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M-Polynomials and Zagreb Indices for i-Iterated Subdivided-Line Graphs

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Abstract

The i-iterated subdivided-line graph $\Gamma^i(G)$ of a base graph G is the graph obtained from G by iteratively applying the subdivided-line graph operation i times. The M-polynomial of a graph G is a bivariate polynomial that encodes the degree-based properties of G. In this paper, we present a general formula expressing the M-polynomial of $\Gamma^i(G)$ in terms of the degrees of the vertices of the base graph G. We compute the First and Second Zagreb indices from the M-polynomial of i-iterated subdivided-line graphs $\Gamma^i(G)$ when G belongs to several graph classes, such as wheel, ladder, Δ-regular, cycle, and tadpole graphs. The obtained results generalize those of Ranjini et al. (2011). Additionally, we analyse the impact of the vertex of maximum degree on the value of the First and Second Zagreb indices, providing asymptotic upper bounds for i-iterated subdivided-line graphs of general graphs.

1 Introduction

Chemical Graph Theory is a branch of mathematical chemistry concerned with analyzing all consequences of connectivity in graphs representing chemical structures – chemical graph (Trinajstić [27]). If the chemical structures under consideration are molecules, we call this type of chemical graph a *molecular graph*. *Molecular descriptors* are mathematical quantities that describe the structure or shape of molecules, helping to predict the activity and properties of molecules in complex experiments (Ahmadi et al. [1]). Among molecular descriptors, topological indices play a significant role, as described by Das [8]. The concept of the topological index originated from the work of Wiener [29] on the boiling points of paraffins. He initially named this index the "path number", which later became known as the *Wiener index*.

A *topological index* is a numeric quantity associated with a graph that characterizes the topology of graph and is invariant under graph automorphism (Baca et al. [3]). According to Waterbeemd et al. [28], a topological index is a numerical value associated with chemical constitution used for correlating chemical structure with various physical properties, chemical reactivity or biological activity. Topological indices are widely used to predict the physico-chemical and bioactivity properties of a molecule or molecular compound in the quantitative structure-property/structure-activity relationship (QSPR/QSAR) modeling (Devillers and Balaban [11]).

The first topological index based on the line graph was introduced by Bertz in 1981 [5]. In recent years, numerous results concerning topological indices that use the subdivision concept in line graphs have emerged. Additional results are provided in [4, 19–22, 24–26] and in the references therein.

In 2016, Nadeem et al. [22] computed topological indices like the generalized Randić, general Zagreb, general sum-connectivity, ABC, GA, ABC_4 and GA_5 indices of the line graphs of subdivision graphs of 2D lattice of nanotube and nanotorus.

Belay et al. [4] computed the first, second, and third Zagreb coindices, the F-coindex, the first and second multiplicative Zagreb coindices and the hyper Zagreb coindex of the subdivision graph and the line graph of subdivision graph of the wheel graph. Ranjini et al. [25] calculated the Zagreb indices and coindices of the line graph of the subdivision graph of wheel, ladder and tadpole graphs. In 2015, Su and Xu [26] generalized the results of Ranjini et al. [25] by calculating the general sum-connectivity index and general product-connectivity index of the line graph of subdivision graph of the tadpole, wheel, and ladder graphs.

Gutman et al. [13, 17] introduced the Zagreb indices of a graph G presented in Table 1, where d_u and d_v are the degrees of the vertices u and v in G respectively.

Topological Index	*Formula*	*Derivation from $M(G)$*
First Zagreb	$M_1(G) = \sum_{uv \in E(G)} d_u + d_v$	$(D_x + D_y)(M(G))$
Second Zagreb	$M_2(G) = \sum_{uv \in E(G)} d_u d_v$	$(D_x D_y)(M(G))$

Table 1. Degree based topological indices and the corresponding formulas computed from their M-polynomial.

