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Research Paper

Neighborhood M-Polynomial of Graph Operations: Exploring Nanostructure Applications and Correcting Cycle-Related Graph Results

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Abstract

Mathematical chemistry is a field of mathematics where chemical compounds are studied by associating a graph to it. A topological index serves as a mathematical invariant that elucidates the underlying topological arrangement of molecules or networks. This paper explores the neighborhood M-Polynomial concerning various graph operations of regular graphs. Additionally, it addresses and rectifies several erroneous results pertaining to cycle-related graphs that were previously reported. Furthermore, we examine the applications of the neighborhood M-Polynomial to the $VPHX[m,n]$ nanotubes and $VPHY[m,n]$ nanotori, presenting their potential in real-world. Through this comprehensive investigation, we aim to advance the understanding of topological indices and their practical implications.

1 Introduction

Topological indices serve as concise mathematical descriptors that provide quantitative insights into the topological characteristics and structural properties of molecules or networks. The exploration of topological indices can be traced back to 1947, when H. Wiener introduced the Wiener index, a graph invariant recognized for its ability to model the physical properties of alkanes [1]. Over the past few decades, an extensive range of topological indices has been formulated and employed in correlation analysis across diverse fields such as theoretical chemistry, pharmacology, toxicology, and environmental chemistry.

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Despite the wide adoption of topological indices, calculating these indices directly for every molecule can be a formidable task. The complexity escalates as molecules or networks increase in size and intricacy. Consequently, researchers have turned to leveraging graph polynomials as a popular and valuable strategy to derive topological indices. This approach offers a more efficient and manageable pathway to extract valuable information about the topological arrangements and structural properties of molecules or networks.

The concept of topological indices has played a pivotal role in providing quantitative information about the topological characteristics and structural properties of molecules or networks. In 2015, Deutsch and Klavžar introduced the M-polynomial, which laid the foundation for determining numerous degree-based topological indices [2]. Building upon this idea, Mondal et al. further expanded the scope of the M-polynomial by introducing the concept of the neighborhood M-polynomial in 2020 [3]. Their groundbreaking work successfully derived the neighborhood M-polynomial and related topological indices based on the sum of neighborhood degrees for the molecular graph of bismuth tri-iodide (BiI_3) chain and sheets. This breakthrough paved the way for mathematicians to generate topological indices based on neighborhood degrees, as exemplified by applications to Cuprous Oxide's (Cu_2O) crystalline structure and the face-centered cubic lattice [4–6].

The effectiveness of a topological index lies in its ability to accurately predict molecules properties or activities. Notably, the study conducted by Mondal et al. identified the neighborhood second modified Zagreb index as the optimal choice for predicting molar refractivity and polarizability in COVID-19 drugs [4]. Similarly, Havare determined the neighborhood harmonic index as the most suitable option for predicting the molar volume of cancer drugs [7]. These findings underscore the critical importance of selecting the appropriate index tailored to specific properties of interest.

Carbon nanotubes (CNTs) are small cylindrical carbon structures endowed with exceptional properties, including high strength, conductivity, and a large surface area. These unique attributes make CNTs highly versatile for numerous applications in pharmacy and medicine. In the pharmaceutical domain, CNTs have proven to be effective in targeted drug delivery and gene therapy through efficient adsorption or conjugation with therapeutic and diagnostic agents. Additionally, CNTs have found utility in tissue regeneration, biosensors, drug separation techniques, pollutant analysis, and have even shown promise as antioxidants.

The primary objectives of our work are threefold. Firstly, in Section 3 of this paper, we derive the neighborhood M-polynomials for some classical graph operations such as cartesian product, composition, Kronecker product, etc. of regular graphs. These operations hold significance in graph theory and find practical applications in network analysis and optimization. Secondly, we address and rectify erroneous results of specific cycle-related graphs in Section 4. The accuracy of topological indices heavily relies on precise calculations, necessitating the correction of any inconsistencies. Furthermore, we determine the neighborhood M-polynomial and associated topological indices for novel cycle-related graphs, expanding the understanding of their properties. Lastly, in Section 5, we apply our findings to obtain the neighborhood M-polynomial and associated topological indices for the $VPHX[m,n]$ nanotubes and $VPHY[m,n]$ nanotori structures. These applications demonstrate the practical implications of our research in fields such as chemistry, molecular property prediction, drug design, network optimization, and vulnerability identification [8, 9]. We have also thoughtfully included preliminaries in Section 2 to assist the reader in better comprehending the content.

2 Preliminaries

Definition 2.1. The neighborhood M-polynomial for a graph G is represented as $NM(G;x,y)$ and can be defined as follows:

$$NM(G;x,y) = \sum_{i\leq j} m_{ij} x^i y^j,$$

here, m_{ij} refers to the count of edges $uv \in E(G)$ in the graph such that $\{\gamma(u),\gamma(v)\} = \{i,j\}$ and x and y are arbitrary variables. The coefficients m_{ij} perform an edge partition. It creates the equivalence classes of edges such that their end vertices have the same neighborhood degree sum. For example, in the case of a Wheel graph $\mathscr{W}_n$ on $n+1$ vertices, the edges can be partitioned as $m_{n+6,n+6}$ and $m_{n+6,3n}$. Each equivalence class contains n number of edges. By analyzing the coefficients of neighborhood M-polynomial, one can gain insights into a graph's complexity, connectivity and combinatorial properties. $\gamma(u)$ denotes the neighborhood degree sum of vertex u in graph G. The neighborhood degree sum can be calculated using the given MATLAB code in the appendix.

A graph product is a creative fusion where the vertices and edges of the original graphs intertwine, unveiling new patterns and relationships within the resulting graph. Graph products provide a powerful framework for analyzing complex systems, modeling interactions, and uncovering hidden connections, enabling us to explore the intricate web of relationships that exist in diverse domains, from social networks to quantum information theory. In what follows, we define various types of graph operations :

Definition 2.2. Let G_1 and G_2 be two graphs with vertex sets $V(G_1)$ and $V(G_2)$, respectively. Let $a_i \in V(G_1)$, $b_i \in V(G_2)$, and $(a_i,b_i) \in V(G_1)\times V(G_2)$ for $i = 1,2$. Graph products are defined on the vertex set $V(G_1)\times V(G_2)$ as follows:

- **Cartesian product** $(G_1 \times G_2)$**:** $(a_1,b_1) \sim (a_2,b_2)$ if and only if $a_1 = a_2$; $b_1 \sim b_2$ or $a_1 \sim a_2$; $b_1 = b_2$.

