Gutman index of the Mycielskian and its complement

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Abstract

Let $G$ be a finite connected simple graph. The Gutman index $\text{Gut}(G)$ of $G$ is defined as $\sum_{\{u,v\} \subseteq V(G)} d_G(u,v) \deg_G(u) \deg_G(v)$, where $\deg_G(u)$ is the degree of vertex $u$ in $G$ and $d_G(u,v)$ is the distance between two vertices $u$ and $v$ in $G$. In this paper, we determine exact value of the Gutman index of Mycielskian of graphs with diameter two. Also, we determine exact value of the Gutman index of the complement of arbitrary Mycielskian graphs.

1 Introduction

Throughout this paper we consider (non trivial) simple graphs, that are finite and undirected graphs without loops or multiple edges. Let $G = (V(G), E(G))$ be a connected graph of order $n = |V(G)|$ and of size $m = |E(G)|$. The distance between two vertices $u$ and $v$ is denoted by $d_G(u,v)$ and is the length of a shortest path between $u$ and $v$ in $G$. The diameter of $G$ is $\max\{d_G(u,v) : u, v \in V(G)\}$. It is well known that almost all graphs have diameter two. The degree of vertex $u$ is the number of edges adjacent to $u$ and is denoted by $\deg_G(u)$.

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A chemical graph is a graph whose vertices denote atoms and edges denote bonds between those atoms of any underlying chemical structure. A topological index for a (chemical) graph $G$ is a numerical quantity invariant under automorphisms of $G$ and it does not depend on the labeling or pictorial representation of the graph. Topological indices and graph invariants based on the distances between vertices of a graph or vertex degrees are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds, and making their chemical applications.

The concept of topological index came from work done by Harold Wiener in 1947 while he was working on boiling point of paraffin [8]. The Wiener index $W(G)$ of $G$ is defined as $W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)$. Two important topological indices introduced about forty years ago by Ivan Gutman and Trinajstić [4] are the first zagreb index $M_1(G)$ and the second zagreb index $M_1(G)$ which are defined as

$$M_1(G) = \sum_{uv \in E(G)} (\deg_G(u) + \deg_G(v)) = \sum_{x \in V(G)} (\deg_G(x))^2, \quad M_2(G) = \sum_{uv \in E(G)} \deg_G(u) \deg_G(v).$$

The degree distance was introduced by Dobrynin and Kochetova [11] and Gutman [3] as a weighted version of the Wiener index. The degree distance of $G$, denoted by $DD(G)$, is defined as follows and it is computed for important families of graphs (see [5] for instance):

$$DD(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)(\deg_G(u) + \deg_G(v)).$$

The Gutman index (another variant of the well known and much studied Wiener Index) was introduced in 1994 by Gutman [3] as

$$Gut(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v) \deg_G(u) \deg_G(v).$$

For more results in this subject or related subjects see [6].

For a graph $G = (V, E)$, the Mycielskian of $G$ is the graph $\mu(G)$ (or simply, $\mu$) with the disjoint union $V \cup X \cup \{x\}$ as its vertex set and $E \cup \{v_i x_j : v_i v_j \in E\} \cup \{x x_j : 1 \leq j \leq n\}$ as its edge set, where $V = \{v_1, v_2, ..., v_n\}$ and $X = \{x_1, x_2, ..., x_n\}$, see [7]. The Mycielskian and generalized Mycielskians have fascinated graph theorists a great deal. This has resulted in studying several graph parameters of these graphs [2].

