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The Maximal Gutman Index of Bicyclic Graphs

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Abstract

Let G be a simple connected graph. The Gutman index $S(G)$ is defined as

$$S(G) = \sum_{u,v \in V(G)} d_G(u) d_G(v) d(u\ v)$$

where $d_G(u)$ is the degree of u, $d(u\ v)$ is the distance between u and v and the summation goes over all pairs of vertices in G. In this paper, we determine that among all bicyclic graphs of order n, the graph formed from two triangles linked by a path has maximal Gutman index.

1 Introduction

Topological indices and graph invariants based on the distances between the vertices of a graph are widely used in theoretical chemistry to establish relations between the structure and the properties of molecules. They provide correlations with physical, chemical and thermodynamic parameters of chemical compounds [9].

We follow standard notations in graph theory in [1]. Let $G = (V(G), E(G))$ be a simple undirected graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. For $u \in V(G)$, we use $d_G(u)$ (or just $d(u)$ for short) to denote the degree of u. The distance $d(v, u)$ between vertices v and u is defined as the length of a shortest path between them. The *diameter* of G, denoted by $diam(G)$, is the maximum distance over all pairs of vertices in G. A connected graph G is called *unicyclic* if $n = m$. Similarly, a connected graph G is called *bicyclic* if $n = m - 1$.

The Wiener index is defined as the sum of all distances between unordered pairs of vertices

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

The Wiener index is considered as one of the most used topological index with high correlation with many physical and chemical indices of molecular compounds (for the recent survey on Wiener index see [10] and [11]).

The parameter $D'(G)$ is called the *degree distance* of G and it was introduced by Dobrynin and Kochetova [12] and Gutman [14] as a graph-theoretical descriptor for characterizing alkanes by an integer, it can be considered as a weighted version of the Wiener index

$$D'(G) = \sum_{u,v \in V(G)} (d_G(u) + d_G(v))d(u, v) = \sum_{v \in V(G)} d_G(v) \cdot D_G(v),$$

where the summation goes over all pairs of vertices in G and $D(v) = \sum_{u \in V(G)} d(u, v)$. In fact, when G is a tree on n vertices, it has been demonstrated that Wiener index and degree distance are closely related by (see [14, 16]) $D'(G) = 4W(G) - n(n - 1)$.

The Gutman index is put forward in [14] and called there the *Schultz index of the second kind*, but for which the name *Gutman index* has also sometimes been used [18]. It is defined as

$$S(G) = \sum_{u,v \in V(G)} d_G(u)d_G(v)d(u, v),$$

where the summation goes over all pairs of vertices in G. When G is a tree on n vertices, Wiener index and Gutman index are closely related by (see [14]) $S(G) = 4W(G) - (2n - 1)(n - 1)$.

The Gutman index of C_n and P_n can be calculated as

$$S(C_n) = 4W(C_n) = \begin{cases} \frac{1}{2}n^3, & \text{if } n \text{ is even} \\ \frac{1}{2}(n^3 - n), & \text{if } n \text{ is odd} . \end{cases}$$

$$S(P_n) = \frac{1}{3}(n-1)(2n^2 - 4n + 3).$$

The degree distance of graphs is well studied in the literature. Dankelmann et al. [7] presented an asymptotically sharp upper bounds of degree distance of graphs with given order and diameter. In [8], the degree distance of polyhex nanotubes was obtained. Tomescu [20] got the degree distance of graphs with small cyclomatic number. Tomescu [19] presented the graph with minimum degree distance among all connected graphs and disproved a conjecture posed in [12]. Zhou [24] reported some bounds for the degree distance. In [21], Tomescu obtained the minimum degree distance of unicyclic and bicyclic graphs. In [17], Ilić, Stevanović and Klavžar characterized the degree distance of partial Hamming graphs.