- **Lexicographic Product or Composition of Graphs** $(G_1[G_2])$**:** $(a_1,b_1) \sim (a_2,b_2)$ if and only if $a_1 \sim a_2$ or $a_1 = a_2$; $b_1 \sim b_2$.

- **Direct Product or Kronecker Product** $(G_1 \otimes G_2)$**:** $(a_1,b_1) \sim (a_2,b_2)$ if and only if $a_1 \sim a_2$ and $b_1 \sim b_2$.

- **Strong Product** $(G_1 \cdot G_2)$**:** $(a_1,b_1) \sim (a_2,b_2)$ if and only if $a_1 \sim a_2$; $b_1 = b_2$ or $a_1 = a_2$; $b_1 \sim b_2$ or $a_1 \sim a_2$; $b_1 \sim b_2$.

For a comprehensive understanding of these graph operations, we kindly refer the reader to the relevant literature [10].

A cycle-related graph is a graph representation where cycles, or closed paths are presented. It is commonly used to model molecular structures and network systems, providing insights into connectivity patterns, stability, and properties of the system. The study of cycle-related graphs plays a vital role in graph theory, chemistry, and network analysis. For more one can refer to [11].

The general expression of the neighborhood degree sum based indices of a graph G is

$$TI(G) = \sum_{e=uv\in E(G)} f(\gamma(u),\gamma(v)).$$

Table 1: Operators to derive neighborhood degree-based topological indices from neighborhood M-polynomial.

Topological Index	**Notation**	$f(\gamma(u),\gamma(v))$	**Derivation from** $NM(G)$
Third version of Zagreb	$M_1'(G)$	$\gamma(u)+\gamma(v)$	$(D_x+D_y)(NM(G;x,y))_{x=y=1}$
Neighborhood Harmonic	$\acute{H}(G)$	$\frac{2}{\gamma(u)+\gamma(v)}$	$2S_xJ(NM(G;x,y))_{x=1}$
Neighborhood second Zagreb	$M_2'(G)$	$\gamma(u)\gamma(v)$	$D_xD_y(NM(G;x,y))_{x=y=1}$
Neighborhood inverse sum	$I\acute{S}I(G)$	$\frac{\gamma(u)\gamma(v)}{\gamma(u)+\gamma(v)}$	$S_xJD_xD_y(NM(G;x,y))_{x=1}$
Neighborhood forgotten	$\acute{F}(G)$	$\gamma(u)^2+\gamma(v)^2$	$(D_x^2+D_y^2)_{x=y=1}$
Third NDe	$NDe_3(G)$	$\gamma(u)\gamma(v)\{\gamma(u)+\gamma(v)\}$	$D_xD_y(D_x+D_y)_{x=y=1}$
Fifth NDe	$ND_5(G)$	$\frac{\gamma(u)}{\gamma(v)}+\frac{\gamma(v)}{\gamma(u)}$	$(D_xS_y+S_xD_y)_{x=y=1}$
Neighborhood second modified Zagreb	$m\acute{M}_2(G)$	$\frac{1}{\gamma(u)\gamma(v)}$	$S_xS_y(NM(G;x,y))_{x=y=1}$

The computation of these topological indices involves an appropriately chosen function $f(x,y)$. Table 1 provides several examples of such indices.

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

3 Neighborhood M-polynomial of some graph operations

This section focuses on finding the neighborhood M-polynomial for different graph operations of regular graphs. Additionally, we calculate the neighborhood M-polynomial for the complete bipartite graph $K_{m,n}$.

Lemma 3.1. *Let G be any r-regular graph of order n and size m. Then the neighborhood M-polynomial of G is given by*

$$NM(G;x,y) = mx^{r^2}y^{r^2}.$$

Proof. Since graph G is r-regular for all $u \in V(G)$

$$\gamma(u) = r + r + \ldots + r = r^2.$$

Hence, the required neighborhood M-polynomial is

$$NM(G;x,y) = \sum_{i\leq j} m_{ij}x^iy^j,$$

thus,

$$NM(G;x,y) = mx^{r^2}y^{r^2}.$$

∎

Theorem 3.2. *Let G_1 be an r_1-regular graph of order n_1 and G_2 be an r_2-regular graph of order n_2. Then*
$$NM(G_1 \times G_2; x, y) = \frac{n_1 n_2 (r_1 + r_2)}{2} x^{(r_1+r_2)^2} y^{(r_1+r_2)^2}.$$

Proof. Since G_1 is r_1-regular and G_2 is r_2-regular of order n_1 and n_2, respectively, the neighborhood degree sum of each vertex is $(r_1 + r_2)^2$ in $G_1 \times G_2$. The order and the size of $G_1 \times G_2$ are $n_1 n_2$ and $\frac{n_1 n_2 (r_1+r_2)}{2}$, respectively. Hence by Lemma 3.1

$$NM(G_1 \times G_2; x, y) = \frac{n_1 n_2 (r_1 + r_2)}{2} x^{(r_1+r_2)^2} y^{(r_1+r_2)^2}.$$

■

Theorem 3.3. *Let G_1 be an r_1-regular graph of order n_1 and G_2 be an r_2-regular graph of order n_2. Then*
$$NM(G_1[G_2]; x, y) = \frac{n_1 n_2^2 r_1 + n_1 n_2 r_2}{2} (xy)^{(n_2 r_1 + r_2)^2}.$$

Proof. Since G_1 is r_1-regular of order n_1 and G_2 is r_2-regular of order n_2, the degree of each vertex is $(n_2 r_1 + r_2)$ and neighborhood degree sum of each vertex in $G_1[G_2]$ is $(n_2 r_1 + r_2)^2$. Size of $G_1[G_2]$ is $\frac{n_1 n_2^2 r_1 + n_1 n_2 r_2}{2}$. So by Lemma 3.1 we get

$$NM(G_1[G_2]; x, y) = \frac{n_1 n_2^2 r_1 + n_1 n_2 r_2}{2} (xy)^{(n_2 r_1 + r_2)^2}.$$

■

Theorem 3.4. *Let G_1 be an r_1-regular graph of order n_1 and G_2 be an r_2-regular graph of order n_2. Then*
$$NM(G_1 \otimes G_2; x, y) = \frac{n_1 n_2 r_1 r_2}{2} (xy)^{(r_1 r_2)^2}.$$

