac{\delta d}{2})(n - \frac{\delta d}{2} - 1)}{2} - b. \tag{8}$$

Note that all pairs $\{x,y\}, x,y \in M(w) - \mathbf{A}$ and all pairs $\{x,y\}, x,y \in M(z) - \mathbf{A}$ (where $M(w)$ and $M(z)$ are the open neighbourhoods of w and z respectively). are in $\mathcal{B}$. Since

w (and z) can be adjacent to at most one vertex in S and to neighbours of at most 2 vertices of S, it follows that w (and z) is adjacent to at most 2δ vertices in $\mathbf{A}$. Then we have

$$\begin{aligned} b &\geq \binom{\deg(w)-2\delta}{2}+\binom{\deg(z)-2\delta}{2} \\ &= \frac{1}{2}([\deg(w)]^2+[\deg(z)]^2)-\frac{4\delta+1}{2}(\deg(w)+\deg(z))+4\delta^2+2\delta \\ &\geq \frac{1}{4}t^2-\frac{4\delta+1}{2}t+4\delta^2+2\delta. \end{aligned}$$

Hence from (8), we get

$$a \leq \frac{(n-\frac{\delta d}{2})(n-\frac{\delta d}{2}-1)}{2}-\frac{1}{4}t^2-\frac{4\delta+1}{2}t+4\delta^2+2\delta.$$

From (7), we have

$$\begin{aligned} \sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y) &\leq \sum_{\{x,y\}\in\mathcal{A}} \frac{t^2 d}{4}=\frac{t^2 ad}{4} \\ &\leq \frac{t^2 d}{4}\left[\frac{(n-\frac{\delta d}{2})(n-\frac{\delta d}{2}-1)}{2}-\frac{1}{4}t^2-\frac{4\delta+1}{2}t+4\delta^2+2\delta\right]. \end{aligned}$$

By Lemma 1, $t \leq n-\frac{\delta d}{2}+4\delta$. Subject to this condition $\frac{t^2 d}{4}\left[\frac{(n-\frac{\delta d}{2})(n-\frac{\delta d}{2}-1)}{2}-\frac{1}{4}t^2-\frac{4\delta+1}{2}t+4\delta^2+2\delta\right]$. is maximized for $t=n-\frac{\delta d}{2}+4\delta$ to give

$$\begin{aligned} &\sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y) \\ &\leq \frac{d}{4}\Big(n-\frac{\delta d}{2}+4\delta\Big)^2\Big[\frac{1}{2}\Big(n-\frac{\delta d}{2}\Big)\Big(n-\frac{\delta d}{2}-1\Big)-\frac{1}{4}\Big(n-\frac{\delta d}{2}+4\delta\Big)^2+O(n)\Big] \\ &= \frac{d}{16}\Big(n-\frac{\delta d}{2}\Big)^4+O(n^4). \end{aligned}$$

which completes the proof of Claim 3.

From Claims 1, 2 and 3, we get

$$\begin{aligned} \mathrm{Gut}(G) &= \sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y)+\sum_{\{x,y\}\in\mathcal{B}} \deg(x)\deg(y)d(x,y) \\ &+ \sum_{\{x,y\}\in\mathcal{P}} \deg(x)\deg(y)d(x,y) \\ &\leq \frac{1}{16}d\Big(n-\frac{\delta d}{2}\Big)^4+O(n^4)+O(n^4)+O(n^4) \\ &= \frac{1}{16}d\Big(n-\frac{\delta d}{2}\Big)^4+O(n^4). \end{aligned}$$

The term

$$\frac{1}{16}d\left(n-\frac{\delta d}{2}\right)^4$$

is maximized, with respect to d, for $d=\frac{2n}{5\delta}$ to give

$$\mathrm{Gut}(G)\le\frac{2^5}{5^5\delta}n^5+O\left(n^4\right),$$

as desired.

It remains to show that the bound is asymptotically sharp. We construct the graph $G'_{n,d,\delta}$ for $d\equiv 1 \pmod 4$. Let $V(G')=G_0+G_1+\ldots+G_d$, where

$$G_i=\begin{cases}\overline{K}_{\delta-1} & \text{if} \quad i\equiv 0 \text{ or } 1 \pmod 4 \quad 4\le i\le d-2,\\ \overline{K}_1 & \text{if} \quad i\equiv 2 \text{ or } 3 \pmod 4 \quad 2\le i\le d-2,\\ \overline{K}_{\lceil\frac{1}{4}(n-\frac{\delta(d-5)}{2})\rceil} & \text{if } i=1 \text{ or } d-1,\\ \overline{K}_{\lfloor\frac{1}{4}(n-\frac{\delta(d-5)}{2})\rfloor} & \text{if } i=0 \text{ or } d.\end{cases}$$

Let $d=\frac{2n}{5\delta}$ be an integer. Then the graph $G_{n,\frac{2n}{5\delta},\delta}$ has order n, minimum degree δ and the Gutman index is $\frac{2^5}{5^5\delta}n^5+O(n^4)$. ■

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