

M-POLYNOMIALS AND DEGREE-BASED TOPOLOGICAL INDICES OF SOME FAMILIES OF CONVEX POLYTOPES

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ABSTRACT. In this article, we compute closed forms of M-polynomials for three general classes of convex polytopes. From the M-polynomials, we derive degree-based topological indices such as first and second Zagreb indices, modified second Zagreb index, Symmetric division index, etc.

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1. Introduction

A graph $G(V, E)$ with vertex set $V(G)$ and edge set $E(G)$ are connected, if there exists a connection between any pair of vertices in G . The degree of a vertex is the number of vertices which are connected to that fixed vertex by the edges. In a chemical graph, the degree of any vertex is at most 4. The distance between two vertices u and v is denoted as $d(u, v) = d_G(u, v)$ and is the length of shortest path between u and v in graph G . 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 . The concept of degree in graph theory is closely related (but not identical) to the concept of valence in chemistry. For details on basics of graph theory, any standard text such as [1] can be of great help.

Several algebraic polynomials have useful applications in chemistry such as Hosoya polynomial (also called Wiener polynomial) [2], which plays a vital role in determining distance-based topological indices. Among other algebraic polynomials, M-polynomial [3] introduced in 2015, plays the same role in determining

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closed form of many degree-based topological indices [4, 5, 6, 7, 8]. The main advantage of M-polynomial is the wealth of information that it contains about degree-based graph invariants.

Definition 1.1. [3] The M-polynomial of G is defined as:

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

where $\delta = \text{Min}\{d_v | v \in V(G)\}$, $\Delta = \text{Max}\{d_v | v \in V(G)\}$, and $m_{ij}(G)$ is the edge $vu \in E(G)$ such that $\{d_v, d_u\} = \{i, j\}$.

The first topological index was introduced by Wiener [9] and it was named *path number*, which is now known as *Wiener index*. In chemical graph theory, this is the most studied molecular topological index due to its wide applications; see for details in [10, 11]. Randić index, [12] denoted by $R_{-1/2}(G)$ and introduced by Milan Randić in 1975 is also one of the oldest topological index. The Randić index is defined as

$$R_{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

In 1998, working independently, Bollobas and Erds, [13] and Amic *et al.* [14] proposed the generalized Randić index which has been studied extensively by both chemists and mathematicians [15]. Many mathematical properties have been discussed [16]. For a detailed survey we refer the book [17].

The general Randić index is defined as:

$$R_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^\alpha},$$

and the inverse Randić index is defined as $RR_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$.

Obviously $R_{-1/2}(G)$ is the particular case of $R_\alpha(G)$ when $\alpha = -\frac{1}{2}$.

The Randić index is the most popular most often applied and most studied among all other topological indices. Many papers and books such as [18, 19, 20] are written on this topological index. Randić himself wrote two reviews on his Randić index [21, 22] and there are three more reviews [23, 24, 25]. The suitability of the Randić index for drug design was immediately recognized, and eventually the index was used for this purpose on countless occasions. The physical reason for the success of such a simple graph invariant is still an enigma, although several more-or-less plausible explanations were offered.

Gutman and Trinajstić introduced first Zagreb index and second Zagreb index, which are defined as: $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$ and $M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v)$ respectively. The second modified Zagreb index is defined as:

$${}^m M_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}.$$

For details about these indices we offer [26, 27, 28, 29, 30] for the readers.

The Symmetric division index is defined as:

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

Another variant of Randić index is the harmonic index defined as:

$$H(G) = \sum_{vu \in E(G)} \frac{2}{d_u + d_v}.$$

The Inverse sum index is defined as:

$$I(G) = \sum_{vu \in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

The augmented Zagreb index is defined as:

$$A(G) = \sum_{vu \in E(G)} \left\{ \frac{d_u d_v}{d_u + d_v - 2} \right\}^3,$$

and it is useful for computing heat of formation of alkanes [31, 32].

The following Table 1 relates some well-known degree-based topological indices with M-polynomial [3].