Proof. Since G_1 is r_1-regular of order n_1 and G_2 is r_2-regular of order n_2, the degree of each vertex is $(r_1 r_2)$ and neighborhood degree sum of each vertex in $G_1 \otimes G_2$ is $(r_1 r_2)^2$. Size of $G_1 \otimes G_2$ is $\frac{n_1 n_2 r_1 r_2}{2}$. Using Lemma 3.1 we get

$$NM(G_1 \otimes G_2; x, y) = \frac{n_1 n_2 r_1 r_2}{2} (xy)^{(r_1 r_2)^2}.$$

■

Theorem 3.5. *Let G_1 be an r_1-regular graph of order n_1 and G_2 be an r_2-regular graph of order n_2. Then*
$$NM(G_1 \cdot G_2; x, y) = \frac{n_1 n_2 (r_1 + r_2 + r_1 r_2)}{2} (xy)^{(r_1 + r_2 + r_1 r_2)^2}.$$

Proof. Since G_1 is r_1-regular of order n_1 and G_2 is r_2-regular of order n_2, the degree of each vertex in $G_1.G_2$ is $(r_1 + r_2 + r_1 r_2)$ and neighborhood degree sum of each vertex is $(r_1 + r_2 + r_1 r_2)^2$. Size of $G_1 \cdot G_2$ is $\frac{n_1 n_2 (r_1 + r_2 + r_1 r_2)}{2}$. Using Lemma 3.1 we get

$$NM(G_1 \cdot G_2; x, y) = \frac{n_1 n_2 (r_1 + r_2 + r_1 r_2)}{2} (xy)^{(r_1 + r_2 + r_1 r_2)^2}.$$

■

Theorem 3.6. *Let G_1 be an r_1-regular graph of order n_1 and G_2 be an r_2-regular graph of order n_2. Then*

$$NM(G_1 + G_2; x, y) = \frac{n_1 r_1}{2}(xy)^{r_1(r_1+n_2)} + \frac{n_2 r_2}{2}(xy)^{r_2(r_2+n_1)} + n_1 n_2 x^{r_1(r_1+n_2)} y^{r_2(r_2+n_1)}.$$

Proof. If $u \in V(G_1)$ then $d(u) = r_1 + n_2$. Similarly, $d(u) = r_2 + n_1$ whenever $u \in V(G_2)$. So, $\gamma(u) = r_1(r_1 + n_2)$ for all $u \in V(G_1)$. Also, $\gamma(u) = r_2(r_2 + n_1)$ for all $u \in V(G_2)$.
The number of edges whose both the end vertices are in $V(G_1)$ are $\frac{n_1 r_1}{2}$. Similarly, the number of edges whose both the end vertices are in $V(G_2)$ are $\frac{n_2 r_2}{2}$.
And the number of edges whose one end vertex is in $V(G_1)$ and another end vertex is in $V(G_2)$ are $n_1 n_2$. Hence the neighborhood M-polynomial of join of G_1 and G_2 is

$$NM(G_1 + G_2; x, y) = \frac{n_1 r_1}{2}(xy)^{r_1(r_1+n_2)} + \frac{n_2 r_2}{2}(xy)^{r_2(r_2+n_1)} + n_1 n_2 x^{r_1(r_1+n_2)} y^{r_2(r_2+n_1)}.$$

■

Theorem 3.7. *Let $K_{m,n}$ be the complete bipartite graph. Then the neighborhood M-polynomial of $K_{m,n}$ is*

$$NM(K_{m,n}; x, y) = mn(xy)^{mn}.$$

Proof. Let $V(K_{m,n}) = V_1 \cup V_2$, where $|V_1| = m$ and $|V_2| = n$. Then $\gamma(u) = mn$ for any $u \in V(G)$. Hence neighborhood M-polynomial of $K_{m,n}$ is

$$NM(K_{m,n}; x, y) = mn(xy)^{mn}.$$

■

Theorem 3.8. *If G is a r-regular graph with order n and size m, then neighborhood M-polynomial of the complement of G is*

$$NM(G^c; x, y) = \frac{n(n-r)}{2}(xy)^{(n-r)^2}.$$

Proof. Since G is r-regular graph so the degree of each vertex of G^c is $(n - r)$, the neighborhood degree of each vertex of G^c is $(n - r)^2$. By Handshaking theorem the size of G^c is $\frac{n(n-r)}{2}$. Hence

$$NM(G^c; x, y) = \frac{n(n-r)}{2}(xy)^{(n-r)^2}.$$

■

4 Some remarks on cycle related graphs

Several results presented in [12] were found to be erroneous upon thorough examination. The author erroneously employed vertex degrees to compute the neighborhood M-polynomial, instead of properly assessing the sum of neighborhood degrees for each vertex, which is the correct approach. We have diligently verified and rectified these inaccuracies, providing the corrected and accurate results in this section.

Theorem 4.1. *Let $\mathscr{W}_n$ be a wheel of order $(n+1)$ and size $2n$. Then*

$$NM(\mathscr{W}_n; x, y) = n(xy)^{n+6} + nx^{n+6}y^{3n}.$$

Proof. The edges of $\mathscr{W}_n$ can be divided as

$$m_{n+6,n+6} = n,$$
$$m_{n+6,3n} = n.$$

Hence, the neighborhood M-polynomial of $\mathscr{W}_n$ can be expressed as:

$$NM(\mathscr{W}_n; x, y) = n(xy)^{n+6} + nx^{n+6}y^{3n}.$$

■

Corollary 4.2. *The significant topological indices based on the neighborhood M-polynomial of $\mathscr{W}_n$ are*

1. $M_1'(\mathscr{W}_n) = 6n^2 + 18n$,
2. $\acute{H}(\mathscr{W}_n) = \frac{3n^2+9n}{(n+6)(2n+3)}$,
3. $M_2'(\mathscr{W}_n) = 4n^3 + 30n^2 + 36n$,
4. $I\acute{S}I(\mathscr{W}_n) = \frac{n(n+6)}{2} + \frac{3n^2(n+6)}{4n+6}$,
5. $\acute{F}(\mathscr{W}_n) = 20n^4 + 96n^3 + 180n^2$,
6. $NDe_3(\mathscr{W}_n) = 14n^4 + 126n^3 + 324n^2 + 432n$,
7. $ND_5(\mathscr{W}_n) = \frac{16n^2+48n+36}{3(n+6)}$,
8. $m\acute{M}_2(\mathscr{W}_n) = \frac{4n+6}{3(n+6)^2}$.

