On the Randić and degree distance indices of the Mycielskian of a graph

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Abstract

In a search for triangle-free graphs with arbitrarily large chromatic numbers, Mycielski developed a graph transformation that transforms a graph into a new graph which is called the Mycielskian of that graph. In this paper we provide some sharp bounds for the Randić index of the Mycielskian graphs. Also, we determine the degree distance index of the Mycielskian of each graph with diameter two.

1 Introduction

Throughout this paper we consider 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.

When $u$ is a vertex of $G$, then the neighbor of $u$ in $G$ is the set $N_G(u) = \{v : uv \in E(G)\}$.

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The degree of \( u \) is the number of edges adjacent to \( u \) and is denoted by \( \deg_G(u) \). A graph is said to be regular if all of its vertices have the same degree.

In a search for triangle-free graphs with arbitrarily large chromatic number, Mycielski [11] developed an interesting graph transformation as follows. 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 \( E \cup \{v_iv_j : v_iv_j \in E\} \cup \{xx_j : 1 \leq j \leq n\} \) as its edge set, where \( V = \{v_1, v_2, ..., v_n\} \) and \( X = \{x_1, x_2, ..., x_n\} \). The Mycielskian and generalized Mycielskians have fascinated graph theorists a great deal. This has resulted in studying several graph parameters of these graphs (see for instance [3]).

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. These indices may be used to derive quantitative structure-property or structure-activity relationships (QSPR/QSAR).

The concept of topological index came from work done by Harold Wiener in 1947 while he was working on boiling point of paraffin [13]. He named this index as path number. Later on, path number was renamed as Wiener index and then theory of topological index started. The Wiener index of \( G \) is defined as \( W(G) = \sum_{(u,v) \subseteq V(G)} d_G(u,v) \). The very first and oldest degree based topological index is Randić index [12] denoted by \( R(G) \) and introduced by Milan Randić in 1975 as

\[
R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg_G(u) \deg_G(v)}}
\]

It has been closely correlated with many chemical properties. The general Randić index was proposed by Bollobás and Erdös [2] and Amic et al. [1] independently, in 1998. Then it has been extensively studied by both mathematicians and theoretical chemists [3], [8]. For a survey of results, we refer to the new book by Li and Gutman [10]. An important topological index introduced about forty years ago by Ivan Gutman and Trinajstić [7] is the Zagreb index or more precisely first zagreb index denoted by \( M_1(G) \) and was defined
as the sum of degrees of end vertices of all edges of $G$,

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

The degree distance was introduced by Dobrynin and Kochetova [4] and Gutman [6] 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 [9] for instance):

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

In this paper we provide upper and lower bounds for the Randic index of the Mycielskian graphs. Also, we determine the degree distance index of the Mycielskian of each graph with diameter two. Up to now and as far as we know, these parameters are not determined for the Mycielskian graphs.

2 The Degree Distance index

In order to determine the degree distance index of the Mycielskian graph, we need the following observations. Throughout this paper we suppose that $G$ is a connected graph, $V(G) = \{v_1, v_2, ..., v_n\}$, $X = \{x_1, x_2, ..., x_n\}$, $V(G) \cap X = \emptyset$, $x \notin V(G) \cup X$, and

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

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. Distances between the vertices of the Mycielskian $\mu$ of $G$ are given as follows. For each $u, v \in V(\mu)$ we have

$$d_\mu(u,v) = \begin{cases} 
  1 & u = x, \ v = x_i \\
  2 & u = x, \ v = v_i \\
  2 & u = x_i, \ v = x_j \\
  d_G(v_i, v_j) & u = v_i, \ v = v_j, \ d_G(v_i, v_j) \leq 3 \\
  4 & u = v_i, \ v = v_j, \ d_G(v_i, v_j) \geq 4 \\
  2 & u = v_i, \ v = x_j, \ i = j \\
  d_G(v_i, v_j) & u = v_i, \ v = x_j, \ i \neq j, \ d_G(v_i, v_j) \leq 2 \\
  3 & u = v_i, \ v = x_j, \ i \neq j, \ d_G(v_i, v_j) \geq 3.
\end{cases}$$
Note that there are \(|E(G)|\) unordered pairs of vertices in \(V(G)\) whose distance is 1,
\[
| \{ \{u, v\} \subseteq V(G) : d_G(u, v) = 1 \} | = |E(G)|.
\]
Also,
\[
\sum_{\{u, v\} \subseteq V(G) \atop d_G(u, v) = 1} (\deg_G(u) + \deg_G(v)) = \sum_{uv \in E(G)} (\deg_G(u) + \deg_G(v)) = M_1(G).
\]

