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Computing Certain Topological Indices of Generalised Mycielskian Graphs

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Abstract: The generalized Mycielskians are the generalization of the Mycielski graphs, which were introduced by Mycielski in 1955. A topological index is a numeric parameter mathematically derived from a graph and is invariant under automorphism of graphs. Topological indices are widely used for establishing correlations between the structure of a molecular compound and its different physico-chemical properties. This paper investigates different degree-based topological indices of the generalized Mycielskians of *G*.

Keywords: Topological Index, Degree of a Vertex, Generalized Mycielskian Graphs, Graph Operations

1. Introduction

Let *G* be a simple connected graph with *n* vertices and *m* edges, having no directed or weighted edges. Let $V(G)$ and $E(G)$ respectively denote the vertex set and edge set of *G*. Also let the edge connecting the vertices *u* and *v* is denoted by *uv*. The degree of a vertex $v \in V(G)$ is the number of edges incident with the vertex *v* and is denoted by $d_G(v)$. A graph is called a *r*-regular graph if all the vertices are of degree *r*. Throughout this paper we consider only simple, connected, undirected graphs. In chemical graph theory, a molecular graph is the graphical representation of the structural formula of a chemical compound whose atoms are represented using vertices and the edges represent the chemical bonds between the atoms. A topological index is a numeric parameter mathematically derived from the molecular graph and which characterize the topology of the molecular graph and correlate the physico-chemical properties of the molecular graphs. A topological index has been found to be useful in isomer discrimination, quantitative structure-activity relationship (QSAR) and structure-property relationship (QSPR) and has good application in chemistry, biochemistry and nanotechnology.

There are various types of topological indices. Among which the first and the second Zagreb index of a *G* denoted by $M_1(G)$ and $M_2(G)$ respectively are one of the oldest topological indices introduced in [1] by Gutman and Trinajstić and are defined as

$$M_1(G) = \sum_{v\in V(G)} d_G(u)^2 = \sum_{uv\in E(G)} \left[d_G(u)+d_G(v)\right] \text{ and}$$
$$M_2(G) = \sum_{u,v\in V(G)} d_G(u)d_G(v).$$

These indices are found to be very useful in study of structure property correlation of molecules and extensively studied both with respect to mathematical as well as chemical point of view.

Another degree-based topological index, named as the F-index or the "forgotten topological index" of a graph was also introduced in [1] and recently Furtula and Gutman in [2] reinvestigated this F-index index and showed that the predictive ability of this index is almost similar to that of first Zagreb index. There are many other recent mathematical study of this index also [3-8]. The F-index of a graph *G* is defined as

$$F(G) = \sum_{uv\in E(G)} \left[d_G(u)^2 + d_G(v)^2\right]. \qquad (1)$$

Analogous to classical Zagreb indices, two new variant of Zagreb indices were introduced by Miličević et al. [9] and named them as reformulated Zagreb indices [10-15]. In this case, the vertex degrees are replaced by edge degrees, where the degree of an edge $e = uv \in E(G)$ is given by

$d_G(e) = d_G(u) + d_G(v) - 2$. Thus the first reformulated Zagreb index of a graph G is defined as

$$EM_1(G) = \sum_{e=uv\in E(G)} d_G(e)^2 = \sum_{uv\in E(G)} \left[d_G(u) + d_G(v) - 2\right]^2. \quad (2)$$

There are different other modifications of the original Zagreb index. One of the modified version of the first Zagreb index, named as Hyper-Zagreb index, was introduced by Shirdel et al. [16] and is defined as

$$HM(G) = \sum_{uv\in E(G)} \left[d_G(u) + d_G(v)\right]^2. \quad (3)$$

For different study of this index see [17-19]. Another version of Zagreb index, named as third version of redefined Zagerb index [20] is defined as

$$\mathrm{Re}\,ZG_3(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)\left[d_G(u) + d_G(v)\right]. \quad (4)$$

The imbalance of an edge $e = uv$ of G is defined as $|d_G(u) - d_G(v)|$. The irregularity of a graph is defined as the sum of imbalance of all the edges of G. Thus irregularity of a graph G is given by

$$irr(G) = \sum_{uv\in E(G)} |d_G(u) - d_G(v)|. \quad (5)$$

This graph invariant is also known as third Zagreb index of a graph and was introduced by Albertson [26]. He proved that the irregularity of an arbitrary graph with n vertices is less than $\frac{4n^3}{27}$. There are various recent study of this graph invariant [27-31]. Clearly, the irregularity of a graph is always nonnegative and for a regular graph G, $irr(G) = 0$.