In this paper we determine the Gutman index of the Mycielskian of each graph with diameter two. Also, we determine the Gutman index of the complement of Mycielskian of arbitrary graphs.
2 Gutman index of the Mycielskian

In order to determine the Gutman index of Mycielskian graphs, we need the following observations. From now on we will always assume that $G$ is a connected graph,

$$V(G) = \{v_1, v_2, ..., v_n\}, \quad X = \{x_1, x_2, ..., x_n\}, \quad V(G) \cap X = \emptyset, \quad x \notin V(G) \cup X,$$

and $\mu$ is the Mycielskian of $G$, where

$$V(\mu) = V(G) \cup X \cup \{x\}, \quad E(\mu) = E(G) \cup \{v_ix_j : v_iv_j \in E(G)\} \cup \{xx_i : 1 \leq i \leq n\}.$$

**Observation 1.** Let $\mu$ be the Mycielskian of $G$. Then for each $v \in V(\mu)$ we have

$$\deg_{\mu}(v) = \begin{cases} n & v = x \\ 1 + \deg_{G}(v_i) & v = x_i \\ 2\deg_{G}(v_i) & v = v_i. \end{cases}$$

**Observation 2.** In the Mycielskian $\mu$ of $G$, the distance between two vertices $u, v \in V(\mu)$ are given as follows.

$$d_{\mu}(u, v) = \begin{cases} 1 & u = x, v = x_i \\ 2 & u = x, v = x_i \\ 2 & u = x, v = x_i \\ d_{G}(v_i, v_j) & u = v_i, v = v_j, d_{G}(v_i, v_j) \leq 3 \\ 4 & u = v_i, v = v_j, d_{G}(v_i, v_j) \geq 4 \\ 2 & u = v_i, v = x_j, i = j \\ d_{G}(v_i, v_j) & u = v_i, v = x_j, i \neq j, d_{G}(v_i, v_j) \leq 2 \\ 3 & u = v_i, v = x_j, i \neq j, d_{G}(v_i, v_j) \geq 3. \end{cases}$$

Specially, the diameter of the Mycielskian graph is at most four.

There are $|E(G)|$ unordered pairs of vertices in $V = V(G)$ whose distance is 1, and

$$\sum_{(u,v) \in V \times V, \quad d_{G}(u,v) = 1} (\deg_{G}(u) + \deg_{G}(v)) = 2 \sum_{uv \in E(G)} (\deg_{G}(u) + \deg_{G}(v)) = 2M_1(G).$$

**Lemma 1.** Let $G$ be a graph of size $m$ whose vertex set is $V = \{v_1, v_2, ..., v_n\}$. Then,

$$\sum_{\{v_i, v_j\} \subseteq V} (\deg_{G}(v_i) + \deg_{G}(v_j)) = (n - 1)2m.$$
Proof. For each \( i \in [n] = \{1, 2, ..., n\} \), \( |\{i, j\} \subseteq [n] : j \neq i| = n - 1 \). Therefore,
\[
\sum_{\{i,j\} \subseteq [n]} (\deg_G(v_i) + \deg_G(v_j)) = \sum_{i=1}^{n} (n - 1) \deg_G(v_i) = (n - 1)2m.
\]
\[\Box\]

Lemma 2. Let \( G \) be a graph of size \( m \) whose vertex set is \( V = \{v_1, v_2, ..., v_n\} \). Then,
\[
\sum_{\{v_i,v_j\} \subseteq V} \deg_G(v_i) \deg_G(v_j) = 2m^2 - \frac{1}{2} M_1(G).
\]

Proof. The sum of all vertex degrees equals twice the number of edges, hence
\[
(2m)^2 = \left( \sum_{i=1}^{n} \deg_G(v_i) \right)^2 = \sum_{i=1}^{n} (\deg_G(v_i))^2 + 2 \sum_{\{v_i,v_j\} \subseteq V} \deg_G(v_i) \deg_G(v_j)
\]
\[
= M_1(G) + 2 \sum_{\{v_i,v_j\} \subseteq V} \deg_G(v_i) \deg_G(v_j),
\]
which completes the proof. \[\Box\]

It is a well known fact that almost all graphs have diameter two. This means that graphs of diameter two play an important role in the theory of graphs and their applications.

