M-Polynomial and Degree-Based Topological Indices

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ABSTRACT Let G be a graph and let $m_{ij}(G), i, j \geq 1$, be the number of edges uv of G such that $\{d_v(G), d_u(G)\} = \{i, j\}$ The M-polynomial of G is introduced with $M(G; x, y) = \sum_{i \leq j} m_{ij}(G) x^i y^j$. It is shown that degree-based topological indices can be routinely computed from the polynomial, thus reducing the problem of their determination in each particular case to the single problem of determining the M-polynomial. The new approach is also illustrated with examples.

KEYWORDS degree-based topological index • Zagreb index • Randić index • graph polynomial

1. INTRODUCTION

Numerous graph polynomials were introduced in the literature, several of them turned out to be applicable in mathematical chemistry. For instance, the Hosoya polynomial [19], see also [9, 11, 21], is the key polynomial in the area of distance-based topological indices. In particular, the Wiener index can be computed as the first derivative of the Hosoya polynomial, evaluated at 1, the hyper-Wiener index [5] and the Tratch-Stankevich-Zefirov index can be obtained similarly [4, 16]. Additional chemically relevant polynomials are the matching polynomial [13, 12], the Zhang-Zhang polynomial (also known as the Clar covering polynomial) [25, 6, 24], the Schultz polynomial [18], and the Tutte polynomial [10], to name just a few of them. In this paper we introduce a polynomial called the M-polynomial, and

show that its role for degree-based invariants is parallel to the role of the Hosoya polynomial for distance-based invariants.

In chemical graph theory (too) many topological indices were introduced, in particular (too) many degree-based topological indices. This fact is emphasized in the recent survey [15] which contains a uniform approach to the degree-based indices and a report on a comparative test from [17] how these indices are correlated with physico-chemical parameters of octane isomers. The test indicates that quite many of these indices are inadequate for any structure-property correlation. But it could be that they are still applicable in a combination with other indices.

In the literature one finds many papers that, for a given family of graphs, determine a closed formula for a given (degree-based) topological index. To overcome this particular approach in the area of degree-based indices, in this paper we introduce the *M*-polynomial and demonstrate that in numerous cases a degree-based topological index can be expressed as a certain derivative or integral (or both) of the corresponding *M*-polynomial. This in particular implies that knowing the *M*-polynomial of a given family of graphs, a closed formula for any such index can be obtained routinely. In the remaining cases when the function defining a given topological index is such that it does not allow it to be (routinely) determined from the *M*-polynomial, one can use equality (2) from the following section and try to get a closed formula from it. But in any case, knowing the *M*-polynomial is sufficient, hence the possible future research in the area should concentrate on determining the *M*-polynomial of a relevant family of graphs instead of computing the corresponding indices one by one. Moreover, it is our hope that a closer look to the properties of the *M*-polynomial will bring new general insights.

In the next section the *M*-polynomial is introduced and shown how degree-based indices can be computed from it. In the last section it is discussed how the *M*-polynomial can be computed for (chemical) graphs and typical examples for the use of the new polynomial are presented.

2. THE *M*-POLYNOMIAL

If $G = (V, E)$ is a graph and $v \in V$, then $d_v(G)$ (or d_v for short if G is clear from the context) denotes the degree of v. Let G be a graph and let $m_{ij}(G)$, $i, j \geq 1$, be the number of edges $e = uv$ of G such that $\{d_v(G), d_u(G)\} = \{i, j\}$. As far as we know, the quantities m_{ij} were first introduced and applied in [14]. We now introduce the *M-polynomial* of G as

$$M(G; x, y) = \sum_{i < j} m_{ij}(G) x^i y^j.$$

For a graph $G = (V, E)$, a degree-based topological index is a graph invariant of the form

$$I(G) = \sum_{e=uv \in E} f(d_u, d_v), \tag{1}$$

where $f = f(x, y)$ is a function appropriately selected for possible chemical applications [15]. For instance, the generalized Randić index $R_\alpha(G), \alpha \neq 0$, is defined with (1) by setting $f(x, y) = (xy)^\alpha$ [3]. Collecting edges with the same set of end degrees we can rewrite (1) as

$$I(G) = \sum_{i \leq j} m_{ij}(G) f(i, j) \tag{2}$$

cf. [7, 8, 15, 22].

