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Abstract

The Gutman index (also known as Schultz index of the second kind) of a graph G is defined as $\mathrm{Gut}(G) = \sum_{u,v \in V(G)} d(u)d(v)d(u,v)$. We show that among all graphs on n vertices, the star graph S_n has minimal Gutman index. In addition, we present upper and lower bounds on Gutman index for graphs with minimal and graphs with maximal Gutman index.

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1 Introduction

The *Wiener index*, $W(G) = \sum_{u,v \in V(G)} d(u,v)$, of a connected graph G is a graph invariant much studied in both mathematical and chemical literature; for details see the reviews [1, 4, 6, 9, 10, 11]. In this paper we are concerned with a variant of the Wiener index called the *Schultz index of the second kind* [9], but for which the name *Gutman index* has also been used [12]. Throughout this paper, the latter name is used. Another variant of Wiener index is the *edge-Wiener index*, defined as the sum of the distances between all pairs of edges of a connected graph G, i.e., $W_e(G) = \sum_{e,f \in E(G)} d(e,f)$; where the distance between two edges is the distance between the corresponding vertices in the line graph of G.

For a vertex $v \in V(G)$, we denote by $d_G(v)$ the degree of v in G. For the sake of simplicity, we write $d(v)$ if the graph G is clear from the context. The minimum vertex degree of a graph G we denote by $\delta = \delta(G)$, and the maximum degree we denote by $\Delta = \Delta(G)$. For $v, u \in V(G)$, we denote by $d_G(u,v)$ (or simply $d(u,v)$) the length of a shortest path in G between u and v.

The Gutman index of a connected graph G is defined as

$$\mathrm{Gut}(G) = \sum_{u,v \in V(G)} d(u)d(v)d(u,v).$$

The Gutman index of graphs attracts attention just recently. Dankelmann et al. [3] presented an asymptotic upper bound for the Gutman index and also established the relation between the edge-Wiener index and Gutman index of graphs. Chen and Liu studied the maximal and minimal Gutman index of unicyclic graphs [2], and maximal Gutman index of bicyclic graphs was determined by Feng and Liu [8]. Gutman [9] gave the following relation between the Gutman and the Wiener index for a tree T on n vertices,

$$\mathrm{Gut}(T) = 4W(T) - (2n-1)(n-1). \tag{1}$$

In [5] lower and upper bounds for the Wiener index for a graph G on n vertices were given. Namely, there it was shown that

$$\binom{n}{2} = W(K_n) \le W(G) \le W(P_n) = \binom{n+1}{3}, \tag{2}$$

where K_n and P_n are the complete graph and path, respectively, on n vertices.

The complete bipartite graph $K_{1,n-1}$ is called a star, denote by S_n. A tree T is a *complete* k*-regular* if every vertex has degree 1 or k. The diameter of a graph G is defined as $diam(G) = \max_{u,v\in V(G)} d(u,v)$. A tree where all leaves are on the same distance to the root is called a *balanced tree*.

Here, we present upper and lower bounds on the Gutman index, we prove that among all connected graphs on n vertices a star, S_n, has minimal Gutman index, and a path, P_n, has maximal Gutman index. We also determine bound of Gutman index for a connected graph with bounded minimum or maximum degree.

2 The graph with minimal Gutman index

First, we show a general lower bound on Gutman index.

Theorem 2.1. *For every connected graph G on n vertices, it holds that*

$$(2n-3)(n-1) = \mathrm{Gut}(S_n) \leq \mathrm{Gut}(G).$$

The equality holds if and only if G is star S_n.

Proof. First, consider the case when G has no leaves, i.e., $\delta(G) \geq 2$. Then,

$$\begin{aligned}\mathrm{Gut}(G) &= \sum_{u,v\in V(G)} d(u)d(v)d(u,v) \geq 4 \sum_{u,v\in V(G)} d(u,v)\\ &\geq 4\binom{n}{2} = 2n(n-1) > (2n-3)(n-1) = \mathrm{Gut}(S_n).\end{aligned}$$

The case when $\delta(G) = 1$, we prove by induction on the number of vertices. For $n = 1$ the claim of the proposition is obvious. Assume that the theorem holds for a graph G on n vertices. We construct a graph G' on $n+1$ vertices from G by adding a leaf x incident to $a \in V(G)$. We show that by adding x, the Gutman index increases by at least $4n-3 = \mathrm{Gut}(S_{n+1}) - \mathrm{Gut}(S_n)$.