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

**Lemma 1.** If \(G\) is a graph of diameter 2, then
\[
\sum_{\{v_i, v_j\} \subseteq V(G) \atop d_G(v_i, v_j) = 2} (\deg_G(v_i) + \deg_G(v_j)) = 2(n - 1)|E(G)| - M_1(G).
\]

**Proof.** Since the diameter of \(G\) is two and each vertex \(v_i \in V(G)\) has \(\deg_G(v_i)\) neighbours in \(G\), the number of vertices in \(V\) which their distance to \(v_i\) is two equals \(n - 1 - \deg_G(v_i)\). This implies that
\[
\sum_{\{v_i, v_j\} \subseteq V(G) \atop d_G(v_i, v_j) = 2} (\deg_G(v_i) + \deg_G(v_j)) = \sum_{i=1}^{n} (n - 1 - \deg_G(v_i)) \deg_G(v_i)
\]
\[
= (n - 1) \sum_{i=1}^{n} \deg_G(v_i) - \sum_{i=1}^{n} (\deg_G(v_i))^2
\]
\[
= 2(n - 1)|E(G)| - M_1(G).
\]

\(\square\)

**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 degree distance index of \(\mu\) is given by
\[
DD(\mu) = 4DD(G) - M_1(G) + (7n - 1)n + (8n + 12)m,
\]
where, \(M_1(G)\) is the first Zagreb index of \(G\).

**Proof.** By the definition of degree distance index, we have
\[
DD(\mu(G)) = \sum_{\{u, v\} \subseteq V(\mu)} d_\mu(u, v) (\deg_\mu(u) + \deg_\mu(v)).
\]
Regarding to the different possible cases which \( u \) and \( v \) can be choosen from the set \( V(\mu) \), we consider the following cases. We use the same notations as before. For computing degrees and distances two observations 1 and 2 are applied.

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

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

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

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

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

\[
\sum_{\{x_i, x_j\} \subseteq X} d_{\mu}(x_i, x_j) \left( \deg_{\mu}(x_i) + \deg_{\mu}(x_j) \right) = \sum_{\{x_i, x_j\} \subseteq X} 2 \left((1 + \deg_G(v_i)) + (1 + \deg_G(v_j))\right)
= 2 \left( \sum_{\{x_i, x_j\} \subseteq X} \sum_{\{x_i, x_j\} \subseteq X} \left( \deg_G(v_i) + \deg_G(v_j) \right) \right)
= 2 \left(\frac{n}{2} + \sum_{k=1}^{n} (n - 1) \deg(x_k)\right)
= 2n^2 - 2n + 4(n - 1)m,
\]

Note that for each \( x_k \in X \) we have \(|\{x_k, x_j\} : j \neq k| = n - 1\).

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

Since the diameter of \( G \) is two, Observation 2 implies that \( d_{\mu}(v_i, v_j) = d_G(v_i, v_j) \) for each \( v_i, v_j \in V(G) \). Hence,

\[
\sum_{\{v_i, v_j\} \subseteq V(G)} d_{\mu}(v_i, v_j) \left( \deg_{\mu}(v_i) + \deg_{\mu}(v_j) \right) = \sum_{\{v_i, v_j\} \subseteq V(G)} d_G(v_i, v_j) \left(2 \deg_G(v_i) + 2 \deg_G(v_j)\right)
= 2 \ \text{DD}(G).
\]

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

\[
\sum_{i=1}^{n} d_{\mu}(v_i, x_i) \left( \deg_{\mu}(v_i) + \deg_{\mu}(x_i) \right) = \sum_{i=1}^{n} 2 \left(2 \deg_G(v_i) + 1 + \deg_G(v_i)\right)
= 2 \left(n + 6m\right).
\]
Case 6. \( u = v_i \) and \( v = x_j, i \neq j \):