The Zagreb indices are among the most significant degree-based molecular structure descriptors with many chemical applications. Many results can be found in [6, 7, 9, 14–16, 23] and in the references therein.

Let $m_{\ell,\ell'}(G)$, $\ell, \ell' \geq 1$, be the number of edges $e = uv$ of a graph G such that $\{d_u, d_v\} = \{\ell, \ell'\}$. The *M-polynomial* of G is defined in [10]:

$$M(G; x, y) \quad = \quad \sum_{\ell \leq \ell'} m_{\ell,\ell'}(G) x^{\ell} y^{\ell'}. \tag{1}$$

This polynomial has been one of the key areas of interest in the computational aspects of materials (Ali et al. [2]). Topological indices can be also be directly derived from their M-polynomial (Deutsch and Klavžar [10]), as exemplified in Table 1, where the First and Second Zagreb indices are calculated from the M-polynomial where the operators D_x and D_y are defined on differentiable functions of two variables:

$$D_x = x \frac{\partial M(G; x, y)}{\partial x}\Big|_{x=1, y=1} \text{ and } D_y = y \frac{\partial M(G; x, y)}{\partial y}\Big|_{x=1, y=1}. \tag{2}$$

Ranjini et al. [25] calculated the Zagreb indices and coindices of the line graph of the subdivision graph of wheel, ladder, and tadpole graphs. In

2015, Su and Xu [26] generalized the results of Ranjini et al. [25] by calculating the general sum-connectivity index and general product-connectivity index of the line graph of subdivision graph of the tadpole, wheel, and ladder graphs. In 2015, using the subdivided-line graph operation, Hasunuma [18] described a new definition of i-iterated subdivided-line graph of a graph.

Motivated by these results, we present the following contributions in this paper. In Section 2, we establish a general formula expressing the M-polynomial of i-iterated subdivided-line graphs in terms of the degrees of the vertices of a general base graph G. In Section 3, we compute the First and Second Zagreb indices from the M-polynomial of i-iterated subdivided-line graphs $\Gamma^i(G)$ when G belongs to several graph classes, such as wheel, ladder, Δ-regular, cycle and tadpole graphs. Moreover, the obtained results, calculating these indices for every $i \geq 1$, generalize those of Ranjini et al. [25]. We conclude the paper analyzing the impact of the vertex of maximum degree on the value of the First and Second Zagreb indices, providing asymptotic upper bounds for i-iterated subdivided-line graphs of general graphs.

2 M-polynomial of i-iterated subdivided-line graphs

In this section, we present the characterization of the M-polynomial of i-iterated subdivided-line graphs. Our main theorem provides a general formula for any graph, expressed in terms of the individual vertex degree. First, we provide some definitions and notations.

Let $G = (V, E)$ be a finite, simple, and undirected graph, with vertex set $V = V(G)$ and edge set $E = E(G)$. The *degree* of a vertex $v \in V$ in a graph G, denoted by $d_G(v) = d_v$, is the number of edges incident to v. Two edges are *adjacent* if they share a common endpoint. Let Δ be the *maximum degree* among all the vertices in the graph G. A graph is called *Δ-regular graph* if the degree of each vertex in the graph is Δ. A *complete graph* K_n with n vertices is a graph in which any two vertices are adjacent. A *path* P_n is a graph whose vertices can be arranged in a linear sequence $(v_1, v_2, \ldots, v_n)$ in such a way that two vertices are adjacent if and only if they are consecutive in the sequence. A path with $n \geq 1$ vertices is represented by $P_n = v_1 v_2 \ldots v_n$. Similarly, a *cycle* C_n on three or more vertices is a graph whose vertices can be arranged in a cyclic sequence $(v_1, v_2, \ldots, v_n, v_1)$ in such a way that two vertices are adjacent if and only if they are consecutive in the sequence.

The *line graph* $L(G)$ of graph G is obtained by associating a vertex of $L(G)$ with each edge in $E(G)$, and two vertices are adjacent in $L(G)$ if and only if the corresponding edges of G have a vertex in common.

