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On the Upper Bound of Gutman Index of Graphs

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Abstract

Let G be a finite connected graph of order n. The Gutman index $\mathrm{Gut}(G)$ of G is defined as $\sum_{\{x,y\}\subseteq V(G)} \deg_G(x)\deg_G(y)d_G(x,y)$, where $\deg_G(x)$ is the degree of vertex x in G and $d_G(x,y)$ is the distance between vertices x and y in G. We prove that $\mathrm{Gut}(G) \leq \frac{2^4}{5^5}n^5 + O(n^4)$. Our bound improves on a bound by Dankelmann, Gutman, Mukwembi and Swart [The edge-Wiener index of a graph, *Discr. Math.* **309** (2009) 3452–3457].

1 Introduction

Let $G = (V, E)$ be a finite, connected, simple graph. We denote the order of G by n, the degree of a vertex v in G by $\deg_G(v)$, and for two vertices u, v in G, $d_G(u, v)$ denotes the usual distance between u and v in G, i. e., the minimum number of edges on a path from u to v. The *Gutman index* $\mathrm{Gut}(G)$ of G is defined as $\mathrm{Gut}(G) = \sum_{\{x,y\}\subseteq V} \deg_G(x)\deg_G(y)d_G(x,y)$. The Gutman index, a Schultz-type molecular topological index and a variant of the well-known and much studied Wiener Index, was introduced in 1994 by Gutman [5] as a kind of a vertex-valency-weighted sum of the distances between all pairs of vertices in a graph. Gutman revealed that in the case of acyclic structures, the index is closely related to the Wiener Index and reflects precisely the same structural features of a molecular as the

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Wiener Index does. A question, on whether theoretical investigations on the Gutman index focusing on the more difficult case of polycyclic molecules can be done, was posed.

Since then, several authors [1, 2, 4, 5, 6] have studied the index and its relationship with other graph parameters. Recently, Dankelmann, Gutman, Mukwembi and Swart [3] presented an upper bound on the Gutman index of a graph in terms of its order. We state their result below.

Theorem 1 [3] *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.

The purpose of this note is to show that the $O(n^{9/2})$ in the bound can be replaced by an $O(n^4)$ term and prove that $\mathrm{Gut}(G) \leq \frac{2^4}{5^5}n^5 + O(n^4)$. This improved bound turns out to be quite challenging and the methods used in [3] seem inadequate to establish the bound. To prove this bound, we will carefully engineer an intricate analysis which can adequately account for the contribution made by pairs of vertices with at least one vertex on a diametral path.

The notation that we use is as follows: The diameter of G, i. e., $\max\{d_G(u,v) : u, v \in V\}$, is denoted by d. For a vertex v, $N[v]$ denotes the closed neighbourhood of v in G, i. e., $N[v] = \{x \in V \ : \ d_G(x,v) \leq 1\}$. Throughout this note, we will assume that $\{x, y\}$ is a pair, i. e., $x \neq y$.

The following observation is folklore and will be required later.

Fact 1 *Let G be a connected graph of order n and diameter d. Then:*

(i) For each vertex x in G, $\deg_G(x) \leq n - d + 1$.

(ii) For each x, y in G with $d_G(x,y) \geq 3$, $\deg_G(x) + \deg_G(y) \leq n - d + 3$.

2 Results

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

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

and the bound is best possible.

Proof: Let d be the diameter of G, $P = u_0, u_1, u_2, \ldots, u_d$ a diametral path and denote $\{u_1, u_2, \ldots, u_{d-1}\}$ by Q. 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 $\mathcal{P} := \{\{x, y\} \ : \ x \in Q\}\}$, $\mathcal{A} := \{\{x, y\} \in \mathcal{V} - \mathcal{P} \ : \ d_G(x, y) \geq 3\}$ and $\mathcal{B} := \{\{x, y\} \in \mathcal{V} - \mathcal{P} \ : \ d_G(x, y) \leq 2\}$. Setting $|\mathcal{A}| = a$, $|\mathcal{B}| = b$, we have

$$a + b = \binom{n-d+1}{2}. \tag{1}$$

Claim 1 $\sum_{\{x,y\} \in \mathcal{P}} \deg_G(x)\deg_G(y)d_G(x, y) \leq d(n-1)(n-d+1)(3n-d+1)$.