Theorem 1. Let \( G \) be an \( n \)-vertex graph of size \( m \) whose diameter is 2. If \( \mu \) is the Mycielskian of \( G \), then the Gutman index of \( \mu \) is given by
\[
Gut(\mu) = 6Gut(G) + 3M_1(G) + \text{DD}(G) + 2(n + m)(2m + n) + n(6m - 1) + 6m.
\]

Proof. By the definition of Gutman index, we have
\[
Gut(\mu) = \sum_{\{u,v\} \subseteq V(\mu)} d_{\mu}(u,v) \deg_{\mu}(u) \deg_{\mu}(v).
\]
Regarding to the different possible cases which \( u \) and \( v \) can be choosen from the set \( V(\mu) \), the following cases are considered. In what follows, the notations are as before and two observations [1] and [2] are applied for computing degrees and distances in \( \mu \).

Case 1. \( u = x \) and \( v \in X \):
\[
\sum_{i=1}^{n} d_{\mu}(x,x_i) \deg_{\mu}(x) \deg_{\mu}(x_i) = \sum_{i=1}^{n} n(1 + \deg_G(v_i)) = n^2 + 2m.
\]

Case 2. \( u = x \) and \( v \in V(G) \):
\[
\sum_{i=1}^{n} d_{\mu}(x,v_i) \deg_{\mu}(x) \deg_{\mu}(v_i) = \sum_{i=1}^{n} 2n(2 \deg_G(v_i)) = 8nm.
\]
Case 3. \{u,v\} \subseteq X:

Using Lemma 1 and Lemma 2, we have

\[
\sum_{\{x_i,x_j\} \subseteq X} d_\mu(x_i,x_j) \deg_\mu(x_i) \deg_\mu(x_j) = \sum_{\{x_i,x_j\} \subseteq X} 2(1 + \deg_G(v_i))(1 + \deg_G(v_j)) \\
= \sum_{\{i,j\} \subseteq [n]} 2(1 + \deg_G(v_i))(1 + \deg_G(v_j)) \\
= 2 \sum_{\{i,j\} \subseteq [n]} (1 + (\deg_G(v_i) + \deg_G(v_j)) + \deg_G(v_i) \deg_G(v_j)) \\
= 2 \left( \binom{n}{2} + (n-1)2m + 2m^2 - \frac{1}{2}M_1(G) \right) \\
= n(n-1) + 4(n-1)m + 4m^2 - M_1(G).
\]

Case 4. \{u,v\} \subseteq V(G):

Since the diameter of \(G\) is two, Observation 2 implies that \(d_\mu(v_i,v_j) = d_G(v_i,v_j)\). Hence,

\[
\sum_{\{v_i,v_j\} \subseteq V(G)} d_\mu(v_i,v_j) \deg_\mu(v_i) \deg_\mu(v_j) = \sum_{\{v_i,v_j\} \subseteq V(G)} d_G(v_i,v_j)(2 \deg_G(v_i))(2 \deg_G(v_j)) \\
= 4 \text{ Gut}(G).
\]

Case 5. \(u = v_i\) and \(v = x_i, 1 \leq i \leq n:\)

\[
\sum_{i=1}^{n} d_\mu(v_i,x_i) \deg_\mu(v_i) \deg_\mu(x_i) = \sum_{i=1}^{n} 2(2 \deg_G(v_i))(1 + \deg_G(v_i)) \\
= 4 \sum_{i=1}^{n} (\deg_G(v_i) + (\deg_G(v_i))^2) \\
= 4(2m + M_1(G)).
\]

Case 6. \(u = v_i\) and \(v = x_j, i \neq j:\)

\[
\sum_{\{v_i,x_j\} \subseteq V(\mu) \atop i \neq j} d_\mu(v_i,x_j) \deg_\mu(v_i) \deg_\mu(x_j) = \sum_{\{v_i,x_j\} \subseteq V(\mu) \atop i \neq j} d_\mu(v_i,x_j)(2 \deg_G(v_i))(1 + \deg_G(v_j)) \\
= 2 \sum_{\{v_i,x_j\} \subseteq V(\mu) \atop i \neq j} d_\mu(v_i,x_j) \deg_G(v_i) + d_\mu(v_i,x_j) \deg_G(v_i) \deg_G(v_j).
\]