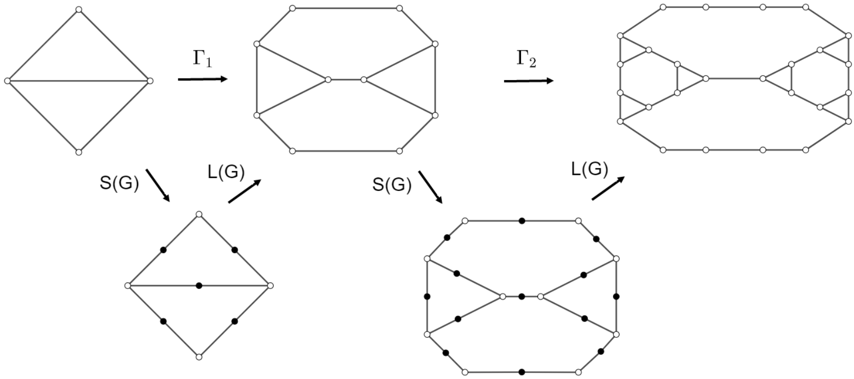

Figure 1. Graphs G, $S(G)$, $\Gamma^1(G)$, $S(\Gamma^1(G))$ and $\Gamma^2(G)$ (2-iterated subdivided-line graph for the graph), respectively.

In this paper, we use the notation and definitions for the subdivided-line graph operation and i-iterated subdivided-line graph as described by Hasunuma [18]. The *subdivision graph* $S(G)$ is the graph obtained from G by replacing each of its edges by a path of length 2, or equivalently, for each edge $uv \in E(G)$, we insert an additional vertex w, delete edge uv and add edges wu and wv. This definition is the same as *barycentric subdivision* $B(G)$ in [18], which says that $B(G)$ is the graph obtained from G by elementary subdividing every edge of G.

The *subdivided-line graph* $\Gamma(G)$ of a graph G is defined as the line graph of the barycentric subdivision of G, i.e., $\Gamma(G) = L(B(G))$. We call Γ the *subdivided-line graph operation.* The *i-iterated subdivided-line graph* $\Gamma^i(G)$

of G is the graph obtained from G by iteratively applying the subdivided-line graph operation i times. We refer to Figure 1 for examples of these graphs when G is the K_4 minus one edge.

The *inflation* or *inflated* graph G_I of the graph G without isolated vertices is obtained as follows (see Favaron [12]). Each vertex $v_j \in V(G)$ of degree $d_G(v_j) = d_{v_j}$ is replaced by a clique X_j such that $G_I[X_j] \cong K_{d_G(v_j)}$. Each edge $(u_j, v_{j'}) \in E(G)$, $j \neq j'$, is replaced by an edge (u, v), in such a way that $u \in X_j$, $v \in X_{j'}$, and two different edges of G are replaced by two non-adjacent edges of G_I. Thus, in G_I, for all $u \in X_j$, we have that $d(u) = d_G(v_j)$, and that G_I is the line graph $L(S(G)) \cong \Gamma^1(G)$. Moreover, $\Gamma^{i+1}(G)$ is the inflated graph of $\Gamma^i(G)$.

Theorem 1. *The M-polynomial of the i-iterated subdivided line graph of the graph G is*

$$M(\Gamma^i(G); x, y) = \sum_{\ell \leq \ell'} m_{\ell,\ell'}(G) x^{\ell} y^{\ell'} + \sum_{w \in V(G)} \left(\frac{d_w(d_w^i - 1)}{2} \right) x^{d_w} y^{d_w} \quad (3)$$

where $m_{\ell,\ell'}(G)$, $\ell, \ell' \geq 1$, *is the number of edges* $uv \in E(G)$ *such that* $\{d_u, d_v\} = \{\ell, \ell'\}$.