To simplify the exposition of the proof, let $D_G(u,v) = d_G(u)d_G(v)d_G(u,v)$, and similarly $D_{G'}(u,v) = d_{G'}(u)d_{G'}(v)d_{G'}(u,v)$.

$$\begin{aligned}\mathrm{Gut}(G') - \mathrm{Gut}(G) = &\sum_{v \in V(G)\setminus\{a\}} [D_{G'}(a,v) - D_G(a,v)] + \sum_{v \in V(G)} D_{G'}(x,v) \\ &+ \sum_{u,v \in V(G)\setminus\{a\}} [D_{G'}(u,v) - D_G(u,v)].\end{aligned}$$

From the construction of the graph G', it is obvious that $d_{G'}(u,v) = d_G(u,v)$, and $d_{G'}(x,v) = 1 + d_G(a,v)$ for every $u, v \in V(G)$. Also notice that the degree of a increases by 1, but all the other vertex degrees are not changed. It is clear that the contribution of $u, v \in V(G) \setminus \{a\}$ is the same in $\mathrm{Gut}(G')$ and in $\mathrm{Gut}(G)$. Hence,

$$\begin{aligned}\mathrm{Gut}(G') - \mathrm{Gut}(G) &= \sum_{v \in V(G)\setminus\{a\}} d_G(v)d_G(a,v) + \sum_{v \in V(G)} d_{G'}(v)(d_G(a,v)+1) \\ &= 2\sum_{v \in V(G)\setminus\{a\}} d_G(v)d_G(a,v) + \sum_{v \in V(G)} d_G(v) + 1.\end{aligned}$$

Since $d_G(a,v) \geq 1$ and $d_G(v) \geq 1$ for every $v \in V(G) \setminus \{a\}$ and $\sum_{v \in V(G)} d_G(v) = 2|E(G)| \geq 2(n-1)$, we infer $\mathrm{Gut}(G') - \mathrm{Gut}(G) \geq 4n - 3$. Moreover the equality holds if and only if $d_G(v) = 1$ for every $v \in V(G) \setminus \{a\}$, which satisfies only the star S_n. □

From (1) and (2) we find that for every tree T on n vertices $\mathrm{Gut}(T) \leq O(n^3)$. Together with Theorem 2.1, we obtain the following result.

Corollary 2.1. *For every tree T on n vertices, it holds that*

$$(n-1)(2n-3) = \mathrm{Gut}(S_n) \leq \mathrm{Gut}(T) \leq \mathrm{Gut}(P_n) = \frac{(n-1)(2n^2-4n+3)}{3}.$$

3 Bounds on graphs with minimal Gutman index

In this section, we consider graphs with minimal Gutman index. First, we show lower and upper bounds for graphs with minimum degree at least two.

Proposition 3.1. *A connected graph G on n vertices with minimum degree at least $\delta \geq 2$ and minimal Gutman index satisfies*

$$\delta(\delta+1)n^2 > \mathrm{Gut}(G) \geq \frac{\delta^2 n}{2}(2n - \delta - 2).$$

Proof. First, we show the lower bound

$$\begin{aligned}\mathrm{Gut}(G) &= \frac{1}{2}\sum_u d(u)\sum_v d(v)\, d(u,v) \geq \frac{n}{2}\min_u \left(d(u)\sum_v d(v)\, d(u,v)\right)\\ &\geq \frac{n\,\delta}{2}\min_u \left(d(u)\sum_v d(u,v)\right).\end{aligned}$$

Since there are $d(u)$ vertices on distance one to u, and $n-d(u)-1$ vertices on distance at least two to u, we have further

$$\mathrm{Gut}(G) \geq \frac{n\,\delta}{2}\min_u \Big(d(u)(d(u)+2(n-d(u)-1))\Big) = \frac{n\,\delta}{2}\min_u \Big(d(u)(2n-d(u)-2)\Big).$$

The quadratic function $f(x) = x(2n-x-2)$ with $\delta \leq x \leq n-1$ has its minimum at δ. Thus,

$$\mathrm{Gut}(G) \geq \frac{n\,\delta}{2}\delta(2n-\delta-2).$$

Now, we show the upper bound. By Erdős-Gallai theorem [7], there exist a graph H on $n-1$ vertices such that

(a) all its vertices are of degree $\delta - 1$ if δ or n is odd; or

(b) a vertex x is of degree δ and all others are of degree $\delta - 1$ if both δ and n are even

exists.