Table 1 Derivation of some degree-based topological indices from M-polynomial

| Topological Index | Derivation from $M(G; x, y)$ |
|--------------------------|--|
| First Zagreb | $(D_x + D_y)(M(G; x, y))_{x=y=1}$ |
| Second Zagreb | $(D_x D_y)(M(G; x, y))_{x=y=1}$ |
| Second Modified Zagreb | $(S_x S_y)(M(G; x, y))_{x=y=1}$ |
| Randić Index | $(D_x^\alpha D_y^\alpha)(M(G; x, y))_{x=y=1}$ |
| Inverse Randić Index | $(S_x^\alpha S_y^\alpha)(M(G; x, y))_{x=y=1}$ |
| Symmetric Division Index | $(D_x S_y + S_x D_y)(M(G; x, y))_{x=y=1}$ |
| Harmonic Index | $2S_x J(M(G; x, y))_{x=1}$ |
| Inverse sum Index | $S_x J D_x D_y(M(G; x, y))_{x=1}$ |
| Augmented Zagreb Index | $S_x^3 Q_{-2} J D_x^3 D_y^3(M(G; x, y))_{x=1}$ |

where

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

$$J(f(x, y)) = f(x, x), \quad Q_\alpha(f(x, y)) = x^\alpha f(x, y).$$

2. Main Results

In this section we give our main results.

2.1. Computational aspects of Convex Polytopes T_n . The graph of convex polytope T_n can be obtained from the graph of convex polytope Q_n by adding new edges. It consists of three-sided faces, five-sided faces and n -sided faces. $a_{i+1}b_i$, i.e., $V(T_n) = V(Q_n)$ and $V(T_n) = V(Q_n) \cup \{a_{i+1}b_i : 1 \leq i \leq n\}$ as shown in figure 1.

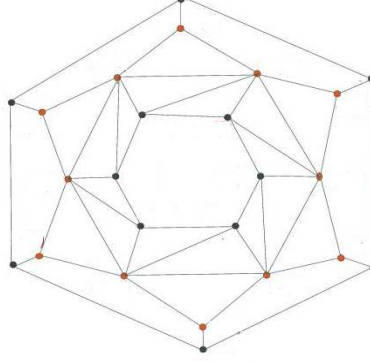


FIGURE 1. Graph of Convex polytope T_6 .

Theorem 2.1. Assume we have a convex polytope T_n , then the M -Polynomial of T_n is

$$M(T_n; x, y) = 2nx^3y^3 + 2nx^3y^6 + nx^4y^4 + 2nx^4y^6 + nx^6y^6.$$

Proof. Let $G = T_n$ be a convex polytope. It is easy to see from Figure 1 that

$$\begin{aligned} |V(T_n)| &= 4n, \\ |E(T_n)| &= 8n. \end{aligned}$$

The vertex set of S_n has two partitions:

$$\begin{aligned} V_1(T_n) &= \{u \in V(T_n) : d_u = 3\}, \\ V_2(T_n) &= \{u \in V(T_n) : d_u = 4\}, \\ V_4(T_n) &= \{u \in V(T_n) : d_u = 6\}, \end{aligned}$$

such that

$$|V_1(T_n)| = 2n, |V_2(T_n)| = n, |V_3(T_n)| = n,$$

The edge set of T_n has three partitions:

$$\begin{aligned} E_1(T_n) &= \{e = uv \in E(T_n) : d_u = d_v = 3\}, \\ E_2(T_n) &= \{e = uv \in E(T_n) : d_u = 3, d_v = 6\}, \end{aligned}$$

$$\begin{aligned}
E_3(T_n) &= \{e = uv \in E(S_n) : d_u = d_v = 4\}, \\
E_4(T_n) &= \{e = uv \in E(T_n) : d_u = 4, d_v = 6\}, \\
E_5(T_n) &= \{e = uv \in E(T_n) : d_u = d_v = 6\},
\end{aligned}$$

From Figure 1,

$$|E_1(T_n)| = 2n, |E_2(T_n)| = 2n, |E_3(T_n)| = n, |E_4(T_n)| = 2n, |E_5(T_n)| = n,$$

From the definition of the M-polynomial

$$\begin{aligned}
M(T_n; x, y) &= \sum_{i \leq j} m_{ij}(T_n) x^i y^j \\
&= \sum_{3 \leq 3} m_{33}(T_n) x^3 y^3 + \sum_{3 \leq 6} m_{36}(T_n) x^3 y^6 + \sum_{4 \leq 4} m_{44}(T_n) x^4 y^4 \\
&\quad + \sum_{4 \leq 6} m_{46}(T_n) x^4 y^6 + \sum_{6 \leq 6} m_{66}(T_n) x^6 y^6 \\
&= \sum_{uv \in E_1} m_{33}(T_n) x^3 y^3 + \sum_{uv \in E_2} m_{36}(T_n) x^3 y^6 + \sum_{uv \in E_3} m_{44}(T_n) x^4 y^4 \\
&\quad + \sum_{uv \in E_4} m_{46}(T_n) x^4 y^6 + \sum_{uv \in E_5} m_{66}(T_n) x^6 y^6 \\
&= |E_1| x^3 y^3 + |E_2| x^3 y^6 + |E_3| x^4 y^4 + |E_4| x^4 y^6 + |E_5| x^6 y^6 \\
&= 2nx^3 y^3 + 2nx^3 y^6 + nx^4 y^4 + 2nx^4 y^6 + nx^6 y^6.
\end{aligned}$$

□

Now we compute some degree-based topological indices of double antiprism from this M-polynomial.