Proof. Let $|E(\Gamma^i(v))|$ be the number of edges added to $E(G)$ by a vertex $v \in V(G)$ after iteratively applying the subdivided-line graph operation i times in G. First, we prove by induction on $i \geq 1$ that:

$$|E(\Gamma^i(v))| = \begin{cases} 0, & \text{if } d(v) = 1; \\ 2^i - 1, & \text{if } d(v) = 2; \\ \frac{d(v)(d(v)^i - 1)}{2}, & \text{if } d(v) \geq 3. \end{cases} \quad (4)$$

If $i = 1$, by definition of inflated graph, we have that $\Gamma^1(G) = L(S(G)) = G_I$. Thus, a vertex $v_j \in V(G)$ of degree $d(v_j)$ is replaced by a clique X_j such that $G_I[X_j] \cong K_{d(v_j)}$. So, the formula is valid: $|E(\Gamma^1(v_j))| = 2^1 - 1 = 1$, if $d(v_j) = 2$; and $|E(\Gamma^1(v_j))| = \frac{d(v_j)(d(v_j)-1)}{2}$, if $d(v_j) \geq 3$.

Suppose, by induction hypothesis, that the statement is valid for $i = k > 1$, that is, $|E(\Gamma^k(v_j))| = 2^k - 1 = 1$, if $d(v_j) = 2$; and $|E(\Gamma^k(v_j))| = \frac{d(v_j)(d(v_j)^k-1)}{2}$, if $d(v_j) \geq 3$. In particular, in $\Gamma^k(G)$, vertex v_j added

$d(v_j)^{k-1}$ cliques of order $d(v_j)$ to G (total of $d(v_j)^k$ vertices), and $d(v_j)$ *external edges*, that is, edges that correspond to the original edges in $E(G)$ incident to do v_j.

Each of this $d(v_j)^k$ vertices $v \in \Gamma^k(G)$ of degree $d(v_j)$ adds a clique of order $d(v_j)$ in $\Gamma^{k+1}(G)$. Now, the number of edges in $\Gamma^{k+1}(v_j)$ is: $|E(\Gamma^{k+1}(v_j))| = |E(\Gamma^k(v_j))| \cdot d(v_j) + \binom{d(v_j)}{2}$, which, by induction hypothesis, implies

$$|E(\Gamma^{k+1}(v_j))| = \left(\frac{d(v_j)(d(v_j)^k - 1)}{2}\right) \cdot d(v_j) + \frac{d(v_j)(d(v_j) - 1)}{2}.$$

Hence, after algebraic manipulation of this expression, we conclude the induction step with

$$|E(\Gamma^{k+1}(v_j))| = \frac{d(v_j)(d(v_j)^{k+1} - 1)}{2}.$$

Thus, considering: the external edges (u, v) (edges that correspond to the original edges in $E(G)$); the edges generated by each vertex in the inflated graph; and $d_v = d(v)$, the edge-generating polynomial $M(\Gamma^i(G); x, y)$ can be expressed as:

$$M(\Gamma^i(G); x, y) \quad = \quad \sum_{\ell \leq \ell'} m_{\ell,\ell'}(G) x^\ell y^{\ell'} + \sum_{w \in V(G)} \frac{d_w(d_w^i - 1)}{2} x^{d_w} y^{d_w}.$$

where $m_{\ell,\ell'}(G)$, $\ell, \ell' \geq 1$, is the number of edges $uv \in E(G)$ such that $\{d_u, d_v\} = \{\ell, \ell'\}$. ■

3 M-polynomial and Zagreb indices for i-iterated subdivided-line graphs

In this section, we calculate the M-polynomial of the i-iterated subdivided-line graphs of G, where the graph G belongs to the wheel, ladder, Δ-regular, cycle, and tadpole graph classes. According to Table 1, and by applying the differential operators D_x and D_y (defined in equation (2)), to the M-polynomials of $\Gamma^i(G)$, we obtain the Zagreb indices for the i-iterated subdivided-line graph of the graphs on these classes.

