The \( M \)-Polynomial and Topological Indices of Generalized Möbius Ladder and Its Line Graph

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Abstract. The \( M \)-polynomial was introduced by Deutsch and Klavžar in 2015 as a graph polynomial to provide an easy way to find closed formulas of degree-based topological indices, which are used to predict physical, chemical, and pharmacological properties of organic molecules. In this paper we give general closed forms of the \( M \)-polynomial of the generalized Möbius ladder and its line graph. We also compute Zagreb Indices, generalized Randić indices, and symmetric division index of these graphs via the \( M \)-polynomial.

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1. Introduction

The \( M \)-polynomial was introduced by E. Deutsch and S. Klavžar in 2015 in [6] as a graph invariant to play a role for degree-based invariants parallel to the role the Hosoya polynomial plays for distance-based invariants.

The \( M \)-polynomial has applications in mathematical chemistry and pharmacology. The most interesting application of the \( M \)-polynomial is that almost all degree-based graph invariants, which are used to predict physical, chemical, and pharmacological properties of organic molecules, can be recovered from it; for more information please see [5, 9, 13, 15, 28, 31, 32].

The \( M \)-polynomial and related topological indices have been studied for several classes of graphs. In 2015 Deutsch and Klavžar gave \( M \)-polynomial, first Zagreb, and second Zagreb indices of polyomino chains, starlike trees, and
Several degree-based topological indices, which play important role in mathematical chemistry, can be recovered from the $M$-polynomial: The most famous degree-based index is the Randić index and was introduced by Milan Randić in 1975 [27]. It is often used in cheminformatics for investigations of organic compounds; for more information, please see [11, 16, 26]. Later in 1998, working independently, Amic et al [2] and Bollobas-Erdos [3] proposed the generalized Randić index; for more information, please see [17, 20]. Gutman and Trinajstić introduced first Zagreb and second Zagreb indices in 1972 [14]. The augmented Zagreb index was proposed by Furtula et al. in 2010 in [8] and is useful for computing heat of information of alkanes [11, 19]. To know more about topological indices, their computing, and their applications we refer the reader to [4, 6, 7, 10, 23, 24, 25, 29, 31, 33].

This article is devoted to study the $M$-polynomial. We not only give the general forms of the $M$-polynomials of the generalized Mőbius ladder and its line graph but also recover first Zagreb, second Zagreb, second modified Zagreb, generalized Randić, reciprocal generalized Randić, and symmetric division indices from them.

2. Preliminary Notes

This section covers the definitions of graph, degree of a vertex, line graph, molecular graph, $M$-polynomial, topological index, Zagreb indices, generalized Randić indices, and generalized Mőbius ladder.

A graph $G$ is a pair $(V, E)$, where $V$ is the set of vertices and $E$ the set of edges. The edge $e$ between two vertices $u$ and $v$ is denoted by $(u, v)$. The degree of a vertex $u$, denoted by $d_u$ is the number of edges incident to it. 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 the length of that path. A graph is said to be connected if there is a path between any two of its vertices.

![Figure 1: A connected graph with $d_u = 4$ to $d_v = 2$](image)

The line graph of a graph $G$, written $L(G)$, is the graph whose vertices are edges of $G$, and when $e = (u, v)$ and $e' = (v, w)$ are adjacent edges of $G$ then $(e, e')$ is an edge of $L(G)$.
A molecular graph is a representation of a chemical compound in terms of graph theory. Specifically, molecular graph is a graph whose vertices correspond to (carbon) atoms of the compound and whose edges correspond to chemical bonds. For instance, Figure 1 represents the molecular graph of 1-bromopropyne (CH$_3$-C≡C-Br).

In the following by $G$ we shall mean a connected graph, $E$ its edge set, $V$ its vertex set, and $e = (u, v)$ its edge joining the vertices $u$ and $v$.