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

\[
= \sum_{\{v_i, x_j\} \subseteq V(\mu)} d_\mu(v_i, x_j) (\deg_G(v_i) + \deg_G(v_j))
+ \sum_{\{v_i, x_j\} \subseteq V(\mu)} d_\mu(v_i, x_j) (1 + \deg_G(v_i)).
\]

Since \( d_\mu(v_i, x_j) = d_\mu(v_j, x_i) \), and using Observation 2 we have

\[
\sum_{\{v_i, x_j\} \subseteq V(\mu)} d_\mu(v_i, x_j) (\deg_G(v_i) + \deg_G(v_j)) = 2 \sum_{\{v_i, v_j\} \subseteq V(G)} d_\mu(v_i, x_j) (\deg_G(v_i) + \deg_G(v_j))
\]

\[
= 2 \sum_{\{v_i, v_j\} \subseteq V(G)} d_G(v_i, v_j) (\deg_G(v_i) + \deg_G(v_j))
= 2 DD(G).
\]

Now since the diameter of \( G \) is two, Lemma 4 implies that

\[
\sum_{\{v_i, x_j\} \subseteq V(\mu)} d_\mu(v_i, x_j) (1 + \deg_G(v_i)) = \sum_{\{v_i, x_j\} \subseteq V(\mu)} 1 (1 + \deg_G(v_i))
\]

\[
+ \sum_{\{v_i, x_j\} \subseteq V(\mu)} 2 (1 + \deg_G(v_i))
\]

\[
= 2m + \sum_{v_i \in V(G)} (\deg_G(v_i) + \deg_G(v_j))
+ 2 \left(2\left(\binom{n}{2} - m\right) + \sum_{\{v_i, v_j\} \subseteq V(G)} (\deg_G(v_i) + \deg_G(v_j))\right)
\]

\[
= 2m + M_1(G)
+ 2(n(n - 1) - 2m + 2(n - 1)m - M_1(G))
= 2n(n - 1) + 2m(2n - 3) - M_1(G).
\]

Thus,

\[
\sum_{\{v_i, x_j\} \subseteq V(\mu)} d_\mu(v_i, x_j) (\deg_\mu(v_i) + \deg_\mu(x_j)) = 2 DD(G) - M_1(G) + 2n(n - 1) + 2m(2n - 3).
\]
Therefore, using the cases 1 to 6, we obtain

\[
DD(\mu) = \left( n(n + 1) + 2m \right) + \left( 2n^2 + 8m \right) + \left( 2n^2 - 2n + 4(n - 1)m \right) + \left( 2 \ DD(G) \right) \\
+ \left( 2n + 12m \right) + \left( 2 \ DD(G) - M_1(G) + 2n(n - 1) + 2m(2n - 3) \right) \\
= 4 \ DD(G) - M_1(G) + (7n - 1)n + (8n + 12)m.
\]

\[\square\]

3 The Randić index

In the following theorem we provide upper and lower bounds for the Randić index of the Mycielskian graph.

**Theorem 2.** Let \( G \) be an \( n \)-vertex graph of size \( m \) with maximum degree \( \Delta \) and minimum degree \( \delta \), whose Mycielskian graph is \( \mu \). Then,

\[
\frac{1}{2} R(G) + \sqrt{\frac{2 m + \sqrt{n\Delta}}{\Delta^2 + \Delta}} \leq R(\mu) \leq \frac{1}{2} R(G) + \sqrt{\frac{2 m + \sqrt{n\delta}}{\delta^2 + \delta}}
\]

Moreover, equalities hold if and only if \( G \) is a regular graph.

**Proof.** By the definition of Randić index and by considering the various types of edges in \( \mu \), one can see that