Proof. From the neighborhood M-polynomial of $\mathscr{W}_n$ we get

$D_x = x\frac{\partial f(x,y)}{\partial x} = n(n+6)x^{x+6}y^{n+6} + n(n+6)x^{n+6}y^{3n}$,
$D_y = y\frac{\partial f(x,y)}{\partial y} = n(n+6)x^{n+6}y^{n+6} + 3n^2x^{n+6}y^{3n}$,
$S_x = \int_0^x \frac{f(t,y)}{t}dt = \frac{n}{n+6}(xy)^{n+6} + \frac{n}{n+6}x^{n+6}y^{3n}$,
$S_y = \int_0^y \frac{f(x,t)}{t}dt = \frac{n}{n+6}(xy)^{n+6} + \frac{1}{3}x^{n+6}y^{3n}$,
$J(f(x,y)) = f(x,x) = nx^{2n+12} + nx^{4n+6}$.

Therefore,

1. $M_1'(\mathscr{W}_n) = (D_x + D_y)(NM(\mathscr{W}_n; x, y))|_{x=1=y} = 6n^2 + 18n$,
2. $\acute{H}(\mathscr{W}_n) = (2S_xJ)(NM(\mathscr{W}_n; x, y))|_{x=1} = \frac{3n^2+9n}{(n+6)(2n+3)}$,
3. $M_2'(\mathscr{W}_n) = (D_xD_y)(NM(\mathscr{W}_n; x, y))|_{x=1=y} = 4n^3 + 30n^2 + 36n$,
4. $I\acute{S}I(\mathscr{W}_n) = (S_xJD_xD_y)(NM(\mathscr{W}_n; x, y))|_{x=1} = \frac{n(n+6)}{2} + \frac{3n^2(n+6)}{4n+6}$,

5. $\acute{F}(\mathscr{W}_n) = (D_x^2 + D_y^2)(NM(\mathscr{W}_n; x, y))|_{x=1=y} = 20n^4 + 96n^3 + 180n^2$,

6. $NDe_3(\mathscr{W}_n) = (D_x D_y (D_x + D_y))(NM(\mathscr{W}_n; x, y))|_{x=1=y} = 14n^4 + 126n^3 + 324n^2 + 432n$,

7. $ND_5(\mathscr{W}_n) = (D_x S_y + S_x D_y)(NM(\mathscr{W}_n; x, y))|_{x=1=y} = \frac{16n^2+48n+36}{3(n+6)}$,

8. $m\acute{M}_2(\mathscr{W}_n) = (S_x S_y)(NM(\mathscr{W}_n; x, y))|_{x=1=y} = \frac{4n+6}{3(n+6)^2}$.

∎

Theorem 4.3. *Let $\mathscr{F}_n$ be a fan graph of order $(n+1)$ and size $(2n-1)$. Then*

$$NM(\mathscr{F}_n; x, y) = 2x^{n+3}y^{n+5} + 2x^{n+5}y^{n+6} + 2x^{n+3}y^{3n-2} + 2x^{n+5}y^{3n-2} + (n-4)x^{n+6}y^{3n-2} + (n-4)x^{n+6}y^{n+6}.$$

Proof. The fan $\mathscr{F}_n$ has $n+1$ vertices and $2n-1$ edges. It is easy to see that

$$\begin{aligned} m_{n+3,n+5} &= 2, \\ m_{n+5,n+6} &= 2, \\ m_{n+3,3n-2} &= 2, \\ m_{n+5,3n-2} &= 2, \\ m_{n+6,3n-2} &= n-4, \\ m_{n+6,n+6} &= n-4. \end{aligned}$$

So the neighborhood M-polynomial of $\mathscr{F}_n$ is

$$NM(\mathscr{F}_n; x, y) = 2x^{n+3}y^{n+5} + 2x^{n+5}y^{n+6} + 2x^{n+3}y^{3n-2} + 2x^{n+5}y^{3n-2} + (n-4)x^{n+6}y^{3n-2} + (n-4)x^{n+6}y^{n+6}.$$

∎

Corollary 4.4. *The topological indices derived from the neighborhood M-polynomial of fan graph $\mathscr{F}_n$ are*

1. $M_1'(\mathscr{F}_n) = 6n^2 + 16n - 18$,

2. $\acute{H}(\mathscr{F}_n) = \frac{96n^6+1264n^5+6114n^4+13731n^3+15868n^2+14700n+5592}{2(n+4)(n+1)(n+6)(4n+1)(4n+3)(2n+11)}$,

3. $M_2'(\mathscr{F}_n) = 4n^3 + 28n^2 - 10n - 38$,

4. $I\acute{S}I(\mathscr{F}_n) = \frac{160n^7+2640n^6+14254n^5+25321n^4+266n^3-4700n^2-6540n-4996}{4(n+4)(n+1)(4n+1)(4n+3)(2n+11)}$,

5. $\acute{F}(\mathscr{F}_n) = 20n^4 + 80n^3 + 80n^2 - 400n + 260$,

6. $NDe_3(\mathscr{F}_n) = 14n^4 + 112n^3 + 82n^2 - 30n - 708$,

7. $ND_5(\mathscr{F}_n) = \frac{10n+14}{n+5} + \frac{3n^2-12n+18}{n+6} + \frac{n^2+6n-8}{3n-2} + \frac{8n+6}{n+3} + 2n - 8$,

8. $m\acute{M}_2(\mathscr{F}_n) = \frac{4n^4+36n^3+130n^2+268n+120}{(n+3)(n+5)(n+6)^2(3n-2)}$.

Proof. From the neighborhood M-polynomial of $\mathscr{F}_n$ we get

$D_x = x\frac{\partial f(x,y)}{\partial x} = 2(n+3)x^{n+3}y^{n+5} + 2(n+5)x^{n+5}y^{n+6} + 2(n+3)x^{n+3}y^{3n-2} + 2(n+5)x^{n+5}y^{3n-2} + (n-4)(n+6)x^{n+6}y^{3n-2} + (n-4)(n+6)x^{n+6}y^{n+6}$,

$D_y = y\frac{\partial f(x,y)}{\partial y} = 2(n+5)x^{n+3}y^{n+5} + 2(n+6)x^{n+5}y^{n+6} + 2(3n-2)x^{n+3}y^{3n-2} + 2(3n-2)x^{x+5}y^{3n-2} + (n-4)(3n-2)x^{n+6}y^{3n-2} + (n-4)(n+6)x^{n+6}y^{n+6}$,
$S_x = \int_0^x \frac{f(t,y)}{t}dt = \frac{2}{n+3}x^{n+3}y^{n+5} + \frac{2}{n+5}x^{n+5}y^{n+6} + \frac{2}{n+3}x^{n+3}y^{3n-2} + \frac{n-4}{n+5}x^{n+5}y^{3n-2} + \frac{n-4}{n+6}x^{n+6}y^{n+6} + \frac{2}{n+5}x^{n+5}y^{3n-2}$,
$S_y = \int_0^y \frac{f(x,t)}{t}dt = \frac{2}{n+5}x^{n+3}y^{n+5} + \frac{2}{n+6}x^{n+5}y^{n+6} + \frac{2}{3n-2}x^{n+3}y^{3n-2} + \frac{n-4}{3n-2}x^{n+6}y^{3n-2} + \frac{n-4}{n+6}(xy)^{n+6} + \frac{2}{3n-2}x^{n+5}y^{3n-2}$,
$J(f(x,y)) = f(x,x) = 2x^{2n+8} + 2x^{2n+11} + 2x^{4n+1} + 2x^{4n+3} + (n-4)x^{4n+4} + (n-4)x^{2n+12}$.