The Gutman index of graphs as well as its application in chemistry attracts attention just recently. In [6], the authors presented an asymptotic upper bound for the Gutman index and also established the relation between the edge–Wiener index and Gutman index. Chen and Liu studied the maximal and minimal Gutman index of unicyclic graphs [2], and they also determined the minimal Gutman index of bicyclic graphs [3]. In [13], the authors derived relations between $W(G)$ and $D'(G)$, $S(G)$ for the (unbranched) hexagonal chain composed of n fused hexagons. In [4, 5, 22, 23], the authors derived the formulas for calculating the modified Schultz index of nanotubes covered by C_4 and polyhex nanotubes, C_4C_8 nanotubes.

In this paper, motivated by the work in [3], we continue to study the Gutman index of bicyclic graphs. We derive sharp upper bounds for the Gutman index of bicyclic graphs and characterize the corresponding extremal graphs.

2 Lemmas and Results

Let us define $D_G^*(v) = \sum_{x \in V(G)} d_G(x) d(v,x)$.

Lemma 2.1 *Let G be a bicyclic graph on $n \geq 4$ vertices and $v \in V(G)$. Then $D_G^*(v) \leq n^2 + 2n - 14$.*

Proof: The proof is by induction on n. If $n = 4$, then $G \cong K_4 - e$ and it is easy to check that statement holds. Similarly, we directly verify the induction hypothesis for $n = 5$ and G is obtained from $K_4 - e$ by attaching one pendant edge or $G \cong C_5 + e$. Let $n \geq 6$.

Case 1: v is a pendant vertex.

Let w be its neighbor. Clearly $G-v$ satisfies the inductive hypothesis, and so

$$\begin{aligned} D^*_G(v) &= \sum_{x\in V(G)\setminus\{v\}} d_G(x)(d(x,w)+1) = D^*_{G-v}(w) + \sum_{x\in V(G)\setminus\{v\}} d_G(x) \\ &\le (n-1)^2 + 2(n-1) - 14 + \ 2(n+1)-1\big) \\ &= n^2+2n-14\ . \end{aligned}$$

Case 2: v is not a pendant vertex.

Since $d_G(v)\ge 2$, there are at least two vertices at distance 1 from v, and the remaining vertices have distance at most $2,3,\dots,n-2$ from v. Let us define f_i to be the sum of the degrees of the vertices at distance i from v in G, where $i\in\{0,1,2,\dots\}$. Clearly,

$$D^*_G(v) = \sum_{i\ge 1} i f_i.$$

Now $\sum_{i\ge1} f_i = 2n+2-d_G(v)\le 2n$. Moreover we have $f_1\ge 3$ since $d_G(v)\ge 2$ and $n\ge 6$, and $f_i\ge 2$ if $f_{i+1}>0$. Since $diam(G)\le n-2$ we have $f_i=0$ for $i\ge n-1$. It is easy to see that, subject to these conditions, the sum $\sum_{i\ge1} i f_i$ is maximized if $f_1=3$, $f_i=2$ for $i=2,3,\dots,n-3$, and $f_{n-2}=5$. Hence

$$D^*_G(v)\le 3\cdot 1 + 2(2+3+\ldots+(n-3)) + 5(n-2) = n^2-3.$$

Now the result follows since $n^2-3 < n^2+2n-14$ for $n\ge 6$. $\square$

Lemma 2.2 *Let G be a connected graph with m edges, v a pendant vertex of G and w its neighbor. Then*

$$S(G) = S(G-v) + 2D^*_{G-v}(w) + 2m - 1.$$

Proof: From the definition, we have

$$\begin{aligned} S(G) &= \sum_{x,y\in V(G)\setminus\{v,w\}} d_G(x)d_G(y)d(x,y) + \sum_{x\in V(G)\setminus\{v,w\}} d_G(x)d_G(w)d(x,w) \\ &\quad + \sum_{x\in V(G)\setminus\{v,w\}} d_G(x)d_G(v)d(x,v) + d_G(w)d_G(v)d(w,v) \\ &= \sum_{x,y\in V(G)\setminus\{v,w\}} d_{G-v}(x)d_{G-v}(y)d_{G-v}(x,y) \end{aligned}$$

