Global Journal of Pure and Applied Mathematics.
ISSN 0973-1768 Volume 12, Number 6 (2016), pp. 5317–5327

http://www.ripublication.com/gjpam.htm

Some Topological Invariants of the Möbius Ladders

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Abstract

In this article we compute many topological indices for the family of Möbius ladder. At first we give general closed form of M-polynomial of this family and recover many degree based topological indices out of it. We also compute Zagreb indices and Zagreb polynomials of this family.

AMS subject classification: 05C12.
Keywords: Möbius ladder, topological indices.

1. Introduction

A number, polynomial or a matrix can uniquely identify a graph. A topological index is a numeric number associated to a graph which completely describes the topology of the graph, and this quantity is invariant under the isomorphism of graphs. The degree-based topological indices are derived from degrees of vertices in the graph. These indices have many correlations to chemical properties. In other words, a topological index remains invariant under graph isomorphism.

The study of topological indices, based on distance in a graph, was effectively employed in 1947 in chemistry by Weiner [25]. He introduced a distance-based topological index called the "Wiener index" to correlate properties of alkenes and the structures of their molecular graphs. Recent progress in nano-technology is attracting attention to the topological indices of molecular graphs, such as nanotubes, nanocones, and fullerenes to cut short experimental labor. Since their introduction, more than 140 topological indices have been developed, and experiments reveal that these indices, in combination, determine the material properties such as melting point, boiling point, heat of formation, toxicity, toughness, and stability [12]. These indices play a vital role in computational and theoretical aspects of chemistry in predicting material properties [4, 5, 9, 15, 16, 23].

Several algebraic polynomials have useful applications in chemistry, such as the Hosoya Polynomial (also called the Wiener polynomial) [7]. It plays a vital role in determining distance-based topological indices. Among other algebraic polynomials, the M-polynomial [3] was introduced recently in 2015 and plays the same role in determining the closed form of many degree-based topological indices. Other famous polynomials are the first Zagreb polynomial and the second Zagreb polynomial.

A graph G is an ordered pair (V, E), where V is the set of vertices and E is the set of edges. A path from a vertex v to a vertex w is a sequence of vertices and edges that starts from v and stops at w. The number of edges in a path is called the length of that path. A graph is said to be connected if there is a path between any two of its vertices. The distance $d(u, v)$ between two vertices u, v of a connected graph G is the length of a shortest path between them. Graph theory is contributing a lion's share in many areas such as chemistry, physics, pharmacy, as well as in industry. We will start with some preliminary facts.

Let G be a simple connected graph and let uv represent the edge between the vertices u and v. The number of vertices of G, adjacent to a given vertex v, is the "degree" of this vertex, and will be denoted by d_v. We define

$$\begin{aligned} V_k &= \{v \in V(G) \mid d_v = k\}, \\ E_{i,j} &= \{uv \in E(G) \mid d_u = j \text{ and } d_v = i\}, \\ \delta &= \min\{d_v \mid v \in V(G)\}, \\ \Delta &= \max\{d_v \mid v \in V(G)\}, \end{aligned}$$

and m_{ij} as the number of edges uv of G such that $\{d_v, d_u\} = \{i, j\}$. The M-polynomial of G is defined as

$$M(G, x, y) = \sum_{\delta \le i \le j \le \Delta} m_{ij} x^i y^j.$$

Active research is in progress, and many authors computed M-polynomials for different types of nonmaterial, for example see [17, 18, 19, 20, 21] and the references therein.

The Wiener index of G is defined as

$$W(G) = \frac{1}{2} \sum_{(u,v)} d(u, v),$$

where (u, v) is any ordered pair of vertices in G. Gutman and Trinajstić [10] introduces important topological index called first Zagreb index, denoted by $M_1(G)$, and is defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

The second Zagreb index $M_2(G)$ and the second modified Zagreb index ${}^m M_2(G)$ are defined as

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v)$$

and

$${}^m M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u \cdot d_v}.$$

Results obtained in the theory of Zagreb indices are summarized in the review [8].