Since \(d_\mu(v_i,x_j) = d_G(v_i,x_j), d_G(v_i,v_i) = 0\), using Observation 2 we see that

\[
\sum_{\{v_i,x_j\} \subseteq V(\mu) \atop i \neq j} d_\mu(v_i,x_j) \deg_G(v_i) = \sum_{\{v_i,x_j\} \subseteq V(\mu) \atop i \neq j} d_G(v_i,x_j) \deg_G(v_i) \\
= \sum_{\{v_i,x_j\} \subseteq V(\mu) \atop i \neq j} d_G(v_i) \deg_G(v_i) \\
= \sum_{\{i,j\} \subseteq [n]} d_G(v_i,v_j)(\deg_G(v_i) + \deg_G(v_j)) \\
= DD(G).
\]
Using similar arguments, it is straightforward to see that

\[
\sum_{\{v_i, x_j\} \subseteq V(\mu)} d_\mu(v_i, x_j) \deg_G(v_i) \deg_G(v_j) = 2 \sum_{\{i, j\} \subseteq [n]} d_G(v_i, x_j) \deg_G(v_i) \deg_G(v_j)
\]

\[
= 2 \sum_{\{i, j\} \subseteq [n]} d_G(v_i, v_j) \deg_G(v_i) \deg_G(v_j)
\]

\[
= 2 \text{Gut}(G).
\]

Now the result follows through these six cases. \(\Box\)

### 3 Gutman index of the complement of Mycielskian

In order to determine the Gutman index of the complement of Mycielskian graphs, we need two following observations.

**Observation 3.** Let \(\overline{\mu}\) be the complement of Mycielskian \(\mu\) of \(G\). Then, for each \(v \in V(\overline{\mu})\)

\[
\deg_{\overline{\mu}}(v) = \begin{cases} 
  n & v = x \\
  2n - (1 + \deg_G(v_i)) & v = x_i \\
  2n - 2 \deg_G(v_i) & v = v_i.
\end{cases}
\]

**Observation 4.** In the complement of Mycielskian \(\mu\) of \(G\), the distance between two vertices \(u, v \in V(\overline{\mu})\) are given as follows.

\[
d_{\overline{\mu}}(u, v) = \begin{cases} 
  2 & u = x, \ v = x_i \\
  1 & u = x, \ v = v_i \\
  1 & u = x_i, \ v = x_j \\
  1 & u = v_i, \ v = v_j, \ d_G(v_i, v_j) > 1 \\
  2 & u = v_i, \ v = v_j, \ d_G(v_i, v_j) = 1 \\
  1 & u = v_i, \ v = x_j, \ i = j \\
  1 & u = v_i, \ v = x_j, \ i \neq j, \ d_G(v_i, v_j) > 1 \\
  2 & u = v_i, \ v = x_j, \ i \neq j, \ d_G(v_i, v_j) = 1.
\end{cases}
\]

Specially, the diameter of \(\overline{\mu}\) is exactly 2.

**Theorem 2.** Let \(G\) be an \(n\)-vertex graph of size \(m\) and let \(\overline{\mu}\) be the complement of the Mycielskian \(\mu\) of \(G\). Then, the Gutman index of \(\overline{\mu}\) is given by

\[
\text{Gut}(\overline{\mu}) = 4M_2(G) - (10n + \frac{5}{2})M_1(G) + 8n^4 - 2n^3 + \frac{1}{2}(n^2 - n) - 4mn(2n^2 - 2n + 3) + 2m(n + 1) + 26m^2.
\]

**Proof.** By the definition, we have

\[
\text{Gut}(\overline{\mu}) = \sum_{\{u, v\} \subseteq V(\overline{\mu})} d_{\overline{\mu}}(u, v) \deg_{\overline{\mu}}(u) \deg_{\overline{\mu}}(v).
\]
We consider the following cases. For computing degrees and distances in $\mu$ two observations $3$ and $4$ are applied.