\[
R(\mu) = \sum_{uv \in E(\mu)} \frac{1}{\sqrt{\deg_{\mu}(u) \deg_{\mu}(v)}} \\
= \sum_{v_iv_j \in E(\mu)} \frac{1}{\sqrt{\deg_{\mu}(v_i) \deg_{\mu}(v_j)}} \\
+ \sum_{x_ix_j \in E(\mu)} \frac{1}{\sqrt{\deg_{\mu}(x) \deg_{\mu}(x_j)}} \\
+ \sum_{xx \in E(\mu)} \frac{1}{\sqrt{\deg_{\mu}(x) \deg_{\mu}(x_i)}}.
\]
Since \( N_\mu(x_i) = N_G(v_i) \cup \{x\} \) and using Observation 1 we get
\[
\sum_{x_i,v_j \in E(\mu)} \frac{1}{\sqrt{\deg_\mu(x_i) \deg_\mu(v_j)}} = \sum_{x_i,v_j \in E(\mu)} \frac{1}{\sqrt{(1 + \deg_G(v_i))(2 \deg_G(v_j))}}
\]
\[
= \sum_{i=1}^{n} \sum_{v_j \in N_G(v_i)} \frac{1}{\sqrt{(\delta + 1)(2\delta)}}
\]
\[
= \sum_{i=1}^{n} \frac{\deg(v_i)}{\sqrt{(\delta + 1)(2\delta)}}
\]
\[
= \frac{2m}{\sqrt{\delta^2 + \delta}}.
\]
Similarly, we can see that
\[
\frac{\sqrt{2m}}{\Delta^2 + \Delta} \leq \sum_{x_i,v_j \in E(\mu)} \frac{1}{\sqrt{\deg_\mu(x_i) \deg_\mu(v_j)}}
\]
Note that
\[
\sum_{xx_i \in E(\mu)} \frac{1}{\sqrt{\deg_\mu(x) \deg_\mu(x_i)}} = \sum_{xx_i \in E(\mu)} \frac{1}{\sqrt{n(1 + \deg_G(v_i))}}
\]
\[
= \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \frac{1}{\sqrt{1 + \deg_G(v_i)}}.
\]
This implies that
\[
\sqrt{\frac{n}{1 + \Delta}} \leq \sum_{xx_i \in E(\mu)} \frac{1}{\sqrt{\deg_\mu(x) \deg_\mu(x_i)}} \leq \sqrt{\frac{n}{1 + \delta}}.
\]
Now since
\[
\sum_{v_i,v_j \in E(\mu)} \frac{1}{\sqrt{\deg_\mu(v_i) \deg_\mu(v_j)}} = \sum_{v_i,v_j \in E(G)} \frac{1}{\sqrt{(2 \deg_G(v_i))(2 \deg_G(v_j))}}
\]
\[
= \frac{1}{2} R(G),
\]
the proof is complete. \(\square\)

References

[1] D. Amic, D. Beslo, B. Lucic, S. Nikolic, N. Trinajstić, The vertex-connectivity index revisited, *J. Chem. Inf. Comput. Sci.*, 38 (1998) 819-822.
[2] B. Bollobás, P. Erdős, Graphs of extremal weights, *Ars Combin.*, **50** (1998) 225-233.

[3] Ş. B. Bozkurt, A. D. Güngör, I. Gutman, A. S. Çevik, Randić matrix and Randić energy, *MATCH Commun. Math. Comput. Chem.*, **64** (2010) 239-250.

[4] A. A. Dobrynin and A. A. Kochetova, Degree Distance of a Graph: A Degree Analogue of the Wiener Index, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 1082-1086.

[5] D.C. Fisher, P.A. McKena, E.D. Boyer, Hamiltonicity, diameter, domination, packing and biclique partitions of the Mycielskis graphs, *Discret. Appl. Math.*, **84** (1998) 93-105.

[6] I. Gutman, Selected Properties of the Schultz Molecular Topological Index, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 1087-1089.

[7] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total $\pi$-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, **17** (1972) 535-538.

[8] Y. Hu, X. Li, Y. Shi, T. Xu, I. Gutman, On molecular graphs with smallest and greatest zeroth-order general Randić index, *MATCH Commun. Math. Comput. Chem.*, **54** (2005) 425-434.

[9] A. Ilić, S. Klavžar, D. Stevanović, Calculating the degree distance of partial Hamming graphs, *MATCH Commun. Math. Comput. Chem.*, **63** (2010) 411-424.

[10] X. Li, I. Gutman, Mathematical aspects of Randić-type molecular structure descriptors, *Mathematical Chemistry Monographs, No. 1, Kragujevac*, 2006.

[11] J. Mycielski, Sur le colouriage des graphes, *Colloq. Math.*, **3** (1955) 161-162.

[12] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.*, **97** (1975) 6609-6615.

[13] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.*, **69** (1947) 17-20.