Proposition 2.2. *Let T_n be the double antiprism, then*

- (1) $M_1(T_n) = 70n$.
- (2) $M_2(T_n) = 154n$
- (3) ${}^m M_2(T_n) = \frac{73}{144}n$.
- (4) $R_\alpha(T_n) = 2 \times 9^\alpha n + 2 \times 18^\alpha n + 16^\alpha n + 2 \times 24^\alpha n + 36^\alpha n$.
- (5) $RR_\alpha(T_n) = \frac{2n}{9^\alpha} + \frac{2n}{16^\alpha} + \frac{n}{16^\alpha} + \frac{2n}{24^\alpha} + \frac{n}{36^\alpha}$.
- (6) $SSD(T_n) = \frac{52}{3}n$.
- (7) $H(T_n) = \frac{98}{45}n$.
- (8) $I(T_n) = \frac{84}{5}n$.
- (9) $A(T_n) = \frac{6534785489}{37044000}n$.

Proof. Let

$$M(T_n; x, y) = f(x, y) = 2nx^3 y^3 + 2nx^3 y^6 + nx^4 y^4 + 2nx^4 y^6 + nx^6 y^6$$

Then

$$D_x(f(x, y)) = 6nx^3 y^3 + 6nx^3 y^6 + 4nx^4 y^4 + 8nx^4 y^6 + 6nx^6 y^6,$$

$$D_y(f(x, y)) = 6nx^3y^3 + 12nx^3y^6 + 4nx^4y^4 + 12nx^4y^6 + 6nx^6y^6,$$

$$(D_y D_x)(f(x, y)) = 18nx^3y^3 + 36nx^3y^6 + 16nx^4y^4 + 48nx^4y^6 + 36nx^6y^6,$$

$$S_x S_y(f(x, y)) = \frac{2}{9}nx^3y^3 + \frac{1}{9}nx^3y^6 + \frac{1}{16}nx^4y^4 + \frac{1}{12}nx^4y^6 + \frac{1}{36}nx^6y^6,$$

$$D_x^\alpha D_y^\alpha(f(x, y)) = 2 \times 9^\alpha nx^3y^3 + 2 \times 18^\alpha nx^3y^6 + 16^\alpha nx^4y^4 + 2 \times 24^\alpha nx^4y^6 + 36^\alpha nx^6y^6,$$

$$S_x^\alpha S_y^\alpha(f(x, y)) = \frac{2n}{9^\alpha}x^3y^3 + \frac{2n}{16^\alpha}x^3y^6 + \frac{n}{16^\alpha}x^4y^4 + \frac{2n}{24^\alpha}x^4y^6 + \frac{n}{36^\alpha}x^6y^6,$$

$$S_y D_x(f(x, y)) = 2nx^3y^3 + nx^3y^6 + nx^4y^4 + \frac{4n}{3}x^4y^6 + nx^6y^6,$$

$$S_x D_y(f(x, y)) = 2nx^3y^3 + 4nx^3y^6 + nx^4y^4 + 3nx^4y^6 + nx^6y^6,$$

$$S_x J f(x, y) = \frac{n}{3}x^6 + \frac{n}{4}x^8 + \frac{2n}{9}x^9 + \frac{n}{5}x^{10} + \frac{n}{12}x^{12},$$

$$S_x J D_x D_y(f(x, y)) = 3nx^6 + 2nx^8 + 4nx^9 + \frac{24}{5}nx^{10} + 3nx^{12},$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3 f(x, y) = \frac{1458}{64}nx^4 + \frac{4096}{216}nx^6 + \frac{11664}{343}nx^7 + \frac{27648}{512}nx^8 + \frac{46656}{1000}nx^{10}.$$