Using the operators D_x and D_y defined on differentiable functions in two variables by

$$D_x(f(x, y)) = x \frac{\partial f(x, y)}{\partial x}, \qquad D_y(f(x, y)) = y \frac{\partial f(x, y)}{\partial y},$$

we have:

Theorem 2.1. Let $G = (V, E)$ be a graph and let $I(G) = \sum_{e=uv \in E} f(d_u, d_v)$, where $f(x, y)$ is a polynomial in x and y. Then

$$I(G) = f(D_x, D_y)(M(G; x, y))\big|_{x=y=1}.$$

Proof. Let $r \geq 0$ and $s \geq 0$ be fixed. Then

$$D_x^r D_y^s(M(G; x, y)) = D_x^r D_y^s\left(\sum_{i \leq j} m_{ij}(G) x^i y^j\right) = D_x^r\left(\sum_{i \leq j} m_{ij}(G) j^s x^i y^j\right)$$

$$= \sum_{i \leq j} m_{ij}(G) i^r j^s x^i y^j.$$

It follows that

$$f(D_x, D_y)(M(G; x, y))\big|_{x=y=1} = \sum_{i \leq j} m_{ij}(G) \sum_{r,s} \alpha_{r,s} i^r j^s = \sum_{i \leq j} m_{ij}(G) f(i, j).$$

The result follows by (2). ∎

In addition to the operators D_x and D_y we will also make use of the operators

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

As in the proof of Theorem 2.1 we infer that the operators $S_x^r S_y^s$, $S_x^r D_y^s$, and $D_x^r S_y^s$ applied to the term $x^i y^j$ of $M(G; x, y)$, and evaluated at $x = y = 1$, return $i^{-r} j^{-s}$, and $i^{-r} j^{-s}$, respectively. Hence, proceeding along the same lines as in the proof of Theorem 2.1, we can state the following extension of Theorem 2.1.

Theorem 2.2. *Let $G = (V, E)$ be a graph and let $I(G) = \sum_{e=uv \in E} f(d_u, d_v)$, where*

$$f(x, y) = \sum_{i,j \in Z} \alpha_{ij} x^i y^j.$$

Then $I(G)$ can be obtained from $M(G; x, y)$ using the operators D_x, D_y, S_x, and S_y.

In the statement of Theorem 2.2, $I(G)$ appears implicitly (contrary to the explicit formula of Theorem 2.1). Hence in Table 1 explicit expressions for some frequent degree-based topological indices are listed. The general case for any function of the form $f(x, y) = \sum_{i,j \in Z} \alpha_{ij} x^i y^j$ should then be clear. Note that for the symmetric division index we can apply Theorem 2.2 because its defining function $f(x, y)$ can equivalently be written as $x/y + y/x$.

Topological index	$f(x, y)$	Derivation from M($G;x,y$)
First Zagreb	$x+y$	$(D_x+D_y)(M(G;x,y))\big|_{x=y=1}$
Second Zagreb	xy	$(D_xD_y)(M(G;x,y))\big|_{x=y=1}$
Second modified Zagreb	$\dfrac{1}{xy}$	$(S_xS_y)(M(G;x,y))\big|_{x=y=1}$
General Randić ($\alpha \in N$)	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(M(G;x,y))\big|_{x=y=1}$
General Randić ($\alpha \in N$)	$\dfrac{1}{(xy)^\alpha}$	$(S_x^\alpha S_y^\alpha)(M(G;x,y))\big|_{x=y=1}$
Symmetric division index	$\dfrac{x^2 + y^2}{xy}$	$(D_xS_y+D_yS_x)(M(G; x,y))\big|_{x=y=1}$

Table 1. Some standard degree based topological indices and the formulas how to compute them from the *M*-polynomial.

In order to handle additional indices that are not covered by Theorem 2.2, we introduce two additional operators as follows:

$$J(f(x, y)) = f(x, x), \qquad Q_\alpha(f(x, y)) = x^\alpha f(x, y), \ \alpha \neq 0.$$

With these two operators we have the following result whose proof again proceeds along the same lines as the proof of Theorem 2.1:

Proposition 2.3. *Let $G = (V;E)$ be a graph and let $I(G) = \sum_{e=uv \in E} f(d_u, d_v)$, where $f(x, y) = \dfrac{x^r y^s}{(x + y + \alpha)^k}$, and $r, s \geq 0, \ t \geq 1$, and $\alpha \in Z$ then*

$$I(G) = S_x^k Q_\alpha J D_x^r D_y^s (M(G; x, y))\big|_{x=1}.$$

In Table 2 three special cases of Proposition 2.3 from the literature are collected.