**Definition 2.1.** [6] The M-polynomial of $G$ is

\[ M(G; x, y) = \sum_{i \leq j} m_{ij} x^i y^j, \]

where $m_{ij}$ is the number of edges $e = (u, v)$ of $G$ with $d_u = i$ and $d_v = j$.

**Definition 2.2.** A function $I$ which assigns to every connected graph $G$ a unique number $I(G)$ is called a graph invariant. Instead of the function $I$ it is custom to say the number $I(G)$ as the invariant. An invariant of a molecular graph which can be used to determine structure-property or structure-activity correlation is called the topological index. A topological index is said to be degree-based if it depends on degrees of the vertices of the graph.

The following are definitions of some those degree-based indices that have connection with the $M$-polynomial.

The first Zagreb, second Zagreb, and second modified Zagreb indices of $G$ are respectively $M_1(G) = \sum_{e \in E} (d_u + d_v)$, $M_2(G) = \sum_{e \in E} d_u \times d_v$, and $MM_2(G) = \sum_{e \in E} \frac{1}{d_u \times d_v}$.

The generalized Randić and reciprocal generalized Randić indices of $G$ are respectively $R_\alpha(G) = \sum_{e \in E} (d_u \times d_v)^\alpha$ and $RR_\alpha(G) = \sum_{e \in E} \frac{1}{(d_u \times d_v)^\alpha}$.

The symmetric division index of $G$ is

\[ SSD(G) = \sum_{e \in E} \left\{ \frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)} \right\}. \]

A remarkable property of the $M$-polynomial is that all the above degree-based indices can be recovered from it, using the relations given in the following table.
Consider the Cartesian product \( P_m \times P_n \) of paths \( P_m \) and \( P_n \) with vertices \( u_1, u_2, \ldots, u_m \) and \( v_1, v_2, \ldots, v_n \), respectively. Take a 180° twist and identify the vertices \( (u_1, v_1), (u_1, v_2), \ldots, (u_1, v_n) \) with the vertices \( (u_m, v_n), (u_m, v_{n-1}), \ldots, (u_m, v_1) \), respectively, and identify the edge \( ((u_1, i), (u_1, i + 1)) \) with the edge \( ((u_m, v_{n+1-i}), (u_m, v_{n-1})) \), where \( 1 \leq i \leq n - 1 \). What we receive is the generalized Möbius ladder \( M_{m,n} \).

You can see \( M_{7,3} \) in the following figure.

![Figure 3: The grid form of the generalized Möbius ladder \( M_{7,3} \)](image)

The original form of \( M_{7,3} \) is:

![Figure 4: The generalized Möbius ladder \( M_{7,3} \)](image)

### 3. Main Results

In this section the general closed formulas of the \( M \)-polynomial of the generalized Möbius ladder and its line graph are given.
Theorem 3.1. The $M$-polynomial of the generalized Möbius ladder $M_{m,n}$, $m \geq 4, n \geq 2$, is

$$M(M_{m,n}, x, y) = 2(m - 1)x^3y^3 + 2(m - 1)x^3y^4 + (m - 1)(2n - 5)x^4y^4.$$ 

Proof. Depending on degrees of the vertices, the edges of $M_{m,n}$ can be divided into three disjoint sets: $E_{(3,3)} = \{e = (u, v) \in E \mid \deg(u) = \deg(v) = 3\}$, $E_{(3,4)} = \{e = (u, v) \in E \mid \deg(u) = 3, \deg(v) = 4\}$, and $E_{(4,4)} = \{e = (u, v) \in E \mid \deg(u) = 4, \deg(v) = 4\}$.