Now from Table 1

$$(1) M_1(T_n) = (D_x + D_y)(f(x, y))|_{x=y=1} = 70n.$$

$$(2) M_2(T_n) = D_x D_y(f(x, y))|_{x=y=1} = 154n.$$

$$(3) {}^m M_2(T_n) = S_x S_y(f(x, y))|_{x=y=1} = \frac{73}{144}n.$$

$$(4) R_\alpha(T_n) = D_x^\alpha D_y^\alpha(f(x, y))|_{x=y=1} = 2 \times 9^\alpha n + 2 \times 18^\alpha n + 16^\alpha n + 2 \times 24^\alpha n + 36^\alpha n.$$

$$(5) RR_\alpha(T_n) = S_x^\alpha S_y^\alpha(f(x, y))|_{x=y=1} = \frac{2n}{9^\alpha} + \frac{2n}{16^\alpha} + \frac{n}{16^\alpha} + \frac{2n}{24^\alpha} + \frac{n}{36^\alpha}.$$

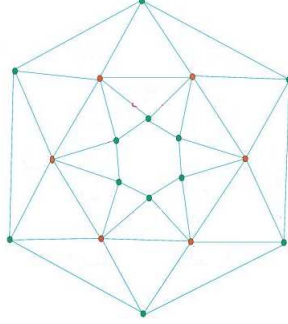
$$(6) SSD(T_n) = (S_y D_x + S_x D_y)(f(x, y))|_{x=y=1} = \frac{52}{3}n.$$

$$(7) H(T_n) = 2S_x J(f(x, y))|_{x=1} = \frac{98}{45}n.$$

$$(8) I(T_n) = S_x J D_x D_y(f(x, y))|_{x=1} = \frac{84}{5}n.$$

$$(9) A(T_n) = S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y))|_{x=1} = \frac{6534785489}{37044000}n.$$

□

FIGURE 2. Graph of double antiprism A_6 .

2.2. Computational aspects of Convex Polytopes A_n . The graph of convex polytope (double antiprism) A_n can be obtained from the graph of convex polytope R_n R_n by adding new edges $b_{i+1}c_i$, i.e., $V(A_n) = V(R_n)$ and $V(A_n) = V(R_n) \cup \{b_{i+1}c_i : 1 \leq i \leq n\}$ as shown in Figure 2.

Theorem 2.3. *Let A_n be the double antiprism, then the M -Polynomial of A_n is*

$$M(A_n, x, y) = 2nx^4y^4 + 4nx^4y^6 + nx^6y^6$$

Proof. Let $G = A_n$ is double antiprism. It is easy to see from figure 2 that

$$\begin{aligned} |V(A_n)| &= 3n, \\ |E(A_n)| &= 7n. \end{aligned}$$

The vertex set of A_n has two partitions:

$$\begin{aligned} V_1(A_n) &= \{u \in V(A_n) : d_u = 4\}, \\ V_2(A_n) &= \{u \in V(A_n) : d_u = 6\}, \end{aligned}$$

such that

$$|V_1(A_n)| = 2n, |V_2(A_n)| = n.$$

The edge set of A_n has three partitions:

$$\begin{aligned} E_1(A_n) &= \{e = uv \in E(A_n) : d_u = d_v = 4\}, \\ E_2(A_n) &= \{e = uv \in E(A_n) : d_u = 4, d_v = 6\}, \\ E_3(A_n) &= \{e = uv \in E(A_n) : d_u = d_v = 6\}, \end{aligned}$$

From Figure 2,

$$|E_1(A_n)| = 2n, |E_2(A_n)| = 4n, |E_3(A_n)| = n,$$

Now from the definition of the M-polynomial

$$\begin{aligned}
M(A_n, x, y) &= \sum_{i \leq j} m_{ij}(A_n) x^i y^j \\
&= \sum_{4 \leq 4} m_{44}(A_n) x^4 y^4 + \sum_{4 \leq 6} m_{46}(A_n) x^4 y^6 + \sum_{5 \leq 5} m_{66}(A_n) x^6 y^6 \\
&= \sum_{uv \in E_1} m_{44}(A_n) x^4 y^4 + \sum_{uv \in E_2} m_{46}(A_n) x^4 y^6 + \sum_{uv \in E_3} m_{66}(A_n) x^6 y^6 \\
&= |E_1| x^4 y^4 + |E_2| x^4 y^6 + |E_3| x^6 y^6 \\
&= 2nx^4 y^4 + 4nx^4 y^6 + nx^6 y^6.
\end{aligned}$$

□

Now we compute some degree-based topological indices of double antiprism from this M-polynomial.