Furthermore, our contributions obtained in Theorems 2, 3 and 6 are valid for any value of $i \geq 1$, which provide a generalization of the results of Ranjini et al. [25] (Theorems 2.4, 3.1 and 2.1, respectively).

Wheel graphs W_{n+1}

The *join* of two graphs G_1 and G_2, denoted by the sum $G_1 + G_2$, is the graph obtained by connecting each vertex of G_1 to every vertex of G_2. Formally, $V(G_1 + G_2) = V(G_1) \cup V(G_2)$ and $E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{(u, v) : u \in V(G_1) \text{ and } v \in V(G_2)\}$. Thus, the join $C_n + K_1$ of a cycle C_n, on n vertices, with a single vertex is referred to as a *wheel graph* W_{n+1}. We refer to Figure 2 for an example of the i-iterated subdivided-line graphs of the wheel graph W_5 for $i \in \{1, 2\}$.

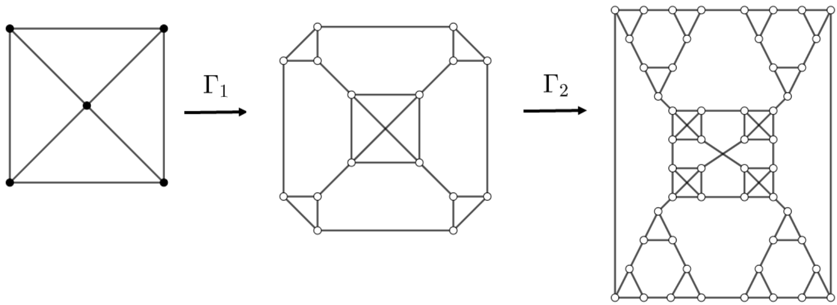

Figure 2. Wheel W_5, and its respective $\Gamma^1(W_5)$ and $\Gamma^2(W_5)$. Zagreb indices $M_1(\Gamma^2(W_5)) = 580$ and $M_2(\Gamma^2(W_5)) = 996$.

Theorem 2. *The M-polynomial and the First and Second Zagreb indices of the i-iterated subdivided-line of the wheel graph W_{n+1}, $n \geq 4$, are*

$$\begin{aligned}
M(\Gamma^i(W_{n+1}); x, y) &= nx^3\left(y^n + \frac{(3^{i+1} - 1)}{2} y^3\right) + \frac{n(n^i - 1)}{2} x^n y^n, \\
M_1(\Gamma^i(W_{n+1})) &= n(n^{i+1} + 3^{i+2}), \\
M_2(\Gamma^i(W_{n+1})) &= n\left(\frac{n^{i+2} - n^2 + 6n + 3^{i+3} - 9}{2}\right).
\end{aligned}$$

Proof. By definition, the wheel graph W_{n+1} has n edges linking the central vertex v_0 (degree n) to the vertices of the cycle C_n (degree 3), and n edges linking pairs of consecutive vertices of the cycle C_n. Thus, $m_{3,n} = m_{3,3} = n$, and $\sum_{\ell\leq\ell'} m_{\ell,\ell'}(G)x^{\ell}y^{\ell'} = nx^3y^n + nx^3y^3 = nx^3(y^n + y^3)$. Now, we have

$$\begin{array}{rcl}\displaystyle\sum_{w\in V(W_{n+1})}\left(\frac{d_w(d_w^i-1)}{2}\right)x^{d_w}y^{d_w} & = & \displaystyle\sum_{w\in V(C_n)}\left(\frac{3(3^i-1)}{2}\right)x^3y^3 \\ & + & \displaystyle\sum_{w\in V(W_{n+1}),w=v_0}\frac{n(n^i-1)}{2}x^ny^n.\end{array}$$