In order to count the number of elements in each of these sets we must consider the grid shape of $M_{m,n}$. The degree-three vertices lie on the top and bottom rows of $M_{m,n}$. Since in each such row there are $m$ vertices, the number of edges whose adjacent vertices are of degree 3 in each such row is $m - 1$. Thus, $|E_{(3,3)}| = 2(m - 1)$. For better understanding, let us have a look at, for instance, the grid shape of $M_{5,6}$:

![Grid of $M_{5,6}$](image)

The degree-three vertices on the top that are adjacent to degree-four vertices determine the edges $(v_{i,1}, v_{i,2})$ for $i \in \{1, \ldots, m - 1\}$, and the degree-three vertices on the bottom that are adjacent to degree-four vertices determine the edges $(v_{i,n-1}, v_{i,n})$ for $i \in \{1, \ldots, m - 1\}$; observe that such edges appear vertically. It follows that $m - 1$ such edges lie on the top and $m - 1$ such edges lie on the bottom of the grid of $M_{m,n}$. Hence $|E_{(3,3)}| = 2(m - 1)$.

The edges whose adjacent vertices have degrees 4 can be split into two types, horizontal and vertical. The horizontal edges determined by degree-four vertices are $(v_{i,j}, v_{i+1,j})$, where for each value of $j$ in $\{2, \ldots, n - 1\}$ $i$ takes values in $\{1, \ldots, m - 1\}$. Hence, the number of horizontal edges is $(m - 1)(n - 2)$. The vertical edges determined by degree-four vertices are $(v_{i,j}, v_{i,j+1})$, where for each value of $i$ in $\{1, \ldots, m - 1\}$ $j$ takes values in $\{2, \ldots, n - 2\}$. Hence, the number of vertical edges is $(m - 1)(n - 3)$. So,
\[ |E_{(4,4)}| = (m-1)(n-2) + (m-1)(n-3) = (m-1)(2n-5), \] and we are done. \(\square\)

**Theorem 3.2.** Let \(M_{m,n}\) be the generalized Möbius ladder for \(m, n \geq 4\). Then

\[
M(L(M_{m,n})) = 2(m-1)x^4y^4 + 4(m-1)x^4y^5 + 6(m-1)x^5y^6 + 6(m-1)(n-3)x^6y^6.
\]

**Proof.** Since the line graph \(L(M_{m,n})\) of the generalized Möbius ladder have only vertices of degrees 4, 5, and 6, the edge set of \(L(M_{m,n})\) can be divided into five disjoint sets:

\[
E_{(4,4)} = \{ e = (u, v) \in E \mid \deg(u) = \deg(v) = 4 \}, \quad E_{(4,5)} = \{ e = (u, v) \in E \mid \deg(u) = 4, \deg(v) = 5 \}, \quad E_{(5,5)} = \{ e = (u, v) \in E \mid \deg(u) = \deg(v) = 5 \}, \quad E_{(5,6)} = \{ e = (u, v) \in E \mid \deg(u) = 5, \deg(v) = 6 \}, \quad E_{(6,6)} = \{ e = (u, v) \in E \mid \deg(u) = \deg(v) = 6 \}.
\]

In order to to count the number of elements in each \(E_{(i,j)}\) we need to consider \(L(M_{m,n})\) in terms of the grid shape of \(M_{m,n}\). The edges of degree 4 appear only on the top and bottom rows of \(L(M_{m,n})\). On the top row each degree-four vertex of \(L(M_{m,n})\) lies on the edge \((v_{1,j}, v_{1,j+1}), \ 1 \leq j \leq m, \) of \(M_{m,n}\), and on the bottom row each degree-four vertex of \(L(M_{m,n})\) lies on the edge \((v_{n,j}, v_{n,j+1}), \ 1 \leq j \leq m, \) of \(M_{m,n}\). Since the number of edges determined by degree-four vertices on the top row of \(L(M_{m,n})\) is \(m-1\) and the number of edges determined by degree-four vertices on the bottom row of \(L(M_{m,n})\) is \(m-1\), \( |E_{(4,4)}| = 2(m-1) \). For better understanding, let us have a look at, for instance, the grid of \(M_{5,6}\) along with its line graph:

![Grid of M5,6](image-url)
Each vertex of degree 4, which is connected to a vertex of degree 5, lies either on the top row or on the bottom row of of $L(M_{m,n})$; see for clarity the line graph of $M_{5,6}$. Each such vertex is connected to two vertices of degree 5; each degree-five vertex of $L(M_{m,n})$ is determined by the edge $(v_{1,j}, v_{2,j}), 1 \leq j \leq m - 1$, on the top and by the edge $(v_{n-1,j}, v_{n,j}), 1 \leq j \leq m - 1$, on the bottom. It follows that the number of edges whose adjacent vertices have degrees 4 and 5 on the top of $L(M_{m,n})$ is $2(m-1)$. Hence, the total number of such edges is $4(m-1)$, i.e., $|E_{(4,5)}| = 4(m-1)$.