$$
\begin{aligned}
&+\sum_{x\in V(G)\setminus\{v,w\}} d_{G-v}(x)(d_{G-v}(w)+1)d_{G-v}(x,w)\\
&+\sum_{x\in V(G)\setminus\{v,w\}} d_{G-v}(x)(d_{G-v}(x,w)+1)+d_{G-v}(w)+1\\
=&\sum_{x,y\in V(G)\setminus\{v,w\}} d_{G-v}(x)d_{G-v}(y)d_{G-v}(x,y)\\
&+\sum_{x\in V(G)\setminus\{v,w\}} d_{G-v}(x)d_{G-v}(w)d_{G-v}(x,w)+\sum_{x\in V(G)\setminus\{v,w\}} d_{G-v}(x)d_{G-v}(x,w)\\
&+\sum_{x\in V(G)\setminus\{v,w\}} d_{G-v}(x)d_{G-v}(x,w)+\sum_{x\in V(G)\setminus\{v,w\}} d_{G-v}(x)+d_{G-v}(w)+1\\
=&\ S(G-v)+2D^*_{G-v}(w)+2m-1\ .
\end{aligned}
$$

So the result follows. □

Lemma 2.3 *Let G be a connected graph with a cut-vertex v such that G_1 and G_2 are two connected subgraphs of G having v as the only common vertex and $G_1\cup G_2=G$. Let $m_i=|E(G_i)|$ for $i=1,2$. Then*

$$S(G)=S(G_1)+S(G_2)+2m_1D^*_{G_2}(v)+2m_2D^*_{G_1}(v).$$

Proof: From the definition of $S(G)$, we have

$$
\begin{aligned}
S(G)\ =&\sum_{x,y\in V(G_1)\setminus\{v\}} d_G(x)d_G(y)d(x,y)+\sum_{x,y\in V(G_2)\setminus\{v\}} d_G(x)d_G(y)d(x,y)\\
&+\sum_{x\in V(G_1)\setminus\{v\}} d_G(x)d_G(v)d(x,v)+\sum_{x\in V(G_2)\setminus\{v\}} d_G(x)d_G(v)d(x,v)\\
&+\sum_{x\in V(G_1)\setminus\{v\},y\in V(G_2)\setminus\{v\}} d_G(x)d_G(y)d(x,y)\\
=&\sum_{x,y\in V(G_1)\setminus\{v\}} d_G(x)d_G(y)d(x,y)+\sum_{x,y\in V(G_2)\setminus\{v\}} d_G(x)d_G(y)d(x,y)\\
&+\sum_{x\in V(G_1)\setminus\{v\}} d_G(x)(d_{G_1}(v)+d_{G_2}(v))d(x,v)\\
&+\sum_{x\in V(G_2)\setminus\{v\}} d_G(x)(d_{G_1}(v)+d_{G_2}(v))d(x,v)
\end{aligned}
$$

$$
\begin{aligned}
& + \sum_{x\in V(G_1)\backslash\{v\}, y\in V(G_2)\backslash\{v\}} d_G(x)d_G(y)(d(x,v)+d(v,y)) \\
= & \sum_{x,y\in V(G_1)\backslash\{v\}} d_G(x)d_G(y)d(x,y) + \sum_{x,y\in V(G_2)\backslash\{v\}} d_G(x)d_G(y)d(x,y) \\
& + \sum_{x\in V(G_1)\backslash\{v\}} d_G(x)d_{G_1}(v)d(x,v) + \sum_{x\in V(G_1)\backslash\{v\}} d_G(x)d_{G_2}(v)d(x,v) \\
& + \sum_{x\in V(G_2)\backslash\{v\}} d_G(x)d_{G_2}(v)d(x,v) + \sum_{x\in V(G_2)\backslash\{v\}} d_G(x)d_{G_1}(v)d(x,v) \\
& + \sum_{x\in V(G_1)\backslash\{v\}, y\in V(G_2)\backslash\{v\}} (d_G(x)d_G(y)d(x,v)+d_G(x)d_G(y)d(y,v)) \\
= & \ S(G_1)+S(G_2)+d_{G_2}(v)D^*_{G_1}(v)+d_{G_1}(v)D^*_{G_2}(v) \\
& +(2m_1-d_{G_1}(v))D^*_{G_2}(v)+(2m_2-d_{G_2}(v))D^*_{G_1}(v) \\
= & \ S(G_1)+S(G_2)+2m_1D^*_{G_2}(v)+2m_2D^*_{G_1}(v)\ .
\end{aligned}
$$