Proof of Claim 1: Partition Q as $Q = V_1 \cup V_2 \cup V_3$, where

$$V_1 = \{u_1,\, u_4,\, u_7,\, \ldots\},\ V_2 = \{u_2,\, u_5,\, u_8,\, \ldots\} \text{ and } V_3 = \{u_3,\, u_6,\, u_9,\, \ldots\}.$$

Since P is a shortest path, for x, $y \in V_i$, $i = 1,\, 2,\, 3$, we have $N[x] \cap N[y] = \emptyset$. Thus

$$\sum_{x \in V_i} \deg_G(x) \leq n - |V_i| \text{ for each } i = 1,\, 2,\, 3\ . \tag{2}$$

For each vertex $x \in Q$ let $s(x) := \sum_{y \in V - \{x\}} \deg_G(x)\deg_G(y)d_G(x, y)$. Thus from Fact 1, we have

$$\begin{aligned} s(x) &= \deg_G(x)\left(\sum_{y \in V-\{x\}} \deg_G(y)d_G(x, y)\right) \\ &\leq \deg_G(x)\left(\sum_{y \in V-\{x\}} (n-d+1)d\right) \\ &\leq \deg_G(x)\left[d(n-1)(n-d+1)\right]. \end{aligned}$$

This, in conjunction with (2), yields that for each $i = 1, 2, 3$,

$$\begin{aligned} \sum_{x \in V_i} s(x) &\leq \sum_{x \in V_i} \left(\deg_G(x)\left[d(n-1)(n-d+1)\right]\right) \\ &= \left[d(n-1)(n-d+1)\right] \sum_{x \in V_i} \deg_G(x) \\ &\leq \left[d(n-1)(n-d+1)\right](n - |V_i|). \end{aligned}$$

Therefore,

$$\begin{aligned} \sum_{\{x,y\} \in \mathcal{P}} \deg_G(x)\deg_G(y)d_G(x, y) &\leq \sum_{x \in Q} s(x) = \sum_{x \in V_1} s(x) + \sum_{x \in V_2} s(x) + \sum_{x \in V_3} s(x) \\ &\leq \left[d(n-1)(n-d+1)\right](n - |V_1|) \\ &\quad + \left[d(n-1)(n-d+1)\right](n - |V_2|) \\ &\quad + \left[d(n-1)(n-d+1)\right](n - |V_3|) \\ &= d(n-1)(n-d+1)(3n-d+1), \end{aligned}$$

as claimed.

Claim 2 $\sum_{\{x,y\}\in\mathcal{B}} \deg_G(x)\deg_G(y)d_G(x,y) \le (n-d)(n-d+1)^3.$

Proof of Claim 2: Since $d_G(x,y)\le 2$ for all $\{x,y\}\in\mathcal{B}$, from Fact 1, we have

$$\begin{aligned}\sum_{\{x,y\}\in\mathcal{B}} \deg_G(x)\deg_G(y)d_G(x,y) &\le \sum_{\{x,y\}\in\mathcal{B}} 2(n-d+1)^2\\ &= 2b(n-d+1)^2.\end{aligned}$$

This, together with (1), yields

$$\sum_{\{x,y\}\in\mathcal{B}} \deg_G(x)\deg_G(y)d_G(x,y) \le (n-d)(n-d+1)^3,$$

as claimed.