From H, we construct the graph H^* by introducing a new vertex y adjacent to all vertices of H. Observe that $e_H = |E(H)| = \left\lceil \frac{(\delta-1)\,(n-1)}{2} \right\rceil$. The contribution of y to $\mathrm{Gut}(H^*)$ is

$$\sum_{v\in V(H)} d_{H^*}(y) d_{H^*}(v) d_{H^*}(y,v) \leq (n-1)((n-2)\delta + \delta + 1).$$

The contribution of x to $\mathrm{Gut}(H^*)$ is

$$\sum_{v\in V(H)} d_{H^*}(x) d_{H^*}(v) d_{H^*}(x,v) \leq (\delta+1)(\delta^2 + 2\delta(n-\delta-2)),$$

and the remaining vertices of H^* contribute with

$$\sum_{u,v\in V(H)\setminus\{x\}} d_{H^*}(u)d_{H^*}(v)d_{H^*}(u,v) = \delta^2\left[e_H - \delta + 2\left(\binom{n-2}{2} - e_H + \delta\right)\right].$$

Thus,

$$\begin{aligned}
\mathrm{Gut}(H^*) \leq &(n-1)((n-2)\delta + \delta + 1) + (\delta+1)(\delta^2 + 2\delta(n-\delta-2)) \\
&+ \delta^2\left[e_H - \delta + 2\left(\binom{n-2}{2} - e_H + \delta\right)\right] \\
=&(n-1)(n\delta - \delta + 1) + (\delta+1)(2n\delta - \delta^2 - 4\delta) + \delta^2\left[2\binom{n-2}{2} - e_H + \delta\right] \\
<&\delta(\delta+1)n^2 - \frac{1}{2}(\delta^3 + 5\delta - 2)n - \frac{\delta^2}{2}(\delta+1) - 3\delta - 1 \\
<&\delta(\delta+1)n^2.
\end{aligned}$$

□

Corollary 3.1. *A connected graph G on n vertices with minimum degree at least $\delta \geq 2$ and minimal Gutman index satisfies*

$$\delta(\delta+1)n^2 - O(n) \geq \mathrm{Gut}(G) \geq \delta^2 n^2 - O(n).$$

Now, we show an upper bound for graphs with minimal Gutman index and maximum degree at most Δ.

Proposition 3.2. *A connected graph G on n vertices with maximum degree at most $\Delta > 2$ and minimal Gutman index satisfies*

$$\mathrm{Gut}(G) < 4(n^2 - 8n + 4)\log_{\Delta-1} n.$$

Proof. Let G is a Δ-regular balanced tree on n vertices. If $\mathrm{diam}(G) = 2k$, then $n - 1 = \Delta\frac{(\Delta-1)^k - 1}{\Delta - 2}$. This tree has $\Delta(\Delta-1)^{k-1} = \frac{(\Delta-2)n+2}{\Delta-1}$ leaves and $\frac{n-2}{\Delta-1}$ inner vertices. Notice that $\log_{\Delta-1}\frac{\Delta-2}{\Delta}n < k < \log_{\Delta-1} n$.

The tree G has three types of vertex pairs: a pair of two leaves, a leaf and an inner vertex, and a pair of two inner vertices. Their contribution to the Gutman index is:

- *Two leaves*: the distance between two leaves is at most $\mathrm{diam}(G) = 2k$, so their contribution to the Gutman index is at most

$$\binom{\frac{(\Delta-2)n+2}{\Delta-1}}{2}2k < \left(\frac{(\Delta-2)n+2}{\Delta-1}\right)^2 k.$$