which implies the result. □

Lemma 2.4 *[2] Let G be a unicyclic graph of order $n \geq 5$. Then*

$$S(G) \leq \frac{2}{3}n^3 - \frac{29}{3}n + 23.$$

The equality holds if and only if G is the graph obtained from C_3 by attaching one pendant path of order $n-3$ to one vertex of C_3.

Lemma 2.5 *Let H be a connected graph with $h \geq 2$ vertices and m edges and C_k be a cycle of order $k \geq 4$. Let F be the graph of order k obtained from C_3 by attaching one pendant path of order $k-3$ to one vertex of C_3. Further suppose G_1 is the graph obtained from H and C_k by identifying one vertex in H and one vertex in C_k; G_2 is the graph obtained from H and F by identifying one vertex in H and the pendant vertex in F. Then we have $S(G_1) < S(G_2)$.*

Proof: Suppose $H \cap C_k = H \cap F = \{v\}$. From Lemma 2.3, we have

$$
\begin{aligned}
S(G_1) &= S(H)+S(C_k)+2mD^*_{C_k}(v)+2kD^*_H(v)\,, \\
S(G_2) &= S(H)+S(F)+2mD^*_F(v)+2kD^*_H(v)\ .
\end{aligned}
$$

Hence

$$S(G_1) - S(G_2) = S(C_k) - S(F) + 2m(D^*_{C_k}(v) - D^*_F(v)).$$

From Lemma 2.4, we have $S(C_k) - S(F) < 0$. And

$$D^*_F(v) = 2D_F(v) + (k-3) = k^2 - 5 > 2\left\lfloor \frac{k^2}{4} \right\rfloor = D^*_{C_k}(v).$$

This completes the proof. □

Let G be a bicyclic graph. The *base* of G, denoted by $\widehat{G}$, is the (unique) minimal bicyclic subgraph of G. It is easy to see that $\widehat{G}$ is the unique bicyclic subgraph of G containing no pendant vertices, while G can be obtained from $\widehat{G}$ by attaching trees to some vertices of $\widehat{G}$.

It is well known that there are the following three types of bicyclic graphs containing no pendant vertices:

Let $B(p,q)$ be the bicyclic graph obtained from two vertex-disjoint cycles C_p and C_q by identifying vertices u of C_p and v of C_q.

Let $B(p,l,q)$ be the bicyclic graph obtained from two vertex-disjoint cycles C_p and C_q by joining vertices u of C_p and v of C_q by a new path $uu_1u_2\ldots u_{l-1}v$ with length l ($l \geq 1$).

Let $B(P_k, P_l, P_m)$, $1 \leq m \leq \min\{k,l\}$ be the bicyclic graph obtained from three pairwise internal disjoint paths from a vertex x to a vertex y. These three paths are $xv_1v_2\ldots v_{k-1}y$ with length k, $xu_1u_2\ldots u_{l-1}y$ with length l, and $xw_1w_2\ldots w_{m-1}y$ with length m.

From the above, one can get that

Lemma 2.6 *Let G be a bicyclic graph of order n. Then at least one of the following holds: (i) G has two vertex disjoint cycles and the minimum degree is 2; (ii) G has a pendant vertex; (iii) G is 2-connected; (iv) G is obtained from two vertex disjoint cycles by identifying two vertices, one from each cycle.*

Let B_n be the graph of order $n \geq 6$ obtained from two triangles linked by a path. It can be checked that

$$S(B_n) = \frac{2}{3}n^3 + 2n^2 - \frac{53}{3}n + 27.$$

Theorem 2.7 *Let G be a bicyclic graph of order $n \geq 6$. Then*

$$S(G) \leq \frac{2}{3}n^3 + 2n^2 - \frac{53}{3}n + 27.$$

The equality holds if and only if $G \cong B_n$.