Therefore,

1. $M_1'(\mathscr{F}_n) = (D_x + D_y)(NM(\mathscr{F}_n;x,y))|_{x=1=y} = 6n^2 + 16n - 18$,
2. $\acute{H}(\mathscr{F}_n) = (2S_xJ)(NM(\mathscr{F}_n;x,y))|_{x=1} = \frac{96n^6+1264n^5+6114n^4+13731n^3+15868n^2}{2(n+4)(n+1)(n+6)(4n+1)(4n+3)(2n+11)} + \frac{14700n+5592}{2(n+4)(n+1)(n+6)(4n+1)(4n+3)(2n+11)}$,
3. $M_2'(\mathscr{F}_n) = (D_xD_y)(NM(\mathscr{F}_n;x,y))|_{x=1=y} = 4n^3 + 28n^2 - 10n - 38$,
4. $I\acute{S}I(\mathscr{F}_n) = (S_xJD_xD_y)(NM(\mathscr{F}_n;x,y))|_{x=1} = \frac{160n^7+2640n^6+14254n^5+25321n^4}{4(n+4)(n+1)(4n+1)(4n+3)(2n+11)} + \frac{266n^3-4700n^2-6540n-4996}{4(n+4)(n+1)(4n+1)(4n+3)(2n+11)}$,
5. $\acute{F}(\mathscr{F}_n) = (D_x^2 + D_y^2)(NM(\mathscr{F}_n;x,y))|_{x=1=y} = 20n^4 + 80n^3 + 80n^2 - 400n + 260$,
6. $NDe_3(\mathscr{F}_n) = (D_xD_y(D_x + D_y))(NM(\mathscr{F}_n;x,y))|_{x=1=y} = 14n^4 + 112n^3 + 82n^2 - 30n - 708$,
7. $ND_5(\mathscr{F}_n) = (D_xS_y + S_xD_y)(NM(\mathscr{F}_n;x,y))|_{x=1=y} = \frac{10n+14}{n+5} + \frac{3n^2-12n+18}{n+6} + \frac{n^2+6n-8}{3n-2} + \frac{8n+6}{n+3} + 2n - 8$,
8. $m\acute{M}_2(\mathscr{F}_n) = (S_xS_y)(NM(\mathscr{F}_n;x,y))|_{x=1=y} = \frac{4n^4+36n^3+130n^2+268n+120}{(n+3)(n+5)(n+6)^2(3n-2)}$.

■

Theorem 4.5. *Let $\mathscr{G}_n$ be a gear graph. Then the neighborhood M-polynomial of $\mathscr{G}_n$ is*

$$NM(\mathscr{G}_n;x,y) = 2nx^6y^{n+4} + nx^{n+4}y^{3n}.$$

Proof. The edges of $\mathscr{G}_n$ can be divided as:

$$m_{6,n+4} = 2n,$$
$$m_{n+4,3n} = n.$$

So the neighborhood M-polynomial is

$$NM(\mathscr{G}_n;x,y) = 2nx^6y^{n+4} + nx^{n+4}y^{3n}.$$

■

Corollary 4.6. *Let $\mathscr{G}_n$ be a gear graph. Then the neighborhood degree based topological indices of $\mathscr{G}_n$ are*

1. $M_1'(\mathscr{G}_n) = 6n^2 + 24n$,
2. $\acute{H}(\mathscr{G}_n) = \frac{9n^2+18n}{2(n+1)(n+10)}$,
3. $M_2'(\mathscr{G}_n) = 3n^3 + 24n^2 + 48n$,
4. $I\acute{S}I(\mathscr{G}_n) = \frac{12n(n+4)}{n+10} + \frac{3n^2(n+4)}{4(n+1)}$,
5. $\acute{F}(\mathscr{G}_n) = 24n^4 + 112n^3 + 320n^2$,
6. $NDe_3(\mathscr{G}_n) = 12n^4 + 72n^3 + 216n^2 + 480n$,
7. $ND_5(\mathscr{G}_n) = \frac{n^2+14n+4}{3}$,
8. $m\acute{M}_2(\mathscr{G}_n) = \frac{n+1}{3(n+4)}$.

Proof. From the neighborhood M-polynomial of $\mathscr{G}_n$ we get

$$D_x = x\frac{\partial f(x,y)}{\partial x} = 12nx^6y^{n+4} + n(n+4)x^{n+4}y^{3n},$$
$$D_y = y\frac{\partial f(x,y)}{\partial y} = 2n(n+4)x^6y^{n+4} + 3n^2x^{n+4}y^{3n},$$
$$S_x = \int_0^x \frac{f(t,y)}{t}dt = \frac{n}{3}x^6y^{n+4} + \frac{n}{n+4}x^{n+4}y^{3n},$$
$$S_y = \int_0^y \frac{f(x,t)}{t}dt = \frac{2n}{n+4}x^6y^{n+4} + \frac{1}{3}x^{n+4}y^{3n},$$
$$J(f(x,y)) = f(x,x) = 2nx^{n+10} + nx^{4n+4}.$$