Hence,

$$\begin{array}{rcl}M(\Gamma^i(W_{n+1});x,y) & = & nx^3(y^n+y^3) \\ & + & n\left(\dfrac{3(3^i-1)}{2}\right)x^3y^3 \\ & + & \dfrac{n(n^i-1)}{2}x^ny^n.\end{array} \tag{5}$$

and, by Theorem 1, the result follows:

$$M(\Gamma^i(W_{n+1});x,y) = nx^3(y^n + \frac{(3^{i+1}-1)}{2}y^3) + \frac{n(n^i-1)}{2}x^ny^n.$$

Applying the differential operators D_x and D_y (defined in equation (2)), we have:

$$\begin{array}{rcl}M_1(\Gamma^i(W_{n+1})) & = & n(n^{i+1}+3^{i+2}), \\ M_2(\Gamma^i(W_{n+1})) & = & n\left(\dfrac{n^{i+2}-n^2+6n+3^{i+3}-9}{2}\right).\end{array}$$

■

Ladder graph L_n

The *Cartesian product* $G_1\square G_2$ of graphs G_1 and G_2 is a graph with vertex set $V_1\times V_2$, and two vertices (u_1,v_1) and (u_2,v_2) are adjacent in $G_1\square G_2$ if and only if either $u_1 = u_2$ and $v_1, v_2 \in E_2$, or $v_1 = v_2$ and $u_1u_2 \in E_1$. The *ladder graph* L_n is constructed from the Cartesian product $L_n = K_2 \square P_n$, where P_n is the path on n vertices. In Figure 3, we present an example of these graphs for $i = 1, 2$.

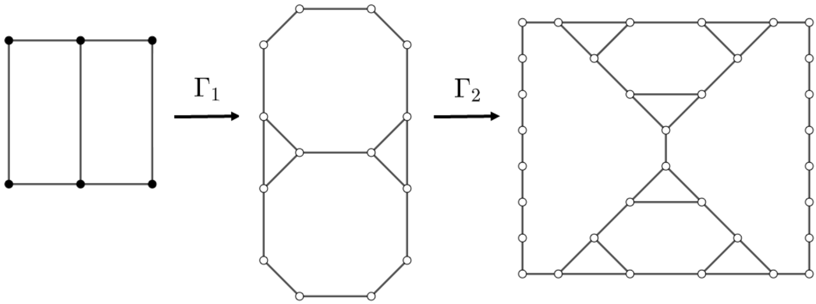

Figure 3. Ladder graph L_3 (obtained by the Cartesian product of $K_2 \square P_3$), and its respective $\Gamma^1(L_3)$ and $\Gamma^2(L_3)$. Zagreb indices $M_1(\Gamma^2(L_3)) = 226$ and $M_2(\Gamma^2(L_3)) = 305$.

Theorem 3. *The M-polynomial and the First and Second Zagreb indices of the i-iterated subdivided-line of the ladder graph* L_n *are*

$$\begin{aligned} M(\Gamma^i(L_n); x, y) &= (2^{i+2} - 2)x^2y^2 + 4x^2y^3 + ((n-2)3^{i+1} - 2)x^3y^3, \\ M_1(\Gamma^i(L_n)) &= 3^i(18n - 36) + 2^{i+4}, \\ M_2(\Gamma^i(L_n)) &= 3^{i+3}(n-2) + 2^{i+4} - 2. \end{aligned}$$

Proof. By definition, the ladder graph $L_n = K_2 \times P_n$ has: 2 edges between vertices of degree 2; 4 edges between vertices of degree 2 and 3; $2(n-3) + (n-2)$ edges between vertices of degree 3; Thus, $m_{2,2} = 2$, $m_{2,3} = 4$, $m_{3,3} = 2(n-3) + (n-2) = 3n - 8$, and

$$\sum_{\ell \leq \ell'} m_{\ell,\ell'}(G) x^{\ell} y^{\ell'} = 2x^2y^2 + 4x^2y^3 + (3n-8)x^3y^3.$$