- *A leave and an inner vertex*: since every inner vertex has degree Δ, and the distance between any two vertices is at most $2k$, these pairs contribution in the sum is less than
$$\frac{(\Delta-2)n+2}{\Delta-1}\cdot\frac{n-2}{\Delta-1}2k\Delta.$$
- *Two inner vertices*: these pair contribute at most
$$\binom{\frac{n-2}{\Delta-1}}{2}2k\Delta^2<\left(\frac{n-2}{\Delta-1}\right)^2\Delta^2k.$$

Now,

$$\begin{aligned}\mathrm{Gut}(G)&<\left(\frac{(\Delta-2)n+2}{\Delta-1}\right)^2k+\frac{(\Delta-2)n+2}{\Delta-1}\cdot\frac{n-2}{\Delta-1}2k\Delta+\left(\frac{n-2}{\Delta-1}\right)^2\Delta^2k\\&=\frac{4k}{(\Delta-1)^2}(\Delta-1)^2(n^2-8n+4)\\&<4(n^2-8n+4)\log_{\Delta-1}n,\end{aligned}$$

and this proves the upper bound. □

Note that if G is a graph with maximum degree $\Delta\le 2$, then G is a path.

4 Bounds on graphs with maximal Gutman index

In this section, we consider graphs with maximal Gutman index. First, we show lower and upper bounds for graphs with maximum degree at most Δ.

Proposition 4.1. *Let G be a connected graph on n vertices with maximum degree $\Delta(G)\le\Delta$, and maximal Gutman index. Then, the following holds:*
$$\frac{(n+1)^3}{27}\Delta^2\le\mathrm{Gut}(G)\le\binom{n+1}{3}\Delta^2.$$

Proof. For the lower bound we consider the graph Q which is illustrated in Figure 1. To simplify the calculation, we assume that $s=(\Delta+1)3$, bn and $3an/(\Delta+1)$ are integers. The graph Q has n vertices, so $2an+bn=n$ holds.

A pair (x,y), where x is a vertex from Q^L and y is a vertex from Q^R, contributes to $\mathrm{Gut}(Q)$ at least $\Delta^2(bn+1)$. Since there are an vertices in bough, Q^L and Q^R, the contribution of these vertices is $(an)^2\Delta^2(bn+1)$. Under the constraint $2a+b=1$,

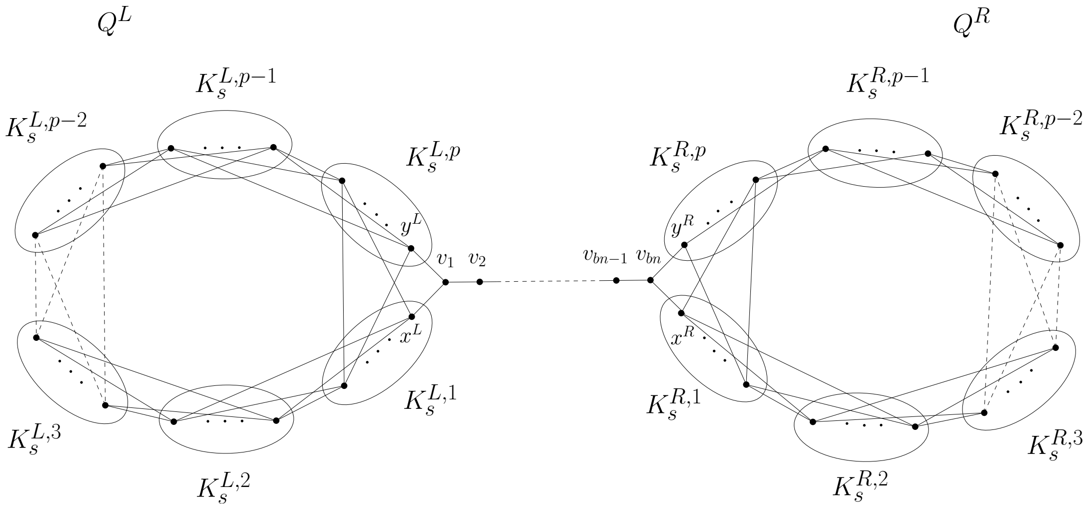

Figure 1: The graph Q consist of two identical parts Q^L and Q^R connected by path on nb vertices. Q^L (resp. Q^R) consists of a lexicographic product $P_p[K_s]$, $s = \frac{\Delta+1}{3}$, plus the all edges between the vertices of $K_s^{L,1}$ and $K_s^{L,p}$ (resp. $K_s^{R,1}$ and $K_s^{R,p}$) except the edge $x^L y^L$ (resp. $x^R y^R$). The vertices x^L and y^L (resp. x^R and y^R) are adjacent to the vertex v_1 (resp. v_{bn}).