Therefore,

1. $M_1'(\mathscr{G}_n) = (D_x + D_y)(NM(\mathscr{F}_n;x,y))|_{x=1=y} = 6n^2 + 24n$,
2. $\acute{H}(\mathscr{G}_n) = (2S_xJ)(NM(\mathscr{F}_n;x,y))|_{x=1} = \frac{9n^2+18n}{2(n+1)(n+10)}$,
3. $M_2'(\mathscr{G}_n) = (D_xD_y)(NM(\mathscr{F}_n;x,y))|_{x=1=y} = 3n^3 + 24n^2 + 48n$,
4. $I\acute{S}I(\mathscr{G}_n) = (S_xJD_xD_y)(NM(\mathscr{G}_n;x,y))|_{x=1} = \frac{12n(n+4)}{n+10} + \frac{3n^2(n+4)}{4(n+1)}$,
5. $\acute{F}(\mathscr{G}_n) = (D_x^2 + D_y^2)(NM(\mathscr{G}_n;x,y))|_{x=1=y} = 24n^4 + 112n^3 + 320n^2$,
6. $NDe_3(\mathscr{G}_n) = (D_xD_y(D_x + D_y))(NM(\mathscr{G}_n;x,y))|_{x=1=y} = 12n^4 + 72n^3 + 216n^2 + 480n$,
7. $ND_5(\mathscr{G}_n) = (D_xS_y + S_xD_y)(NM(\mathscr{G}_n;x,y))|_{x=1=y} = \frac{n^2+14n+4}{3}$,
8. $m\acute{M}_2(\mathscr{G}_n) = (S_xS_y)(NM(\mathscr{G}_n;x,y))|_{x=1=y} = \frac{n+1}{3(n+4)}$.

■

Theorem 4.7. *Let $\mathscr{F}\mathscr{D}_n$ be a friendship graph. Then neighborhood M-polynomial of $\mathscr{F}\mathscr{D}_n$ is*

$$NM(\mathscr{F}\mathscr{D}_n;x,y) = 2nx^{2n}y^{2n+2} + nx^{2n+2}y^{2n+2}.$$

Proof. The edges of $\mathscr{F}\mathscr{D}_n$ can be divided as

$$m_{2n+2,2n} = 2n,$$
$$m_{2n+2,2n+2} = n.$$

Hence the neighborhood M-polynomial is

$$NM(\mathscr{F}\mathscr{D}_n; x, y) = 2nx^{2n}y^{2n+2} + nx^{2n+2}y^{2n+2}.$$

■

Corollary 4.8. *If $\mathscr{F}\mathscr{D}_n$ is a friendship graph, then the neighborhood degree based topological indices are:*

1. $M_1'(\mathscr{F}\mathscr{D}_n) = 12n^2 + 8n$,
2. $\acute{H}(\mathscr{F}\mathscr{D}_n) = \frac{6n^2+5n}{2(n+1)(2n+1)}$,
3. $M_2'(\mathscr{F}\mathscr{D}_n) = 12n^3 + 16n^2 + 4n$,
4. $I\acute{S}I(\mathscr{F}\mathscr{D}_n) = \frac{n(n+1)(6n+1)}{2n+1}$,
5. $\acute{F}(\mathscr{F}\mathscr{D}_n) = 72n^4 + 96n^3 + 40n^2$,
6. $NDe_3(\mathscr{F}\mathscr{D}_n) = 48n^4 + 96n^3 + 64n^2 + 16n$,
7. $ND_5(\mathscr{F}\mathscr{D}_n) = \frac{6n^2+6n+2}{n+1}$,
8. $m\acute{M}_2(\mathscr{F}\mathscr{D}_n) = \frac{3n+2}{(2n+2)^2}$.

Theorem 4.9. *Let $\mathscr{H}_n$ be a helm graph. Then the neighborhood M-polynomial of $\mathscr{H}_n$ is*

$$NM(\mathscr{H}_n; x, y) = nx^{n+9}y^{4n} + nx^{n+9}y^{n+9} + nx^4y^{n+9}.$$

Proof. The partition of the edges based on the neighborhood degree sum can be done as:

$$m_{4,n+9} = n,$$
$$m_{n+9,4n} = n,$$
$$m_{n+9,n+9} = n.$$

So the neighborhood M-polynomial is

$$NM(\mathscr{H}_n; x, y) = nx^{n+9}y^{4n} + nx^{n+9}y^{n+9} + nx^4y^{n+9}.$$

■

Corollary 4.10. *If $\mathscr{H}_n$ is a helm, then*

1. $M_1'(\mathscr{H}_n) = 8n^2 + 40n$,
2. $\acute{H}(\mathscr{H}_n) = \frac{17n^3+226n^2+513n}{(n+9)(5n+9)(n+13)}$,
3. $M_2'(\mathscr{H}_n) = 5n^3 + 58n^2 + 117n$,

4. $I\acute{S}I(\mathscr{H}_n) = \frac{4n^2(n+9)}{5n+9} + \frac{n(n+9)}{2} + \frac{4n(n+9)}{n+13}$,

5. $\acute{F}(\mathscr{H}_n) = 40n^4 + 304n^3 + 808n^2$,

6. $NDe_3(\mathscr{H}_n) = 22n^4 + 274n^3 + 898n^2 + 1926n$,

7. $ND_5(\mathscr{H}_n) = \frac{n^3+43n^2+187n+81}{4(n+9)}$,

8. $m\acute{M}_2(\mathscr{H}_n) = \frac{n^2+14n+9}{4(n^2+18n+81)}$.

Theorem 4.11. *If $\mathscr{C}\mathscr{H}_n$ is a closed helm, then the neighborhood M-polynomial of $\mathscr{C}\mathscr{H}_n$ is*

$$NM(\mathscr{C}\mathscr{H}_n; x, y) = n(xy)^{10} + n(xy)^{n+11} + nx^{10}y^{n+11} + n(xy^n)^{n+11}.$$

Proof. The edges of the closed helm $\mathscr{C}\mathscr{H}_n$ can be divided as:

$$\begin{aligned} m_{10,10} &= n, \\ m_{10,n+11} &= n, \\ m_{n+11,n+11} &= n, \\ m_{n+11,n(n+11)} &= n. \end{aligned}$$

Hence the neighborhood M-polynomial is

$$NM(\mathscr{C}\mathscr{H}_n; x, y) = n(xy)^{10} + n(xy)^{n+11} + nx^{10}y^{n+11} + n(xy^n)^{n+11}.$$

■

Corollary 4.12. *If $\mathscr{C}\mathscr{H}_n$ is a closed helm, then*

1. $M_1'(\mathscr{C}\mathscr{H}_n) = n^3 + 15n^2 + 74n$,

2. $\acute{H}(\mathscr{C}\mathscr{H}_n) = \frac{n^4+63n^3+743n^2+1081n}{10(n+1)(n+11)(n+21)}$,

3. $M_2'(\mathscr{C}\mathscr{H}_n) = n^4 + 23n^3 + 153n^2 + 331n$,

4. $I\acute{S}I(\mathscr{C}\mathscr{H}_n) = 5n + \frac{n(n+1)}{2} + \frac{10n(n+11)}{n+21} + \frac{n^2(n+11)}{n+1}$,

5. $\acute{F}(\mathscr{C}\mathscr{H}_n) = n^6 + 26n^5 + 237n^4 + 1000n^3 + 2788n^2$,

6. $NDe_3(\mathscr{C}\mathscr{H}_n) = n^6 + 34n^5 + 398n^4 + 1770n^3 + 2377n^2 + 6972n$,

7. $ND_5(\mathscr{C}\mathscr{H}_n) = \frac{11n^3+172n^2+671n+110}{10(n+11)}$,

8. $m\acute{M}_2(\mathscr{C}\mathscr{H}_n) = \frac{n^3+32n^2+331n+100}{100(n+11)^2}$.