The construction of the Mycielski graph was introduced in 1955 [21]. Let, $x \in V(G)$, then the Mycielski graph $\mu(G)$ of G (see [22-24]) contains G itself as an isomorphic subgraph, and also *(n + 1)* additional vertices, among which n vertices denoted by x' corresponds to each $x \in V(G)$, connected by an edge to the vertex u, which form a subgraph in the form of $K_{1,n}$. Also for each edge $xy \in E(G)$, $\mu(G)$ includes two edges $x'y$ and xy'. Thus, if $V' = \{x' : x \in V(G)\}$, then the vertex and edge sets of $\mu(G)$ are respectively given by

$$V(\mu(G)) = V(G) \cup V' \cup \{u\} \text{ and}$$
$$E(\mu(G)) = E(G) \cup \{x'y, xy' : xy \in E(G)\} \cup \{x'u : x' \in V'\}.$$

Thus, the degree of the vertices of $\mu(G)$ is given by

$$d_{\mu(G)}(x) = 2d_G(x),\ d_{\mu(G)}(x') = d_G(x) + 1 \text{ and } d_{\mu(G)}(u) = n.$$

As an example, the Mycielskian of the cycle graph C_8 is depicted in figure 1.

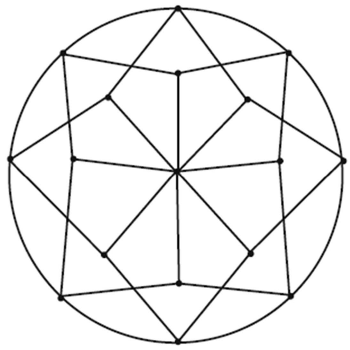

Figure 1. *The Mycielskian of* C_8.

The generalized Mycielskian graph of G is the generalization of the Mycielski graph. Let G be the graph with vertex set V^0 and edge set E^0. Now for an integer $k \geq 1$, the k- Mycielskian of G, denoted by $\mu_k(G)$, is the graph with vertex set

$$V(\mu_k(G)) = V^0(G) \cup \left(\bigcup_{i=1}^{k} V^i(G)\right) \cup \{u\}$$

$$\text{where } V^i(G) = \left\{x^i : x \in V\right\}$$

and the edge set

$$E(\mu_k(G)) = E^0(G) \bigcup_{i=1}^{k} \left\{y^{i-1}x^i; x^{i-1}y^i : xy \in E^0(G)\right\} \cup \left\{x^k u : x^k \in V^k\right\}.$$

Note that, $x^0 = x$ and $y^0 = y$. It is clear that, the original Mycielskian of a graph G is equal to $\mu_1(G)$. From definition of generalized Mycielskian graph $\mu_k(G)$, $(k \geq 0)$ of G, the following lemma follows directly.

Lemma 1.1

(i) $|V(\mu_k(G))| = (k+1)n + 1$ and $|E(\mu_k(G))| = (2k+1)m + n$.

(ii) $d_{\mu_k(G)}(v^i) = 2d_G(v)$, $0 \leq i \leq k-1$,

$d_{\mu_k(G)}(v^k) = d_G(v) + 1$, for all $v \in V(G)$,

$d_{\mu_k(G)}(u) = n$.

A. Jerline et al. in [25] obtain the exact expressions for the first and second Zagreb indices of the generalised Mycielskian of a graph. In this paper, we derive some explicit expression of different topological indices of generalised Mycielskian graphs of a connected graph in terms of different other topological indices of the original graph. Also different topological indices of generalised Mycielskian constructions of cycle and path graphs are analyzed.

2. Main Results

In this section, we proceed to calculate different topological indices such as forgotten topological index, hyper Zagreb index, reformulated first Zagreb index, redefined Zagreb index, irregularity of graphs of generalized Mycielskian of a connected graph G and hence find the explicit expressions of these topological indices of generalised Mycielskian constructions of cycle and path graphs.