Topological index	$f(x, y)$	Derivation from $M(G;x,y)$
harmonic	$\dfrac{2}{x+y}$	$2\,S_x\,J\,(M(G\,;x,y))\big|_{x=1}$
inverse sum	$\dfrac{xy}{x+y}$	$S_x\,J\,D_x\,D_y(M(G\,;x,y))\big|_{x=1}$
augmented Zagreb	$\left(\dfrac{xy}{x+y-2}\right)^3$	$S_x^{\,3}\,Q_{-2}\,J\,D_x^{\,3}D_y^{\,3}(M(G\,;x\,,y))\big|_{x=1}$

Table 2. Three more topological indices and the corresponding formulas.

3. HOW TO COMPUTE THE *M*-POLYNOMIAL

As we have demonstrated in the previous section, the computation of the degree based topological indices can be reduced to the computation of the *M*-polynomial. In this section we first give some general remarks how to compute this polynomial and then derive the polynomial for some typical classes of graphs from the literature. In the general setting we follow an approach of Gutman [14] for which some definitions are needed first.

As we are primarily interested in chemical applications, we will restrict us here to chemical graphs which are the connected graphs with maximum degree at most 4. (However, the statements can be generalized to arbitrary graphs.) For a chemical graph $G = (V, E)$, let $n = |V(G)|$, $m = |E(G)|$, and let n_i, $1 \le i \le 4$, be the number of vertices of degree *i*. Note first that $m_{11} = 0$ whenever *G* has at least three vertices (and is connected). For the other coefficients m_{ij} of the *M*-polynomial Gutman observed that the following relations hold:

$$n_1 + n_2 + n_3 + n_4 = n \tag{3}$$
$$m_{12} + m_{13} + m_{14} = n_1 \tag{4}$$
$$m_{12} + 2m_{22} + m_{23} + m_{24} = 2n_2 \tag{5}$$
$$m_{13} + m_{23} + 2m_{33} + m_{34} = 3n_3 \tag{6}$$
$$m_{14} + m_{24} + m_{34} + 2m_{44} = 4n_4 \tag{7}$$
$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2m \tag{8}$$

These equalities are linearly independent. In some examples, all the quantities m_{ij} (and consequently the *M*-polynomial) can be found directly. On the other hand, one can determine

some of the m_{ij} 's first and then the remaining ones can be obtained from the above relations. We now demonstrate this on several examples.

3.1. Polyomino chains

Let $B(n;r;\ell_1,\ldots,\ell_r)$ be a polyomino chain with n squares, arranged in r segments of lengths $\ell_1,\ldots\ell_r$, $\ell_i \geq 2$, see Figure 1 for the particular case $B(11;6;3,4,2,2,3,2)$.
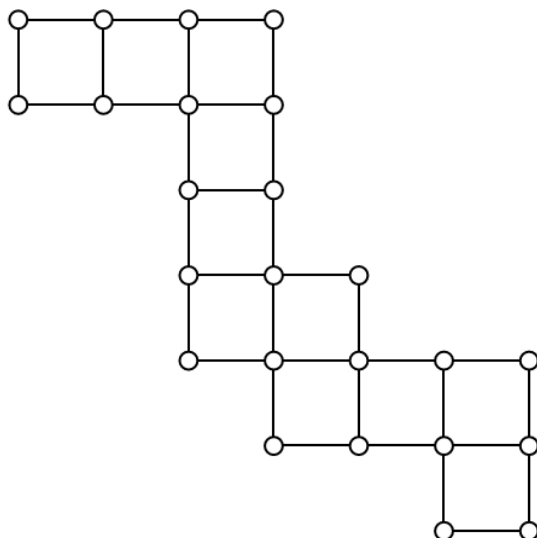

Figure 1. Polyomino chain $B(11; 6; 3; 4; 2; 2; 3; 2)$.

