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On the Gutman index and minimum degree

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ABSTRACT

The Gutman index 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 graphs of order n and minimum degree δ, where δ is a constant, $\mathrm{Gut}(G) \le \frac{2^4\cdot 3}{5^5(\delta+1)}n^5 + O(n^4)$. Our bound is asymptotically sharp for every $\delta \ge 2$ and it extends results of Dankelmann, Gutman, Mukwembi and Swart (2009) and Mukwembi (2012), whose bound is sharp only for graphs of minimum degree 2.

1. Introduction

Graph indices have been studied for decades because of their extensive applications in chemistry. With Wiener's discovery of a close correlation between the boiling points of certain alkanes and the sum of the distances between vertices in graphs representing their molecular structures, it became apparent that graph indices can potentially be used to predict properties of chemical compounds. Like Wiener's original index, Gutman index is also based on distances between vertices of graphs.

The Gutman index is a natural extension of the Wiener index. The Gutman index of a finite connected graph G is defined as

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

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.

The Gutman index has been studied for example in [1,4–6]. In [6] it was presented that for acyclic structures, the Gutman index reflects exactly the same structural features as the Wiener index. The question, whether theoretical investigations on the Gutman index focusing on the more difficult polycyclic molecules can be done, was posed. Feng [4] studied the Gutman index for unicyclic graphs, and Feng and Liu [5] considered bicyclic graphs in their research. Inequalities relating the Gutman index to the edge-Wiener index, i.e., the Wiener index of the graph's line graph, were presented in [2,7,9], and also in [3]. In their investigations, Dankelmann, Gutman, Mukwembi and Swart [3] showed that if G is a connected graph of order n, then

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

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Mukwembi [8] improved this upper bound and presented the result

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

which shows that $O(n^{\frac{9}{2}})$ can be replaced by $O(n^4)$. However all graphs which attain this bound are of minimum degree 2, which was a motivation for us to study the Gutman index of graphs of minimum degree δ, where $\delta \ge 2$. In this note we improve the bound of Mukwembi for $\delta \ge 3$, and show that

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

where n is the order of the graph G and the minimum degree $\delta \ge 2$ is a constant. Moreover we show that our bound is asymptotically sharp for every $\delta \ge 2$.

2. Results

First we present Lemma 2.1, which will be used in the proof of our main result.

Lemma 2.1. *Let G be a connected graph of order n, diameter d and minimum degree δ. Let v, v' be any vertices of G.*

(1) *Then* $\deg(v) \le n - \frac{1}{3}d(\delta+1) + 2\delta$.
(2) *If* $d(v, v') \ge 3$, *then* $\deg(v) + \deg(v') \le n - \frac{1}{3}d(\delta+1) + 4\delta$.

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

$$S := \left\{ v_{3i+1} : i = 0, 1, 2, \ldots, \left\lfloor \frac{d-1}{3} \right\rfloor \right\}.$$

For each $u \in S$, choose any δ neighbours $u_1, u_2, \ldots, u_\delta$ of u and denote the set $\{u, u_1, u_2, \ldots, u_\delta\}$ by $P[u]$. Let $\mathbf{P} = \cup_{u \in S} P[u]$. Then

$$|\mathbf{P}| = (\delta+1)\left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1 \right).$$

Let v be any vertex of G. We denote by $N[v]$ the closed neighbourhood of v, which is the set that consists of v and its neighbours. Note that if $v \notin \mathbf{P}$, 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 $2\delta + 1$ vertices in $\mathbf{P}$. If $v \in \mathbf{P}$, then it can be checked that v can be adjacent to at most 2δ vertices in $\mathbf{P}$. In both cases we obtain $|\mathbf{P} \cap N[v]| \le 2\delta + 1$ which implies

$$\begin{aligned} n &\ge |\mathbf{P}| + |N[v]| - |\mathbf{P} \cap N[v]| \\ &\ge (\delta+1)\left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1 \right) + (\deg(v)+1) - (2\delta+1) \\ &\ge (\delta+1)\frac{d}{3} + \deg(v) - 2\delta. \end{aligned}$$

Rearranging the terms, we obtain $\deg(v) \le n - \frac{1}{3}d(\delta+1) + 2\delta$, which completes the proof of (1).

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

$$\begin{aligned} n &\ge |\mathbf{P}| + |N[v]| + |N[v']| - |\mathbf{P} \cap N[v]| - |\mathbf{P} \cap N[v']| \\ &\ge (\delta+1)\left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1 \right) + (\deg(v)+1) + (\deg(v')+1) - 2(2\delta+1) \\ &\ge (\delta+1)\frac{d}{3} + \deg(v) + \deg(v') - 4\delta, \end{aligned}$$

which implies $\deg(v) + \deg(v') \le n - \frac{1}{3}d(\delta+1) + 4\delta$. $\square$

Now we present our main result.

Theorem 2.1. *Let G be a connected graph of order n and minimum degree δ. Then*

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

and this bound, for a fixed δ, is asymptotically sharp.