the expression $(an)^2\Delta^2(bn+1)$ attains maximum for $a = (n+1)/3n$ and $b = \frac{n-2}{3n}$. Finally we have

$$\mathrm{Gut}(Q) \geq \frac{(n+1)^3}{27}\Delta^2.$$

Now, we show the upper bound. From (2) and $\Delta(G) \leq \Delta$, it follows that

$$\mathrm{Gut}(G) \leq \sum_{u,v} \Delta^2\, d(u,v) = \Delta^2 W(G) \leq \Delta^2 W(P_n) = \Delta^2 \binom{n+1}{3}.$$

□

For graphs with bounded maximum degree, we obtain the following result.

Corollary 4.1. *Let G be a connected graph on n vertices with bounded maximum degree Δ. Then,*

$$O(n^3) \geq \mathrm{Gut}(G) \geq \Omega(n^2 \log n),$$

and those bounds can be attained.

Proof. The lower bound follows directly from Proposition 3.2 and the upper bound from Proposition 4.1. □

In the sequel, we consider lower and upper bounds for graphs with maximal Gutman index and minimum degree at least δ. Dankelmann et al. [3] presented the following upper bound on Gutman index.

Theorem 4.1. *(Dankelmann et al. [3]) Let G be a connected graph on n vertices. 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 the best possible.

Now, we present the lower bound.

Proposition 4.2. *A connected graph G on n vertices with minimum degree at least δ, and maximal Gutman index satisfies*

$$\frac{2^5}{5^5} \frac{(n+\delta-1)^5}{\delta^5} < \mathrm{Gut}(G).$$

Proof. To show the bound consider the graph L given in Figure 2. To simplify the

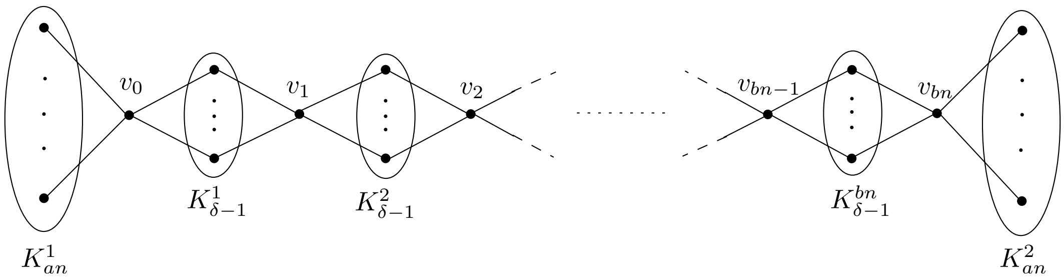

Figure 2: The graph L consists of bn cliques $K^1_{\delta-1}, \ldots, K^{bn}_{\delta-1}$ on $\delta-1$ vertices, and $bn+1$ other vertices $v_0, \ldots, v_{bn}$ such that every vertex of clique $K^i_{\delta-1}$ is adjacent to v_{i-1} and v_i. Moreover, v_0 is adjacent to every vertex of a clique K^1_{an} on an vertices and v_{bn} is adjacent to every vertex of other clique K^2_{an} on an vertices.

calculations, we assume that the parameters $a\,n$ and $b\,n$ of the graph L are integers. Since L has n vertices, $2an + bn\delta + 1 = n$. We consider only the contribution of the pairs (x, y) to $\mathrm{Gut}(L)$, where $x \in V(K^1_{an})$, $y \in V(K^2_{an})$, which is more than $(an)^4 2(bn+1)$. Under the constrain $2an + bn\delta + 1 = n$, the expression $2(an)^4(bn+1)$ attains the maximum at $bn + 1 = \dfrac{n+\delta-1}{5\delta}$ and $an = 2(bn+1)$. Thus, we obtain

$$\mathrm{Gut}(G) > \frac{2^5}{5^5} \frac{(n+\delta-1)^5}{\delta^5}.$$

$\square$

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