Let a denote the number of segments of length 2 that occur at the extremities of the chain ($a = 0$, 1, or 2) and let b denote the number of non-extreme segments of length 2. In Figure 1 we have $a = 1$, $b = 2$. As we shall see, the knowledge of the parameters n, r, a, and b of a chain is sufficient to determine its M-polynomial. It is easy to see that $|V| = 2n + 2$ and $|E| = 3n + 1$. The numbers n_i of vertices of degree i are given by $n_2 = r + 3$ (number of outer corners), $n_4 = r - 1$ (number of inner corners), and $n_3 = |V| - n_2 - n_4 = 2(n - r)$. We have $m_{22} = 2$, $m_{44} = b$ (the edges that halve the non–extreme segments of length 2), and $m_{24} = a + 2b$ (each extreme segment of length 2 contributes 1 and each non–extreme segment of length 2 contributes 2 24–edges). Now, taking into account that there are no vertices of degree 1, from (5)–(7) we obtain the expressions for m_{23}, m_{33}, and m_{34}. Setting $B_n = B(n;r;\ell_1,\ldots,\ell_r)$ this yields

$$M(B_n; x, y) = 2x^2 y^2 + (2r - a - 2b + 2)x^2 y^3 + (a + 2b)x^2 y^4$$
$$+ (3n - 6r + 1 + a + 3b)x^3 y^3 + (4r - a - 4b - 4)x^3 y^4 + bx^4 y^4.$$

For example, for the first Zagreb index (corresponding to $f(x,y) = x + y$), either from (2) or from the first entry of Table 1 we obtain $18n + 2r - 4$, in agreement with [23, Theorem 2.1]. Similarly, for the second Zagreb index (corresponding to $f(x, y) = xy$) we obtain $27n + 6r - 19 - a - b$, in agreement with [23, Theorem 2.4]. For the special case of the linear chain $L_n (n \geq 3)$, corresponding to $r = 1$, $a = b = 0$, we obtain $M(L_n; x, y) = 2x^2 y^2 + 4x^2 y^3 + (3n - 5) x^3 y^3$. For the special case of the zig-zag chain Z_n, corresponding to $r = n - 1$, $a = 2$, $b = r - 2 = n - 3$, we obtain $M(Z_n; x, y) = 2x^2 y^2 + 4x^2 y^3 + 2(n - 2)x^2 y^4 + 2x^3 y^4 + (n - 3)x^4 y^4$. We remark that for the first (second) Zagreb index we obtain $20n-6$ (resp. $32n-24$), in disagreement with the slightly mistaken expressions given in [23, Corollary 2.2(ii)] and [23, Corollary 2.5 (ii)].

3.2. Starlike trees

We next consider starlike trees, i.e. trees having exactly one vertex of degree greater than two [2]. If the degree of this vertex (called center) is n, then we denote a starlike tree by $S(k_1,\ldots,k_n)$, where the k_j's are positive integers representing the number of edges of the rays emanating from the center, see Figure 2 for an example.
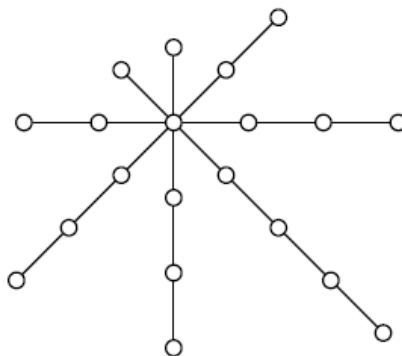

Figure 2. Starlike tree $S(1, 2, 3, 4, 3, 3, 2, 1)$.

Denote $K = \sum_{j=1}^{n} k_j$ and let a be the number of rays having exactly one edge. The possible vertex degrees are 1, 2, and n and it is easy to see that $m_{11} = 0$, $m_{12} = n - a$, $m_{1,n} = a$, $m_{2,n} = n - a$, $m_{n,n} = 0$. Since the total number of edges is K, we have $m_{2,2} = K - (n - a) - a - (n - a) = K + a - 2n$, leading to

$$M(S(k_1,\ldots, k_n); x, y) = (n - a)xy^2 + axy^n + (K + a - 2n) x^2 y^2 + (n - a) x^2 y^n.$$

For example, for the first Zagreb index we obtain (using (2) or Table 1) $n^2 - 3n + 4K$. Similarly, for the second Zagreb index we obtain $2n^2 - 6n - an + 2a + 4K$. Both results are in agreement with those in [2, Corollary 3.7] obtained in a more complicated manner.