There is no edge with adjacent vertices of degree 5; to convince yourself, you may see $L(M_{5,6})$.

The degree-five vertices of $L(M_{m,n})$ that are connected to degree-six vertices of $L(M_{m,n})$ lie at the edges $(v_{1,j}, v_{2,j})$ and $(v_{n-1,j}, v_{n,j})$ for each column $j, 1 \leq j \leq m - 1$, of $M_{m,n}$. Each of degree-five vertex of $L(M_{m,n})$ that lies at the edge $(v_{1,j}, v_{2,j})$ of $M_{m,n}$ is connected with three vertices of degree 6, two are lying at the edges $(v_{1,j}, v_{1,j+1})$ and $(v_{1,j+1}, v_{1,j+2})$ and one is lying at the edge $(v_{i,j}, v_{i+1,j})$ of $M_{m,n}$. Since there are $m - 1$ such vertices, the number of edges, whose adjacent vertices are of degree 5 and 6, determined by them is $3(m-1)$. Similarly, the number of edges, whose adjacent vertices are of degree 5 and 6, determined by degree-five vertices of $L(M_{m,n})$ that lie at the edges $(v_{n-1,j}, v_{n,j})$ of $M_{m,n}$ is $3(m-1)$. Hence $|E_{(5,6)}| = 6(m-1)$.

The edges of $L(M_{m,n})$ whose adjacent vertices have degrees 6 can be divided into three types: the edges that appear horizontally, the edges that appear vertically, and the edges that appear diagonally. Each horizontal edge of $L(M_{m,n})$ with adjacent vertices of degrees 6 appears in row $i, 2 \leq i \leq n - 1$,
Similarly, division indices from the
M\text{Zagreb}, generalized Randić, reciprocal generalized Randić, and symmetric
4. Topological Indices
In this section we recover the first Zagreb, second Zagreb, modified second
Zagreb, generalized Randić, reciprocal generalized Randić, and symmetric
division indices from the \( M \)-polynomials of the generalized Möbius ladder
and its line graph.

Proposition 4.1. The degree-based topological indices of \( M_{m,n} \) are:

1. \( M_1(M_{m,n}) = 16mn - 20m - 16n + 14 \)
2. \( M_2(M_{m,n}) = 16(4n - 3)(n - 1)(m - 1)^2 \)
3. \( MM_2(M_{m,n}) = \frac{1}{144}(6n - 1)(6n + 1)(m - 1)^2 \)
4. \( R_α(M_{m,n}) = [16(4n - 3)(n - 1)(m - 1)^2]^α \)
5. \( RR_α(M_{m,n}) = [\frac{1}{144}(6n - 1)(6n + 1)(m - 1)^2]^α \)
6. \( SDD(M_{m,n}) = \frac{1}{72}(48n^2 - 42n + 1)(m - 1)^2 \)

Proof. From the \( M \)-polynomial of \( M_{m,n} \) we get

\[
D_x = x\left[\frac{\partial M(M_{m,n})}{\partial x}\right]
\]
\[
= x\left[\frac{\partial}{\partial x}(2(m - 1)x^3y^3 + 2(m - 1)x^3y^4 + (m - 1)(2n - 5)x^4y^4]\right]
\]
\[
= x[6(m - 1)x^2y^3 + 6(m - 1)x^2y^4 + 4(m - 1)(2n - 5)x^3y^4]
\]
\[
= 6(m - 1)x^3y^3 + 6(m - 1)x^3y^4 + 4(m - 1)(2n - 5)x^4y^4.
\]