Proposition 2.4. *Let A_n be the double antiprism, then*

- (1) $M_1(A_n) = 68n$.
- (2) $M_2(A_n) = \frac{23}{72}n$.
- (3) ${}^m M_2(A_n) = \frac{23}{72}n$.
- (4) $R_\alpha(A_n) = n(4 \times 24^\alpha + 36^\alpha + 2 \times 16^\alpha)$.
- (5) $RR_\alpha(A_n) = n\left(\frac{2}{16^\alpha} + \frac{4}{24^\alpha} + \frac{1}{36^\alpha}\right)$.
- (6) $SSD(A_n) = \frac{44}{3}n$.
- (7) $H(A_n) = \frac{11}{15}n$.
- (8) $I(A_n) = \frac{83}{5}n$.
- (9) $A(A_n) = \frac{649964}{3375}n$.

2.3. Computational aspects of Convex Polytopes. S_n

The graph of convex polytope (double antiprism) S_n can be obtained from the graph of convex polytope Q_n by adding new edges $c_i c_{i+1}$, i.e., $V(S_n) = V(Q_n)$ and $E(S_n) = E(Q_n) \cup \{c_i c_{i+1} : 1 \leq i \leq n\}$ as shown in Figure 3.

Theorem 2.5. *Let S_n be the double antiprism, then the M-Polynomial of S_n is*

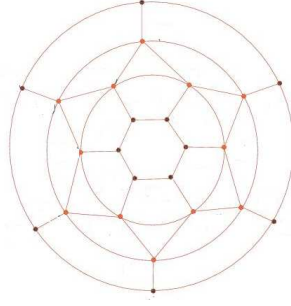
$$M(S_n; x, y) = 2nx^3 y^3 + 2nx^3 y^5 + 4nx^5 y^5.$$

Proof. Let $G = S_n$ be the double antiprism. It is easy to see from Figure 3 that

$$\begin{aligned}
|V(S_n)| &= 4n, \\
|E(S_n)| &= 8n.
\end{aligned}$$

The vertex set of S_n has two partitions:

$$V_1(S_n) = \{u \in V(S_n) : d_u = 3\},$$

FIGURE 3. Graph of double antiprism S_6 .

$$V_2(S_n) = \{u \in V(S_n) : d_u = 5\},$$

such that

$$|V_1(S_n)| = 2n, |V_2(S_n)| = 2n.$$

The edge set of A_n has three partitions:

$$\begin{aligned} E_1(S_n) &= \{e = uv \in E(S_n) : d_u = d_v = 3\}, \\ E_2(S_n) &= \{e = uv \in E(S_n) : d_u = 3, d_v = 5\}, \\ E_3(S_n) &= \{e = uv \in E(S_n) : d_u = d_v = 5\}, \end{aligned}$$

From Figure 3,

$$|E_1(S_n)| = 2n, |E_2(S_n)| = 2n, |E_3(S_n)| = 4n,$$

Now from the definition of the M-polynomial

$$\begin{aligned} M(S_n; x, y) &= \sum_{i \leq j} m_{ij}(S_n) x^i y^j \\ &= \sum_{uv \in E_1} m_{33}(S_n) x^3 y^3 + \sum_{uv \in E_2} m_{35}(S_n) x^3 y^5 + \sum_{uv \in E_3} m_{55}(S_n) x^5 y^5 \\ &= |E_1| x^3 y^3 + |E_2| x^3 y^5 + |E_3| x^5 y^5 \\ &= 2n x^3 y^3 + 2n x^3 y^5 + 4n x^5 y^5. \end{aligned}$$

□

Now we compute some degree-based topological indices of double antiprism from this M-polynomial.

Proposition 2.6. *Let A_n be the double antiprism, then*

- (1) $M_1(S_n) = 68n$.
- (2) $M_2(S_n) = 148n$.
- (3) ${}^m M_2(S_n) = \frac{116}{225}n$.
- (4) $R_\alpha(S_n) = 2n(9^\alpha + 15^\alpha + 2 \times 25^\alpha)$.
- (5) $RR_\alpha(S_n) = 2n\left(\frac{1}{9^\alpha} + \frac{1}{15^\alpha} + \frac{2}{25^\alpha}\right)$.
- (6) $SSD(S_n) = \frac{248}{15}n$.
- (7) $H(S_n) = \frac{59}{60}n$.
- (8) $I(S_n) = \frac{67}{4}n$.
- (9) $A(S_n) = \frac{22541}{128}n$.

3. Conclusions and Discussions

We computed closed forms of M-polynomial of three general classes of convex polytopes at first. Then we derived as many as nine degree-based topological indices such as first and second Zagreb indices, modified second Zagreb index, Symmetric division index, Augmented Zagreb index, Inverse-sum index etc.

Competing Interest

The authors declare no competing interest.

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