3.3. Triangulanes

We consider the family of triangulanes T_n, defined in Figure 3, where the auxiliary triangulane G_n is defined recursively in the following manner (see also [1, 9, 20]). Let G_1 be a triangle and denote one of its vertices by y_1. We define G_n as the circuit of the graphs G_{n-1}, G_{n-1}, and K_1 (the 1-vertex graph) and denote by y_n the vertex where K_1 has been placed (see Figure 3 again).
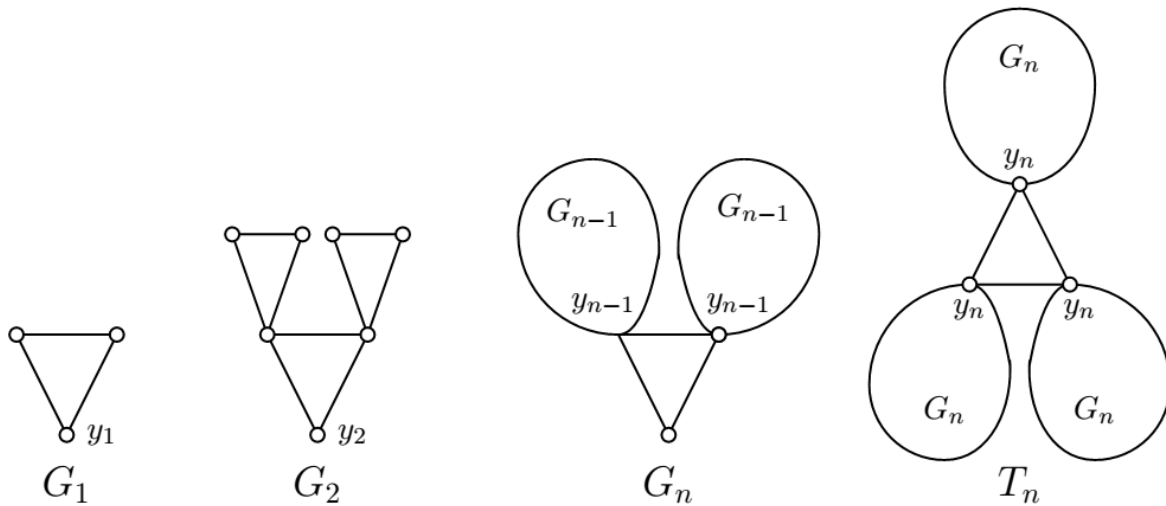

Figure 3. Graphs G_1, G_2, G_n, and T_n.

The possible vertex degrees of G_n are 2, 4 and, using the notation μ_{ij} instead of m_{ij}, it is easy to see that $\mu_{22} = 2^{n-1}$ and $\mu_{24} = 2 + 2^n$. We have $\mu_{22} + \mu_{24} + \mu_{44} = |E(G_n)| = 3(2^n - 1)$ since G_n consists of $2^n - 1$ triangles. From here we obtain $\mu_{44} = 3 \cdot 2^{n-1} - 5$. Thus, as a by-product,

$$M(G_n; x, y) = 2^{n-1}x^2y^2 + (2 + 2^n)x^2y^4 + (3 \cdot 2^{n-1} - 5)x^4y^4 .$$

Now, in order to find the m_{ij}'s of T_n from its defining picture, we note that at the attachment of each G_n to the starting triangle, two 24-edges of G_n turn into two 44-edges of T_n. Consequently,

$$m_{22} = 3\mu_{22} = 3 \cdot 2^{n-1}; \ m_{24} = 3(\mu_{24} - 2) = 3 \cdot 2^n; \ m_{44} = 3(\mu_{44}+2) + 3 = 3(3 \cdot 2^{n-1} - 2)$$

and

$$M(T_n; x, y) = 3 \cdot 2^{n-1} x^2 y^2 + 3 \cdot 2^n x^2 y^4 + 3(3 \cdot 2^{n-1} - 2) x^4 y^4 \,.$$

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