Similarly,

\[
D_y = y\left[\frac{\partial M(M_{m,n})}{\partial y}\right]
\]
\[
= 6(m - 1)x^3y^3 + 8(m - 1)x^3y^4 + 4(m - 1)(2n - 5)x^4y^4.
\]
Now
\[ S_x = \int_0^x \frac{M(t,y)}{t} dt \]
\[ = \int_0^x \frac{1}{t} \left[ 2(m-1)t^3y^3 + 2(m-1)t^3y^4 + (m-1)(2n-5)t^4y^4 \right] dt \]
\[ = \left( \frac{2m-2}{3} \right)x^3y^3 + \left( \frac{2m-2}{4} \right)x^3y^4 + \frac{(2n-5)(m-1)}{4}x^4y^4. \]

Similarly,
\[ S_y = \left( \frac{2m-2}{3} \right)x^3y^3 + \left( \frac{2m-2}{4} \right)x^3y^4 + \frac{(2n-5)(m-1)}{4}x^4y^4. \]

Finally,
1. \[ M_1 = (D_x + D_y)_{x=y=1} \]
   \[ = (8mn - 8m - 8n + 8) + (8mn - 12m - 8n + 6) \]
   \[ = 16mn - 20m - 16n + 14 \]

2. \[ M_2 = (D_x)_{x=y=1}(D_y)_{x=y=1} \]
   \[ = (8mn - 8m - 8n + 8)(8mn - 12m - 8n + 6) \]
   \[ = 16(4n - 3)(n - 1)(m - 1)^2 \]

3. \[ MM_2 = (S_x)_{x=y=1}(S_y)_{x=y=1} \]
   \[ = \left( \frac{6mn + m - 6n - 1}{12} \right)\left( \frac{6mn - m - 6n + 1}{12} \right) \]
   \[ = \frac{1}{144}(6n - 1)(6n + 1)(m - 1)^2 \]

4. \[ R_\alpha(G) = [D^\alpha_x]_{x=y=1}[D^\alpha_y]_{x=y=1} \]
   \[ = [16(4n - 3)(n - 1)(m - 1)^2]^\alpha \]

5. \[ RR_\alpha(G) = [S^\alpha_x]_{x=y=1}[S^\alpha_y]_{x=y=1} \]
   \[ = \left[ \frac{1}{144}(6n - 1)(6n + 1)(m - 1)^2 \right]^\alpha \]
6. \[ SDD = (D_xS_y)_{x=y=1} + (S_xD_y)_{x=y=1} \]
\[ = (8mn - 8m - 8n + 8)(\frac{6mn - m - 6n + 1}{12}) \]
\[ + (\frac{6mn + m - 6n - 1}{12})(8mn - 12m - 8n + 6) \]
\[ = \frac{1}{72}(48n^2 - 42n + 1)(m - 1)^2 \]

**Proposition 4.2.** The degree-based topological indices of \( L(M_{m,n}) \) are:
1. \( M_1(L(M_{m,n})) = 2(36n - 49)(m - 1) \)
2. \( M_2(L(M_{m,n})) = 72(9n - 11)(2n - 3)(m - 1)^2 \)
3. \( MM_2(L(M_{m,n})) = \frac{1}{100}(10n - 3)(10n - 7)(m - 1)^2 \)
4. \( R_\alpha(L(M_{m,n})) = [\frac{72(9n - 11)(2n - 3)(m - 1)^2}{\alpha}]^\alpha \)
5. \( RR_\alpha(L(M_{m,n})) = [\frac{1}{100}(10n - 3)(10n - 7)(m - 1)^2]^\alpha \)
6. \( SDD(L(M_{m,n})) = \frac{1}{72}(48n^2 - 42n + 1)(m - 1)^2 \)

**Proof.** The proof is similar to the proof of Proposition 4.1.

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