Claim 3

$$\begin{aligned}\sum_{\{x,y\}\in\mathcal{A}} \deg_G(x)\deg_G(y)d_G(x,y) &\le \frac{1}{16}d(n-d)^4+\frac{3}{4}d(n-d)^3+\frac{21}{8}d(n-d)^2\\ &\quad +\frac{9}{4}d(n-d)-\frac{27}{16}d.\end{aligned}$$

Proof of Claim 3: Let $\{w,z\}$ be a pair in $\mathcal{A}$ such that $\deg_G(w)+\deg_G(z)$ is maximum. Denote $\deg_G(w)+\deg_G(z)$ by t. Thus since

$$\deg_G(x)\deg_G(y)\le\frac{1}{4}\left(\deg_G(x)+\deg_G(y)\right)^2,$$

we have

$$\deg_G(x)\deg_G(y)\le\frac{1}{4}t^2. \tag{3}$$

We first find an upper bound on a, the cardinality of $\mathcal{A}$. Note that from (1),

$$a=\binom{n-d+1}{2}-b. \tag{4}$$

Note that all pairs $\{x,y\},\ x,y\in N[w]-Q$ and all pairs $\{x,y\},\ x,y\in N[z]-Q$ are in $\mathcal{B}$. Since w and z can be adjacent to at most 3 vertices in Q, it follows that

$$\begin{aligned} b &\ge \binom{\deg_G(w)+1-3}{2}+\binom{\deg_G(z)+1-3}{2}\\ &= \frac{1}{2}\left([\deg_G(w)]^2+[\deg_G(z)]^2\right)-\frac{5}{2}\left(\deg_G(w)+\deg_G(z)\right)+6\\ &\ge \frac{1}{4}t^2-\frac{5}{2}t+6.\end{aligned}$$

Hence from (4), we get

$$a \leq \binom{n-d+1}{2} - \frac{1}{4}t^2 + \frac{5}{2}t - 6.$$

Thus, from (3), we now have

$$\begin{aligned}\sum_{\{x,y\}\in\mathcal{A}} \deg_G(x)\deg_G(y)d_G(x,y) &\leq \sum_{\{x,y\}\in\mathcal{A}} \frac{1}{4}t^2 d \\ &\leq \frac{1}{4}t^2 d\left[\binom{n-d+1}{2} - \frac{1}{4}t^2 + \frac{5}{2}t - 6\right].\end{aligned}$$

By Fact 1, $t \leq n-d+3$. Subject to this condition, a simple differentiation shows that the function $\frac{1}{4}t^2 d\left[\binom{n-d+1}{2} - \frac{1}{4}t^2 + \frac{5}{2}t - 6\right]$ is maximized for $t = n-d+3$ to give

$$\begin{aligned}\sum_{\{x,y\}\in\mathcal{A}} \deg_G(x)\deg_G(y)d_G(x,y) &\leq \frac{1}{16}d(n-d)^4 + \frac{3}{4}d(n-d)^3 + \frac{21}{8}d(n-d)^2 \\ &\quad + \frac{9}{4}d(n-d) - \frac{27}{16}d\end{aligned}$$

as claimed.

Combining Claim 1, 2 and 3, we get

$$\begin{aligned}\mathrm{Gut}(G) &= \sum_{\{x,y\}\in\mathcal{A}} \deg_G(x)\deg_G(y)d_G(x,y) + \sum_{\{x,y\}\in\mathcal{B}} \deg_G(x)\deg_G(y)d_G(x,y) \\ &+ \sum_{\{x,y\}\in\mathcal{P}} \deg_G(x)\deg_G(y)d_G(x,y) \\ &\leq \frac{1}{16}d(n-d)^4 + \frac{3}{4}d(n-d)^3 + \frac{21}{8}d(n-d)^2 + \frac{9}{4}d(n-d) - \frac{27}{16}d \\ &+ (n-d)(n-d+1)^3 + d(n-1)(n-d+1)(3n-d+1) \\ &= \frac{1}{16}d(n-d)^4 + O(n^4)\ .\end{aligned}$$

The term $\frac{1}{16}d(n-d)^4$ is maximized for $d = \frac{1}{5}n$ to give

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

as desired.

The graph G_n constructed in [3] shows that the bound is sharp. Precisely for n a multiple of 5, G_n is 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. $\square$

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