Theorem 2.1 Let G be a simple connected graph with n vertices and m edges, then

$$F(\mu_k(G)) = (8k+1)F(G) + 3M_1(G) + 6m + n^3 + n .$$

Proof. By definition (1) and using lemma 1 we have

$$F(\mu_k(G)) = \sum_{uv\in E(\mu_k(G))}\left[d_{\mu_k(G)}(u)^2 + d_{\mu_k(G)}(v)^2\right]$$

$$= \sum_{uv\in E(G)}\left[4d_G(u)^2 + 4d_G(v)^2\right] + 2(k-1)\sum_{uv\in E(G)}\left[4d_G(u)^2 + 4d_G(v)^2\right]$$

$$+ \sum_{uv\in E(G)}\left[\{4d_G(u)^2 + (d_G(v)+1)^2\} + \{4d_G(v)^2 + (d_G(u)+1)^2\}\right]$$

$$+ \sum_{v\in V(G)}\left[(d_G(v)+1)^2 + n^2\right]$$

$$= 4\sum_{uv\in E(G)}\left[d_G(u)^2 + d_G(v)^2\right] + 8(k-1)\sum_{uv\in E(G)}\left[d_G(u)^2 + d_G(v)^2\right]$$

$$+ \sum_{uv\in E(G)}\left[\{5d_G(u)^2 + 5d_G(v)^2\} + 2(d_G(u)+d_G(v)) + 2\right]$$

$$+ \sum_{v\in V(G)}\left[d_G(v)^2 + 2d_G(v) + 1 + n^2\right]$$

$$= (8k+1)F(G) + 3M_1(G) + 6m + n(n^2+1).$$

Hence the desired follows.

Corollary 2.1 If G be r-regular graph, then

$$F(\mu_k(G)) = (8k+1)nr^3 + 3nr^2 + 3nr + n(n^2+1).$$

Example 2.1

(i) $F(\mu_k(C_n)) = n^3 + 64nk + 27n$

(ii) $F(\mu_k(P_n)) = n^3 + 64nk + 27n - 112k - 38$.

In the following now we calculate hyper-Zagreb index of the generalised Mycielskian graph.

Theorem 2.2 Let G be a simple connected graph with n vertices and m edges, then

$$HM(\mu_k(G)) = (8k-4)HM(G) + 5F(G) + 7M_1(G) + 8M_2(G) + n(n+1)^2 + 4mn + 6m .$$

Proof. By definition and using lemma 1 we have

$$HM(\mu_k(G)) = \sum_{uv\in E(\mu_k(G))}\left[d_{\mu_k(G)}(u) + d_{\mu_k(G)}(v)\right]^2$$

$$= \sum_{uv\in E(G)}\left[2d_G(u) + 2d_G(v)\right]^2 + 2(k-1)\sum_{uv\in E(G)}\left[2d_G(u) + 2d_G(v)\right]^2$$

$$+ \sum_{uv\in E(G)}\left[\{2d_G(u) + (d_G(v)+1)\}^2 + \{2d_G(v) + (d_G(u)+1)\}^2\right]$$

$$+ \sum_{v\in V(G)}\left[(d_G(v)+1) + n\right]^2$$

$$= 4\sum_{uv\in E(G)}\left[d_G(u) + d_G(v)\right]^2 + 8(k-1)\sum_{uv\in E(G)}\left[d_G(u) + d_G(v)\right]^2$$

$$+ \sum_{uv\in E(G)}\left[\{5d_G(u)^2 + 5d_G(v)^2\} + 6(d_G(u)+d_G(v)) + 8d_G(u)d_G(v) + 2\right]$$

$$+\sum_{v\in V(G)}\left[d_G(v)^2+2(n+1)d_G(v)+(n+1)^2\right]$$

$$=(8k-4)HM(G)+5F(G)+7M_1(G)+8M_2(G)+n(n+1)^2+4mn+6m\ .$$

Hence the desired result follows.

Corollary 2.2 Let G be a r-regular graph, then

$$HM(\mu_k(G))=(16k+1)nr^3+5nr+n(n+1)^2.$$

Example 2.2

(i) $HM(\mu_k(C_n))=n^3+6n^2+128nk+15n$

(ii) $HM(\mu_k(P_n))=n^3+6n^2+128nk+11n-240k-20.$

In the next theorem, we calculate reformulated first Zagreb index of generalised Mycielskian of a connected graphs.

Theorem 2.3 Let G be a simple connected graph with n vertices and m edges, then

$$EM_1(\mu_k(G))=2(4k-1)EM_1(G)+F(G)+2HM(G)+(16k-5)M_1(G)$$

$$-6m(4k-1)+4m(n-1)+n(n-1)^2.$$

Proof. From definition (2) and using Lemma 1, we have

$$EM_1(\mu_k(G))=\sum_{uv\in E(\mu_k(G))}\left[d_{\mu_k(G)}(u)+d_{\mu_k(G)}(v)-2\right]^2$$