Now, we have

$$\sum_{w\in V(L_n)} \left(\frac{d_w(d_w^i-1)}{2}\right) x^{d_w}y^{d_w} = 4\left(\frac{2(2^i-1)}{2}\right)x^2y^2 + (2n-4)\left(\frac{3(3^i-1)}{2}\right)x^3y^3.$$

Hence, by Theorem 1, we have

$$M(\Gamma^i(L_n);x,y) = (2^{i+2}-2)x^2y^2 + 4x^2y^3 + ((n-2)3^{i+1}-2)x^3y^3$$

Applying the differential operators D_x and D_y (defined in equation (2)), we have:

$$\begin{aligned} M_1(\Gamma^i(L_n)) &= 3^i(18n-36) + 2^{i+4}, \\ M_2(\Gamma^i(L_n)) &= 3^{i+3}(n-2) + 2^{i+4} - 2. \end{aligned}$$

■

Regular graphs G_Δ

Theorem 4. *The M-polynomial and the First and Second Zagreb indices of the i-iterated subdivided-line graph of the Δ-regular graph G_Δ with n vertices is*

$$\begin{aligned} M(\Gamma^i(G_\Delta);x,y) &= \frac{n}{2}\Delta^{i+1}x^\Delta y^\Delta, \\ M_1(\Gamma^i(G_\Delta)) &= n\Delta^{i+2}, \\ M_2(\Gamma^i(G_\Delta)) &= \frac{n\Delta^{i+3}}{2}. \end{aligned}$$

Proof. By Theorem 1, we have

$$\begin{aligned} M(\Gamma^i(G_\Delta);x,y) &= \sum_{\ell\le\ell'} m_{\ell,\ell'}(G_\Delta)x^\ell y^{\ell'} + \sum_{w\in V(G_\Delta)} \frac{d_w(d_w^i-1)}{2}x^{d_w}y^{d_w} \\ &= \frac{n\Delta}{2}x^\Delta y^\Delta + \frac{n\Delta(\Delta^i-1)}{2}x^\Delta y^\Delta \\ &= \frac{n}{2}\Delta^{i+1}x^\Delta y^\Delta. \end{aligned}$$

Applying the differential operators D_x and D_y (defined in equation (2)), we have that

$$M_1(\Gamma^i(G_\Delta)) = n\Delta^{i+2} \text{ and } M_2(\Gamma^i(G_\Delta)) = \frac{n\Delta^{i+3}}{2}$$

■

Corollary 5. *The M-polynomial and the First and Second Zagreb indices of the i-iterated subdivided-line of the cycle graph C_n are*

$$\begin{aligned} M(\Gamma^i(C_n);x,y) &= 2^i n x^2 y^2, \\ M_1(\Gamma^i(C_n)) &= n2^{i+2}, \\ M_2(\Gamma^i(C_n)) &= n2^{i+2}. \end{aligned}$$

Tadpole graphs $T_{n,k}$

A *tadpole graph* $T_{n,k}$ is a graph obtained by linking, by an edge, a vertex of a cycle graph C_n to a degree one vertex of a path P_k. In Figure 4, is shown the 2-iterated subdivided-line graph for the tadpole graph $T_{n,k}$ as example.

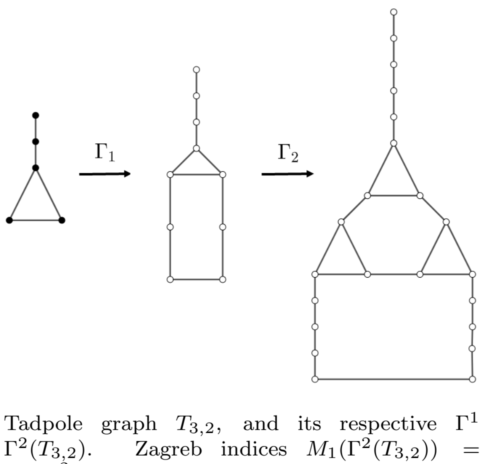

Figure 4. Tadpole graph $T_{3,2}$, and its respective $\Gamma^1(T_{3,2})$ and $\Gamma^2(T_{3,2})$. Zagreb indices $M_1(\Gamma^2(T_{3,2})) = 130$ and $M_2(\Gamma^2(T_{3,2})) = 168$.