In 1998, working independently, Bollobas and Erdos [2] and Amic et al. [1] proposed general Randić index. It has been extensively studied by both mathematicians and theoretical chemists (see, for example, [13, 14]). The Randić index denoted by $R_\alpha(G)$ is the sum of $(dud_v)^\alpha$, that is,

$$R_\alpha(G) = \sum_{uv \in E(G)} (dud_v)^\alpha,$$

Table 1: Derivation of topological indices from M-polynomial.

Topological Index	$f(x, y)$	Derivation from $M(G, x, y)$
First Zagreb	$x + y$	$(D_x + D_y)(M(G; x, y))\|_{x=y=1}$
Second Zagreb	xy	$(D_x D_y)(M(G; x, y))\|_{x=y=1}$
${}^m M_2(G)$	$\frac{1}{xy}$	$(S_x D_y)(M(G; x, y))\|_{x=y=1}$
General Randić $\alpha \in N$	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(M(G; x, y))\|_{x=y=1}$
General Randić $\alpha \in N$	$\frac{1}{xy}^\alpha$	$(S_x^\alpha S_y^\alpha)(M(G; x, y))\|_{x=y=1}$
Symmetric Division Index	$\frac{x^2 + y^2}{xy}$	$(D_x S_y + D_y S_x)(M(G; x, y))\|_{x=y=1}$

where α is any constant.

The symmetric division index is defined by

$$SDD(G) = \sum_{uv \in E(G)} \left(\frac{\min\{d_u, d_v\}}{\max\{d_u, d_v\}} + \frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}} \right).$$

These indices can help to characterize the chemical and physical properties of molecules (see [7]).

Table 1 enlist some standard degree-based topological indices and their derivation from M-polynomial [3].

Here

$$D_x(f(x, y)) = x\frac{\partial f(x, y)}{\partial x},$$
$$D_y(f(x, y)) = y\frac{\partial f(x, y)}{\partial y},$$
$$S_x(f(x, y)) = \int_0^x \frac{f(t, y)}{t} dt,$$
$$S_y(f(x, y)) = \int_0^y \frac{f(x, t)}{t} dt.$$

For a simple connected graph, the first Zagreb polynomial is defined as

$$M_1(G, x) = \sum_{uc \in E(G)} x^{[d_u + d_v]}$$

and the second Zagreb polynomial is defined as

$$M_2(G, x) = \sum_{uc \in E(G)} x^{[d_u \times d_v]}.$$

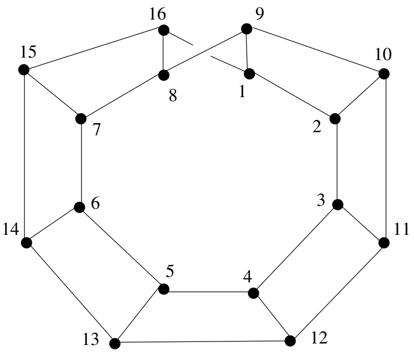


Figure 1: Möbius ladder M_{16}

In 2013, Shirdel et al. [24] proposed the hyper-Zagreb index, which is also degree-based, given as

$$HM(G) = \sum_{uc \in E(G)} [d_u + d_v]^2.$$

In 2012, Ghorbani and Azimi [6] proposed two new variants of Zagreb indices; namely, the first multiple Zagreb index $PM_1(G)$ and the second multiple Zagreb index $PM_2(G)$, which are defined as

$$PM_1(G) = \prod_{uv \in E(G)} [d_u + d_v],$$

$$PM_2(G) = \prod_{uv \in E(G)} [d_u \times d_v].$$

The Möbius ladder M_n which is a cubic circulant graph with an even number of vertices, formed from an n-cycle by adding edges (called "rungs") connecting opposite pair of vertices in the cycle. It is so-named because (with the exception of $M_6 = K_{3,3}$) M_n has exactly $\frac{n}{2}$ 4-cycles which link together by their shared edges to form a topological Möbius strip. Möbius ladders can also be viewed as a prism with one twisted edge. Two different views of Möbius ladders M_n have been shown in Figure 1. Möbius ladders have many applications in chemistry, chemical stereography, electronics and computer science.