Theorem 4.13. *Let $\mathscr{C}\mathscr{W}_n$ be a crown. Then the neighborhood M-polynomial of $\mathscr{C}\mathscr{W}_n$ is*

$$NM(\mathscr{C}\mathscr{W}_n; x, y) = nx^3y^7 + n(xy)^7.$$

Proof. The edges of $\mathscr{CW}_n$ can be divided as:

$$m_{3,7} = n,$$
$$m_{7,7} = n.$$

Hence the required polynomial is

$$NM(\mathscr{CW}_n; x, y) = nx^3y^7 + n(xy)^7.$$

■

Corollary 4.14. *If $\mathscr{CW}_n$ is a crown, then*

1. $M_1'(\mathscr{CW}_n) = 24n$,
2. $\acute{H}(\mathscr{CW}_n) = \frac{12n}{35}$,
3. $M_2'(\mathscr{CW}_n) = 70n$,
4. $I\acute{S}I(\mathscr{CW}_n) = \frac{28n}{5}$,
5. $\acute{F}(\mathscr{CW}_n) = 296n^2$,
6. $NDe_3(\mathscr{CW}_n) = 896n$,
7. $ND_5(\mathscr{CW}_n) = \frac{100n}{21}$,
8. $m\acute{M}_2(\mathscr{CW}_n) = \frac{10n}{147}$.

Theorem 4.15. *Let $\mathscr{FL}_n$ be a flower graph. Then the neighborhood M-polynomial of $\mathscr{FL}_n$ is*

$$NM(\mathscr{FL}_n; x, y) = n(xy)^{2n+10} + nx^{2n+10}y^{6n} + nx^{2n+4}y^{6n}.$$

Proof. The edges can be partitioned as

$$m_{2n+4,6n} = n,$$
$$m_{2n+10,6n} = n,$$
$$m_{2n+10,2n+10} = n.$$

Hence the neighborhood M-polynomial is

$$NM(\mathscr{FL}_n; x, y) = n(xy)^{2n+10} + nx^{2n+10}y^{6n} + nx^{2n+4}y^{6n}.$$

■

Corollary 4.16. *If $\mathscr{FL}_n$ is a flower graph, then*

1. $M_1'(\mathscr{FL}_n) = 20n^2 + 34n$,
2. $\acute{H}(\mathscr{FL}_n) = \frac{16n^3+61n^2+40n}{2(n+5)(4n+5)(2n+1)}$,
3. $M_2'(\mathscr{FL}_n) = 28n^3 + 124n^2 + 100n$,
4. $I\acute{S}I(\mathscr{FL}_n) = \frac{n(32n^3+159n^2+135n+250)}{(4n+5)(2n+1)}$,

5. $\acute{F}(\mathscr{F}\mathscr{L}_n) = 232n^4 + 568n^3 + 676n^2$,

6. $NDe_3(\mathscr{F}\mathscr{L}_n) = 208n^4 + 1080n^3 + 1896n^2 + 2000n$,

7. $ND_5(\mathscr{F}\mathscr{L}_n) = \frac{26n^3+126n^2+129n+70}{3(n+5)(n+2)}$,

8. $m\acute{M}_2(\mathscr{F}\mathscr{L}_n) = \frac{5n^2+23n+35}{3(2n+10)^2(n+2)}$.

5 Applications to nanotubes and nanotori

In this section, we focus on the computation of the several topological indices (TIs) of carbon nanotubes and nanotori. TIs serve as numerical indicators that provide valuable insights into a compound's characteristics, forming a crucial link between physio-chemical properties and mathematics. Our research focuses explicitly on carbon nanostructures. Referring to important sources like [13–15], we have seen that topological indices play a crucial role in figuring out details about these carbon nanostructures' physical and chemical properties. Considering the widespread use of carbon nanostructures in various physical applications, as highlighted in [16–21], the evaluation of topological indices becomes pivotal. This assessment aids in streamlining the selection process for compounds in practical applications, determining which ones are better suited for specific purposes.

Among carbon nanomaterials, carbon nanotubes and nanotori are widely utilized in various applications. The primary uses of these nanostructures encompass biomolecule and drug delivery to targeted organs, biosensor diagnostics, and analysis. They demonstrate outstanding chemical and physical characteristics, including high tensile strength, extremely low weight, unique electronic structures, elevated chemical and thermal stability, extensive surface area, numerous antibacterial and antifungal properties, capacity to serve as protein carriers, and possession of exposed functional groups. These remarkable attributes have sparked significant interest in these nanomaterials among scientists. The considerable potential of multiwalled carbon nanotubes (MWCNT) in biosensors arises from their ability to facilitate protein immobilization with ease while preserving the inherent activity of the proteins. Some significant applications are as follows:

In a study by Beden et al. [16], they created an electrochemical sensor using MWCNTs and Gold Nanoparticles (AuNPs) to detect dopamine at very low levels. This was achieved by including electroactive adducts, which improved the sensor's analytical capabilities. Additionally, Gutierrez et al. [17] used MWCNTs on a glassy carbon electrode (GCE) to detect albumin, glucose, and amino acids both qualitatively and quantitatively. The sensor could identify glucose with a limit as low as 182 nM. It also successfully recognized carbohydrates, amino acids, and albumin in real samples, indicating its practical usefulness and suggesting potential commercial applications. For a more in-depth understanding of how carbon nanotubes and nanotori are applied, we recommend checking out [18–21].

5.1 Computational aspects of VPHX[m,n]

In this sub-section, we obtain the general forms of neighborhood M-polynomials of V-Phenylenic nanotubes $VPHX[m,n]$ with m and n taking only positive integral value and rapidly compute some topological indices from the polynomial obtained.