$$=\sum_{uv\in E(G)}\left[2d_G(u)+2d_G(v)-2\right]^2+2(k-1)\sum_{uv\in E(G)}\left[2d_G(u)+2d_G(v)-2\right]^2$$

$$+\sum_{uv\in E(G)}\left[\{2d_G(u)+(d_G(v)+1)-2\}^2+\{2d_G(v)+(d_G(u)+1)-2\}^2\right]$$

$$+\sum_{v\in V(G)}\left[(d_G(v)+1)+n-2\right]^2$$

$$=4\sum_{uv\in E(G)}\left[d_G(u)+d_G(v)-2\right]^2+4\sum_{uv\in E(G)}\left[2(d_G(u)+d_G(v)-2)+1\right]$$

$$+8(k-1)\sum_{uv\in E(G)}\left[d_G(u)+d_G(v)-2\right]^2+8(k-1)\sum_{uv\in E(G)}\left[2(d_G(u)+d_G(v)-2)+1\right]^2$$

$$+2\sum_{uv\in E(G)}\left[d_G(u)+d_G(v)-2\right]^2+4\sum_{uv\in E(G)}\left[(d_G(u)+1)^2+(d_G(v)+1)^2\right]$$

$$+2\sum_{uv\in E(G)}\{\left[d_G(u)+d_G(v)-2\right](d_G(u)+1)+\left[d_G(u)+d_G(v)-2\right](d_G(v)+1)\}$$

$$+\sum_{v\in V(G)}\left[(d_G(v)+(n-1)\right]^2$$

$$=4EM_1(G)+4(2M_1(G)-3m)+8(K-1)EM_1(G)+8(K-1)(2M_1(G)-3m)$$

$$+EM_1(G)+\sum_{uv\in E(G)}\left[d_G(u)^2+2d_G(u)+1+d_G(v)^2+2d_G(v)+1\right]$$

$$+2\sum_{uv\in E(G)}\left[d_G(u)+d_G(v)-2\right]\left[d_G(u)+d_G(v)+2\right]+EM_1(G)+M_1(G)$$

$$+4m(n-1)+n(n-1)^2$$

$$=(8k-2)EM_1(G)+(16k-7)M_1(G)+F(G)+2M_1(G)+2m+2HM(G)$$

$$-8m+4m(n-1)+n(n-1)^2-3((8k-8)+4)m,$$

from where the desired result follows.

Corollary 2.3 Let G be a r-regular graph, then

$$EM_1(\mu_k(G))=4nr(4k-1)(r-1)^2+5nr^3+(16k-5)nr^2-3nr(4k-1)+2nr(n-1)+n(n-1)^2.$$

Example 2.3

(i) $EM_1(\mu_k(C_n))=n^3+2n^2+72nk+15n$,

(ii) $EM_1(\mu_k(P_n))=n^3+2n^2+72nk+11n-152k-26$.

In the next theorem, we calculate third redefined Zagreb index of generalised Mycielskian of a connected graphs.

Theorem 2.4 Let G be a simple connected graph with n vertices and m edges, then

$$\operatorname{Re}ZG_3(\mu_k(G))=(16k-2)\operatorname{Re}ZG_3(G)+2HM(G)+2F(G)+(n+2)M_1(G)$$

$$+2M_2(G)+2mn(n+2)+n^2(n+1).$$

Proof. From definition and using Lemma 1, we have

$$\operatorname{Re}ZG_3(\mu_k(G))=\sum_{uv\in E(\mu_k(G))} d_{\mu_k(G)}(u)d_{\mu_k(G)}(v)\left[d_{\mu_k(G)}(u)+d_{\mu_k(G)}(v)\right]$$

$$=\sum_{uv\in E(G)}2d_G(u).2d_G(v)\left[2d_G(u)+2d_G(v)\right]$$

$$+2(k-1)\sum_{uv\in E(G)}2d_G(u).2d_G(v)\left[2d_G(u)+2d_G(v)\right]$$

$$+\sum_{uv\in E(G)}2d_G(u)(d_G(v)+1)\left[2d_G(u)+(d_G(v)+1)\right]$$

$$+\sum_{uv\in E(G)}2d_G(v)(d_G(u)+1)\left[2d_G(v)+(d_G(u)+1)\right]$$

$$+\sum_{v\in V(G)}n(d_G(v)+1)\left[(d_G(v)+1)+n\right]$$

$$=8\sum_{uv\in E(G)}d_G(u)d_G(v)\left[d_G(u)+d_G(v)\right]$$

$$+16(k-1)\sum_{uv\in E(G)}d_G(u)d_G(v)\left[d_G(u)+d_G(v)\right]$$

$$+2\sum_{uv\in E(G)}(d_G(u)d_G(v)+d_G(u))\left[(d_G(u)+d_G(v))+(d_G(u)+1)\right]$$