Proof: The proof is based on induction on n. If $n = 6$, then it is easy to verify that the theorem holds, so let $n \geq 7$. We distinguish into the following four cases by Lemma 2.6.

Case 1: G has two vertex disjoint cycles and the minimum degree is 2. By applying Lemma 2.5, we easily get that $S(G) \leq S(B_n)$.

Case 2: G has a pendant vertex. Let v be a pendant vertex of G and let w be its neighbor. Clearly $G - v$ satisfies the inductive hypothesis, and so we have

$$S(G-v) \leq \frac{2}{3}(n-1)^3 + 2(n-1)^2 - \frac{53}{3}(n-1) + 27.$$

By Lemma 2.1, Lemma 2.2 and the induction hypothesis, we obtain

$$\begin{aligned} S(G) &= S(G-v) + 2D^*_{G-v}(w) + 2m - 1\ . \\ &\leq \left(\frac{2}{3}(n-1)^3 + 2(n-1)^2 - \frac{53}{3}(n-1) + 27\right) \\ &\quad +2\ \ (n-1)^2 + 2(n-1) - 14) + 2n + 1 \\ &= \frac{2}{3}n^3 + 2n^2 - \frac{53}{3}n + 17 < \frac{2}{3}n^3 + 2n^2 - \frac{53}{3}n + 27\,, \end{aligned}$$

as desired.

Case 3: G is 2-connected. From Lemma 2.6, G must be of the form $B(P_k, P_l, P_m)$, $1 \leq m \leq \min\{k, l\}$. Similar as Case 2 in Lemma 2.1, we need the expression $D^*_G(v) = \sum_{i\geq 1} i f_i$.

Now $\sum_{i\geq 1} f_i = 2n + 2 - d_G(v) \leq 2n$. Moreover we have $f_1 \geq 4$ since $d_G(v) \geq 2$ and $n \geq 6$, and $f_i \geq 2$ if $f_{i+1} > 0$. Since $diam(G) \leq \lfloor \frac{n}{2} \rfloor$ we have $f_i = 0$ for $i > \lfloor \frac{n}{2} \rfloor$. It is easy to see that, subject to these conditions, the sum $\sum_{i\geq 1} i f_i$ is maximized if $f_i = 4$ for $i = 1, 2, 3, \ldots, \lfloor \frac{n}{2} \rfloor - 1$, and $f_{\lfloor \frac{n}{2} \rfloor} = 2n - 4\lfloor \frac{n}{2} \rfloor + 4$. Hence

$$\begin{aligned} D^*_G(v) &\leq 4\left(1 + 2 + 3 + \ldots + \left(\lfloor\frac{n}{2}\rfloor - 1\right)\right) + \lfloor\frac{n}{2}\rfloor\left(2n - 4\lfloor\frac{n}{2}\rfloor + 4\right) \\ &\leq 4\left(1 + 2 + 3 + \ldots + \left(\frac{n}{2} - 2\right)\right) + 6 \cdot \frac{n}{2} = \frac{1}{2}(n^2 + 8)\ . \end{aligned}$$

Therefore,

$$\begin{aligned} S(G) &= \frac{1}{2} \sum_{u \in V(G)} d_G(u) \sum_{v \in V(G)} d_G(v) d(u,v) \\ &= \frac{1}{2} \sum_{u \in V(G)} d_G(u) D^*_G(u) \\ &\leq \frac{1}{2}\frac{1}{2}(n^2 + 8)(2n + 2) = \frac{1}{2}n^3 + \frac{1}{2}n^2 + 4n + 4\,, \end{aligned}$$

and since $\frac{1}{2}n^3 + \frac{1}{2}n^2 + 4n + 4 < \frac{2}{3}n^3 + 2n^2 - \frac{53}{3}n + 27$ for $n \geq 7$, the statement follows.

CASE 4: G is the union of two cycles that have exactly one vertex in common. Similar as in CASE 1, by applying Lemma 2.5, we easily get that $S(G) \leq S(B_n)$. $\square$

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