For our convenience, we view the Möbius ladder M_n which is a cubic circulant graph with an even number of vertices, formed from an n-cycle by adding edges (called "rungs") connecting opposite pair of vertices in the cycle.

In this report we are interested to find the closed form of algebraic polynomials and topological indices defined above.

2. Main results

Theorem 2.1. Let M_n be Möbius ladder. Then the M-polynomial of M_n is

$$M(M_n, x, y) = 3nx^3y^3.$$

Proof. Let M_n be Möbius ladder. From the structure of Möbius ladder M_n we can see that only one partition $V_3 = \{v \in V(M_n)|d_v = 3\}$. By definition of M-polynomial, we can see edge set of M_n can be partition as follows:

$$E_{3,3} = \{e = uv \in E(M_n) \mid d_u = d_v = 3\} \to |E_{\{3,3\}}| = 3n.$$

In Figure 1 the size of $E_{\{3,3\}}$ is equal to $3n$. Thus M-polynomial of M_n

$$\begin{aligned} M(M_n, x, y) &= \sum_{i \le j} m_{ij}(M_n)x^iy^j \\ &= \sum_{3 \le 3} m_{ij}(M_n)x^3y^3 \\ &= |E_{\{3,3\}}|x^3y^3 \\ &= 3nx^3y^3. \end{aligned}$$

■

Now we derive topological indices which are directly derivable from M-polynomial.

Theorem 2.2. Let M_n be Möbius ladder. Then

(a) $M_1(M_n) = 18n$.

(b) $M_2(M_n) = 27n$.

(c) ${}^mM_2(M_n) = \frac{n}{3}$.

(d) $R_\alpha(M_n) = 3^{2\alpha+1}$.

(e) $R_\alpha(M_n) = \frac{1}{3^{2\alpha-1}}$.

(f) $SDD(M_n) = 6n$.

Proof. Let $f(x, y) = 3nx^3y^3$. Then

$$\begin{aligned} D_x(f(x, y)) &= 9nx^3y^3, \\ D_y(f(x, y)) &= 9nx^3y^3, \\ S_x(f(x, y)) &= S_y(f(x, y)) = nx^3y^3. \end{aligned}$$

Now from Table 1.

(a)
$$M_1(M_n) = (D_x + D_y)f(x, y))(M(M_n; x, y))|_{x=y=1} = 18n.$$

(b)
$$M_2(M_n) = (D_x D_y)f(x, y))(M(M_n; x, y))|_{x=y=1} = 27n.$$

(c)
$$^{m}M_2(M_n) = (S_x S_y)f(x, y))(M(M_n; x, y))|_{x=y=1} = \frac{n}{3}.$$

(d)
$$R_\alpha(M_n) = (D_x D_y)^\alpha f(x, y))(M(M_n; x, y))|_{x=y=1} = 3^{2\alpha+1}.$$

(e)
$$R_\alpha(M_n) = (S_x S_y)^\alpha f(x, y))(M(M_n; x, y))|_{x=y=1} = \frac{1}{3^{2\alpha-1}}.$$

(f)
$$SDD(M_n) = (D_x S_y + D_y S_x)(M(M_n; x, y))|_{x=y=1} = 6n.$$

■

Theorem 2.3. Let M_n be Möbius ladder. Then

(a) $PM_1(M_n) = 6^{3n}$.

(b) $PM_2(M_n) = 9^{3n}$.

(c) $HM(M_n) = 36(3n)$.

Proof. Let M_n be Möbius ladder. Edge set of M_n has one partition based on degree of vertices. The edge partition has $3n$ edges uv where $d_u = d_v = 3$ it can easy to see that $|E_1(M_n)| = d_{33}$.