**Case 1.** $u = x$ and $v \in X$:

$$\sum_{i=1}^{n} d_{\mu}(x, x_i) \deg_{\mu}(x) \deg_{\mu}(x_i) = \sum_{i=1}^{n} 2n(2n - 1 - \deg_{G}(v_i))$$

$$= 2n((2n - 1)n - 2m).$$

**Case 2.** $u = x$ and $v \in V(G)$:

$$\sum_{i=1}^{n} d_{\mu}(x, v_i) \deg_{\mu}(x) \deg_{\mu}(v_i) = \sum_{i=1}^{n} n(2n - 2 \deg_{G}(v_i))$$

$$= 2n (n^2 - 2m).$$

**Case 3.** $\{u, v\} \subseteq X$:

Using Lemma $1$ and Lemma $2$ we see that

$$\sum_{\{x_i, x_j\} \subseteq X} d_{\mu}(x_i, x_j) \deg_{\mu}(x_i) \deg_{\mu}(x_j) = \sum_{\{x, x\} \subseteq X} (2n - 1 - \deg_{G}(v_i)) (2n - 1 - \deg_{G}(v_j))$$

$$= \sum_{\{i, j\} \subseteq [n]} (2n - 1 - \deg_{G}(v_i)) (2n - 1 - \deg_{G}(v_j))$$

$$= \sum_{\{i, j\} \subseteq [n]} \left((2n - 1)^2 - (2n - 1)(\deg_{G}(v_i) + \deg_{G}(v_j)) + \deg_{G}(v_i) \deg_{G}(v_j)\right)$$

$$= \left(\frac{n}{2}\right)(2n - 1)^2 - (2n - 1)(n - 1)2m + 2m^2 - \frac{1}{2}M_1(G).$$

**Case 4.** $\{u, v\} \subseteq V(G)$:

By Observation $4$, $d_{\mu}(v_i, v_j)$ is 1 whenever $v_i v_j \notin E(G)$ and is 2 otherwise. Also,

$$\{\{v_i, v_j\} \subseteq V : i \neq j, v_i v_j \notin E(G)\} = \{\{v_i, v_j\} \subseteq V : i \neq j\} \setminus \{\{v_i, v_j\} \subseteq V : v_i v_j \in E(G)\}.$$

Thus,

$$\sum_{\{v_i, v_j\} \subseteq V(G)} d_{\mu}(v_i, v_j) \deg_{\mu}(v_i) \deg_{\mu}(v_j) = \sum_{v_i v_j \notin E(G)} 1(2n - 2 \deg_{G}(v_i))(2n - 2 \deg_{G}(v_j))$$

$$+ \sum_{v_i v_j \in E(G)} 2(2n - 2 \deg_{G}(v_i))(2n - 2 \deg_{G}(v_j))$$

$$= \sum_{\{v_i, v_j\} \subseteq V(G)} (2n - 2 \deg_{G}(v_i))(2n - 2 \deg_{G}(v_j))$$

$$+ \sum_{v_i v_j \in E(G)} (2n - 2 \deg_{G}(v_i))(2n - 2 \deg_{G}(v_j)).$$
Now, two lemmas 1 and 2 imply that
\[
\sum_{\{v_i, v_j\} \subseteq V} (2n - 2 \deg_G(v_i))(2n - 2 \deg_G(v_j)) = 4n^2 \left(\frac{n}{2}\right) - 4n(n - 1)2m + 4(2m^2 - \frac{1}{2} M_1(G)).
\]

Also, the definitions of first and second Zagreb indices imply that
\[
\sum_{v_i, v_j \in E(G)} (2n - 2 \deg_G(v_i))(2n - 2 \deg_G(v_j)) = 4n^2m - 4n \ M_1(G) + 4 \ M_2(G).
\]