Theorem 6. *The M-polynomial and the First and Second Zagreb indices of the i-iterated subdivided-line graph of the tadpole graph $T_{n,k}$ is*

$$\begin{aligned} M(\Gamma^i(T_{n,k});x,y) &= xy^2+3x^2y^3+(2^i(n+k-2)-2)x^2y^2 \\ &+ \frac{(3^{i+1}-3)}{2}x^3y^3, \\ M_1(\Gamma^i(T_{n,k})) &= 2^{i+2}(n+k-2)+3^{i+2}+1, \\ M_2(\Gamma^i(T_{n,k})) &= 2^{i+2}(n+k-2)+\frac{3^{i+3}-3}{2}. \end{aligned}$$

Proof. By definition, the tadpole graph $T_{n,k}$ has: 1 edge between a vertex of degree 1 and 2 of the P_k; 3 edges between vertices of degree 2 and 3; $n-2$ edges between vertices of degree 2 of the cycle C_n; and $k-2$ edges between vertices of degree 2 of the path P_k.

Thus, $m_{1,2}=1$, $m_{2,3}=3$, $m_{2,2}=n+k-4$, $\sum_{\ell\le\ell'} m_{\ell,\ell'}(G)x^\ell y^{\ell'} = 1x^1y^2+3x^2y^3+(n+k-4)x^2y^2$, and

$$\begin{aligned} \sum_{w\in V(L_n)} \left(\frac{d_w(d_w^i-1)}{2}\right) x^{d_w}y^{d_w} &= 1\left(\frac{1(1^i-1)}{2}\right)x^1y^1 \\ &+ (n+k-2)\left(\frac{2(2^i-1)}{2}\right)x^2y^2 \\ &+ 1\left(\frac{3(3^i-1)}{2}\right)x^3y^3. \end{aligned}$$

Hence, by Theorem 1, we have $M(\Gamma^i(T_{n,k});x,y) = xy^2+3x^2y^3+(2^i(n+k-2)-2)x^2y^2+\frac{(3^{i+1}-3)}{2}x^3y^3$. Thus, applying the differential operators D_x and D_y (defined in equation (2)), we have that

$$\begin{aligned} M_1(\Gamma^i(T_{n,k})) &= 2^{i+2}(n+k-2)+3^{i+2}+1, \\ M_2(\Gamma^i(T_{n,k})) &= 2^{i+2}(n+k-2)+\frac{3^{i+3}-3}{2}. \end{aligned}$$

∎

4 Conclusions

Topological indices have meaningful role in the chemical-mathematical literature, as they have potential for predicting the physico-chemical properties of molecules. In this paper, we present the First and Second Zagreb indices of i-iterated subdivided-line graphs of various graph classes, calculated from their M-polynomial.

In particular, we compute the Zagreb indices for the i-iterated subdivided-line graph of wheel, ladder, Δ-regular, cycle, and tadpole graphs. These results are significant, as they generalize the findings of Ranjini et al. [25] for these classes, corroborating new methods for computing topological indices that can be widely applied to other indices in future research.

Finally, we analyze the impact of the maximum degree on the topological index metrics, observing that Theorem 4 establishes asymptotic upper bounds for both First and Second Zagreb indices of the i-iterated subdivided-line graph of general graphs G.

Theorem 7. *If G is a graph of maximum degree Δ and $\Gamma^i(G)$ is i-iterated subdivided-line graph of a graph G, then $M_1(\Gamma^i(G)) = O(\Delta^i)$ and $M_2(\Gamma^i(G)) = O(\Delta^i)$.*

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