$$+2\sum_{uv\in E(G)}(d_G(u)d_G(v)+d_G(v))\left[(d_G(u)+d_G(v))+(d_G(v)+1)\right]$$

$$+n\sum_{v\in V(G)}(d_G(v)^2+d_G(v)+(n+1)d_G(v)+(n+1))$$

$$=8\operatorname{Re}ZG_3(G)+16(k-1)\operatorname{Re}ZG_3(G)+4\sum_{uv\in E(G)}d_G(u)d_G(v)\left[d_G(u)+d_G(v)\right]$$

$$+\sum_{uv\in E(G)}\left[d_G(u)(d_G(u)+d_G(v))+d_G(v)(d_G(u)+d_G(v))\right]$$

$$+\sum_{uv\in E(G)}\left[d_G(u)(d_G(u)+1)+d_G(v)(d_G(v)+1)\right]$$

$$+\sum_{uv\in E(G)}\left[d_G(u)d_G(v)(d_G(u)+1)+d_G(u)d_G(v)(d_G(v)+1)\right]$$

$$+n\sum_{v\in V(G)}(d_G(v)^2+(n+2)d_G(v)+(n+1))$$

$$=(16k-4)\operatorname{Re}ZG_3(G)+2HM(G)+2F(G)+2M_1(G)+nM_1(G)$$

$$+2\operatorname{Re}ZG_3(G)+2M_2(G)+2mn(n+2)+n^2(n+1),$$

from where the desired result follows.

Corollary 2.4 Let G be a r-regular graph, then

$$\operatorname{Re}ZG_3(\mu_k(G))=2(8k-1)nr^4+nr(n+2)(n+r)+7nr^3+n^2(n+1).$$

Example 2.4

(i) $\operatorname{Re}ZG_3(\mu_k(C_n))=3n^3+5n^2+265nk+32n$

(ii) $\operatorname{Re}ZG_3(\mu_k(P_n))=3n^3+7n^2+265nk+22n-576k-20.$

In the following now we calculate irregularity index of the generalised Mycielskian graph.

Theorem 2.5 Let G be a simple connected graph with n vertices and m edges, then

$$irr(\mu_k(G))\geq(4k+1)irr(G)+n(n-1)-2m\ .$$

Proof. From definition (5) and lemma 1, and also using triangle inequality, we have

$$irr(\mu_k(G))=\sum_{uv\in E(\mu_k(G))}|\,d_{\mu_k(G)}(u)-d_{\mu_k(G)}(v)\,|$$

$$=\sum_{uv\in E(G)}|\,2d_G(u)-2d_G(v)\,|+2(k-1)\sum_{uv\in E(G)}|\,2d_G(u)-2d_G(v)\,|$$

$$+\sum_{uv\in E(G)}\left[|\,2d_G(u)-(d_G(v)+1)\,|+|\,(d_G(u)+1)-2d_G(v)\,|\right]$$

$$+\sum_{v\in V(G)}|\,n-(d_G(v)+1)\,|$$

$$\geq 2\sum_{uv\in E(G)}|\,d_G(u)-d_G(v)\,|+4(k-1)\sum_{uv\in E(G)}|\,d_G(u)-d_G(v)\,|$$

$$+3\sum_{uv\in E(G)}|\,d_G(u)-d_G(v)\,|+n(n-1)-2m$$

$$=(4k+1)irr(G)+n(n-1)-2m.$$

Hence the desired result follows. Note that, in the desired inequality, equality holds if both and $[(d_G(u)+1)-2d_G(v)]$, for all $uv\in E(G)$ are either both positive or both negative. For example, in case of path graph with three vertices, P_3, the above conditions are true and hence using the previous result we get $irr(\mu_k(P_3))=4(2k+1).$

Corollary 2.5 Let G be a r-regular graph, then

$$irr(\mu_k(G))\geq n(n-r-1).$$

3. Conclusions

In this paper, we calculate some explicit expression of different topological indices such as forgotten topological index, hyper Zagreb index, reformulated first Zagreb index, redefined Zagreb index, irregularity of graphs of generalised Mycielskian transformation of a connected graph in terms of different other topological indices of the original graph. Note that in the above derived results if we put $k=1$, we get the results for original Mycielski graph. Similarly the generalised Mycielskian transformation of some other topological indices can be computed in future study.

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