**Case 5.** \(u = v_i\) and \(v = x_i, 1 \leq i \leq n:\)
\[
\sum_{i=1}^{n} d_\mathcal{P}(v_i, x_i) \deg_\mathcal{P}(v_i) \deg_\mathcal{P}(x_i) = \sum_{i=1}^{n} (2n - 2 \deg_G(v_i))(2n - 1 - \deg_G(v_i)) = 2n^2(2n - 1) - (6n - 2)2m + 2M_1(G).
\]

**Case 6.** \(u = v_i\) and \(v = x_j, i \neq j:\)
By Observation 1 \(d_\mathcal{P}(v_i, x_j) = d_\mathcal{P}(v_j, x_i)\) is 1 when \(v_i v_j \notin E(G)\), otherwise is 2. Also,
\[
\{(v_i, v_j) : i \neq j, v_i v_j \notin E(G)\} = \{(v_i, v_j) : i \neq j\} \setminus \{(v_i, v_j) : v_i v_j \in E(G)\}.
\]
Thus,
\[
\sum_{\{v_i, x_j\} \subseteq V(\mathcal{G}) \atop i \neq j} d_\mathcal{P}(v_i, x_j) \deg_\mathcal{P}(v_i) \deg_\mathcal{P}(x_j) = \sum_{(v_i, v_j) \atop v_i, v_j \notin E(G)} 1(2n - 2 \deg_G(v_i))(2n - 1 - \deg_G(v_j))
+ \sum_{(v_i, v_j) \atop v_i v_j \in E(G)} 2(2n - 2 \deg_G(v_i))(2n - 1 - \deg_G(v_j))
= \sum_{(v_i, v_j) \atop i \neq j} (2n - 2 \deg_G(v_i))(2n - 1 - \deg_G(v_j))
+ \sum_{(v_i, v_j) \atop v_i v_j \in E(G)} (2n - 2 \deg_G(v_i))(2n - 1 - \deg_G(v_j))
\]

Each vertex \(v_j\) can be paired with \(n-1\) vertices \(v_i\) as \((v_i, v_j), i \neq j\). Hence \(\sum_{(v_i, v_j)} \deg_G(v_j) = (n-1) \sum_{j=1}^{n} \deg_G(v_j)\) which is equal to \((n-1)2m\). Also, note that \(\sum_{(v_i, v_j)} \deg_G(v_i) \deg_G(v_j)\) equals \(2 \sum_{(v_i, v_j)} \deg_G(v_i) \deg_G(v_j)\). Now, since \(|\{(v_i, v_j) : i \neq j\}| = n(n - 1)\), we obtain
\[
\sum_{(v_i, v_j) \atop i \neq j} (2n - 2 \deg_G(v_i))(2n - 1 - \deg_G(v_j)) = 2n(2n - 1)n(n - 1) - 2n(n - 1)2m
- 2(2n - 1)(n - 1)2m + 4(2m^2 - \frac{1}{2} M_1(G)).
\]
Note that $\left| \{(v_i, v_j) : v_i v_j \in E(G)\} \right| = 2m$ and $\sum_{(v_i, v_j) \in E(G)} \deg_G(v_i) = \sum_{i=1}^{n} (\deg_G(v_i))^2$, because each vertex $v_i$ has $\deg_G(v_i)$ neighbours and appears $\deg_G(v_i)$ times in the desired summation. Thus, using Lemma [2] we see that

$$\sum_{(v_i, v_j) \in E(G)} (2n - 2 \deg_G(v_i))(2n - 1 - \deg_G(v_j)) = 2n(2n - 1)2m - 2nM_1(G)$$

$$= -2(2n - 1)M_1(G) + 4(2m^2 - \frac{1}{2}M_1(G)).$$

Now the result follows through the cases 1 to 6. \qed

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