Now by definition,

(a)
$$\begin{aligned} PM_1(M_n) &= \prod_{uv \in E(M_n)} [d_u + d_v] \\ &= \prod_{uv \in E_1(M_n)} [d_u + d_v] \\ &= 6^{|E_1(M_n)|} \\ &= 6^{3n}. \end{aligned}$$

(b)

$$\begin{aligned} PM_2(M_n) &= \prod_{uv\in E(M_n)} [d_u \times d_v] \\ &= \prod_{uv\in E_1(M_n)} [d_u \times d_v] \\ &= 9^{|E_1(M_n)|} \\ &= 9^{3n}. \end{aligned}$$

(c)

$$\begin{aligned} HM(M_n &= \sum_{uv\in E(M_n)} [d_u + d_v]^2 \\ &= \sum_{uv\in E_1(M_n)} [d_u + d_v]^2, \\ &= 36|E_1(M_n)|, \\ &= 36(3n). \end{aligned}$$

■

Theorem 2.4. Let M_n be Möbius ladder. Then

(a) $M_1(M_n, x) = 3nx^6$.

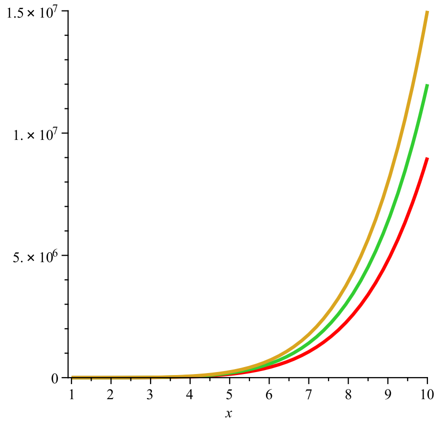
(b) $M_2(M_n, x) = 3nx^9$.

Proof. Let M_n be Möbius ladder. Edge set of M_n has one partition based on degree of vertices. The edge partition has $3n$ edges uv where $d_u = d_v = 3$ it can easy to see that $|E_1(M_n)| = d_{33}$.

Now by definitions we have

(a)

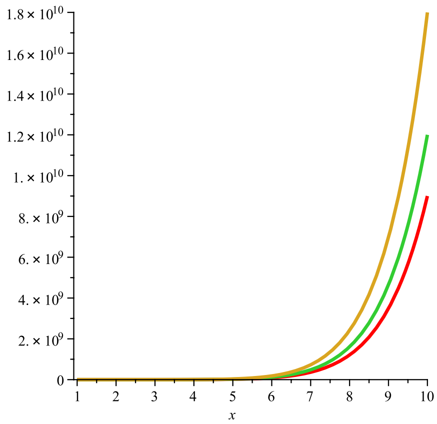
$$\begin{aligned} M_1(M_n) &= \sum_{uv\in E(M_n)} x^{[d_u+d_v]} \\ &= \sum_{uv\in E_1(M_n)} x^{[d_u+d_v]} \\ &= |E_1(M_n)|x^6 \\ &= 3nx^6. \end{aligned}$$



Zagreb 1st polynomial of M_n for n=3 Red,n=4 Green and n=5 Golden

(b)

$$\begin{aligned} PM_2(M_n) &= \sum_{uv\in E(M_n)} x^{[d_u \times d_v]} \\ &= \sum_{uv\in E_1(M_n)} x^{[d_u \times d_v]} \\ &= |E_1(M_n)|x^9 \\ &= 3nx^9. \end{aligned}$$



2nd polynomial of M_n n=3.Red n=4 Green and n=6 Golden

■

3. Conclusion

Closed forms of M-polynomial, first Zagreb polynomial, second Zagreb polynomial of Möbius ladder is determined. We recovered many degree-based topological indices from the M-polynomial. Our nest target is two determine M-polynomial and some degree based topological indices of circulant graphs [11, 22].

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