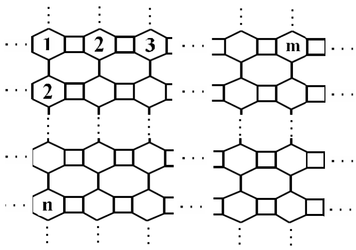

Figure 1: V-Phenylenic nanotubes VPHX[m,n].

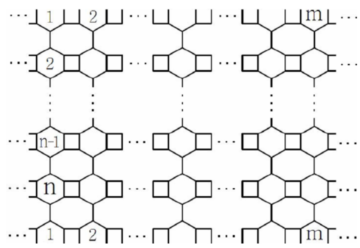

Figure 2: V-Phenylenic nanotori VPHY[m,n].

Theorem 5.1. *Let $G = VPHX[m,n]$ be the V-Phenylenic nanotube. Then the neighborhood M-polynomial is given by*

$$NM(G;x,y) = 4mx^6y^8 + 2(m-1)(xy)^8 + 4mx^8y^9 + (9mn-11m-2n+2)(xy)^9.$$

Proof. We see from Figure 1 that the graph has $6mn$ number of vertices and $9mn$ number of edges. The edge partition of the graph G can be realized as:

$$m_{6,8} = 4m,$$
$$m_{8,9} = 4m,$$
$$m_{8,8} = 2(m-1),$$
$$m_{9,9} = 9mn - 11m - 2n + 2.$$

Hence the neighborhood M-polynomial of G is

$$NM(G;x,y) = 4mx^6y^8 + 2(m-1)(xy)^8 + 4mx^8y^9 + (9mn-11m-2n+2)(xy)^9.$$

■

Corollary 5.2. *If G is the graph of $VPHX[m,n]$, then*

1. $M_1'(G) = -42m + 162mn - 36n + 4,$
2. $\acute{H}(G) = -\frac{35}{612}m + \frac{9mn-2n}{9} - \frac{1}{36},$
3. $M_2'(G) = -283m + 729mn - 162n + 34,$
4. $I\acute{S}I(G) = \frac{-2581m+9639mn-2142n+238}{238},$
5. $\acute{F}(G) = 954m^2 - 6804m^2n + 2160mn - 168m + 13122m^2n^2 - 5832mn^2 + 648n^2 - 144n + 8,$
6. $NDe_3(G) = 1613m + 6561mn - 1458n - 590,$
7. $ND_5(G) = \frac{493}{18}m + 18mn - 4n - 14,$
8. $m\acute{M}_2(G) = -\frac{367}{36}m + 9mn - 2n + \frac{571}{324}.$

5.2 Computational aspects of $VPHY[m,n]$

In this sub-section, we obtain the general forms of neighborhood M-polynomials of V-Phenylenic nanotubes $VPHY[m,n]$ with m and n taking only positive integral value and rapidly compute some topological indices from this polynomial.

Theorem 5.3. *Let $G = VPHY[m,n]$ be the V-Phenylenic nanotorus. Then the neighborhood M-polynomial is given by*

$$NM(G;x,y) = 9mn(xy)^9.$$

Proof. We see from Figure 2 that the graph has $6mn$ number of vertices and $9mn$ number of edges. The edge partition of the graph G can be realized as

$$m_{9,9} = 9mn.$$

Hence the neighborhood M-polynomial is

$$NM(G;x,y) = 9mn(xy)^9.$$

■

Corollary 5.4. *If G is the graph of $VPHY[m,n]$, then*

1. $M_1'(G) = 162mn$,
2. $\acute{H}(G) = mn$,
3. $M_2'(G) = 9mn$,
4. $I\acute{S}I(G) = \frac{81mn}{2}$,
5. $\acute{F}(G) = 13122(mn)^2$,
6. $NDe_3(G) = 13122mn$,
7. $ND_5(G) = 18mn$,
8. $m\acute{M}_2(G) = \frac{mn}{9}$.

5.3 Graph representation of $VPHX[1,1]$ and $VPHY[1,1]$

The surface of the neighborhood M-polynomial of $VPHX[1,1]$ and $VPHY[1,1]$ have been plotted using Maple 13. This implies that the values derived from the neighborhood M-polynomial exhibit distinct patterns corresponding to varying parameters x and y. These values can be controlled through parameters. Clearly, Figure 3 shows the hyperboloid of two sheets and Figure 4 indicates that on one side, the intercept forms an upward-opening parabola, while on the other side, it forms a downward-opening parabola. Moreover, we see that all indices are linearly related with the structural parameters m and n as the following Figure 5 and Figure 6 suggests. It is observed that this index increases as m and n increase. We also tried to compare different topological indices keeping one parameter constant. The following Figures 7 and 8 demonstrate the comparison.

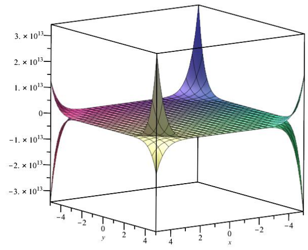

Figure 3: Plotting of neighborhood M-polynomial of $VPHX[1,1]$.

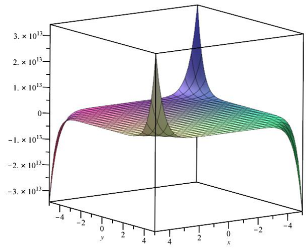

Figure 4: Plotting of neighborhood M-polynomial of $VPHY[1,1]$.

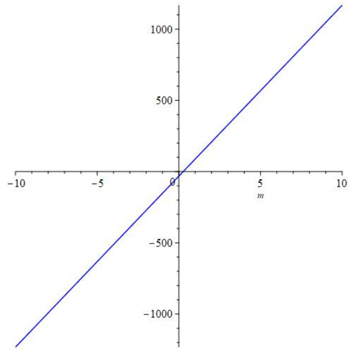

Figure 5: Linear relationship between M_1' and m.

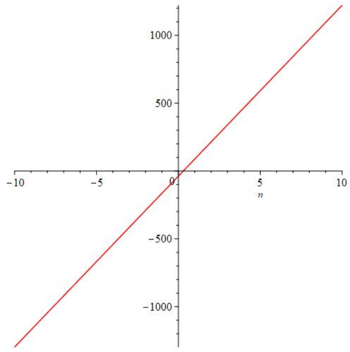

Figure 6: Linear relationship between M_1' and n.

6 Discussions

To sum up, our work has successfully achieved its three main objectives. Through the derivation of neighborhood M-polynomials for classical graph operations of regular graphs, we have provided valuable tools for network analysis and optimization, which have practical significance in various domains. The primary benefit of utilizing graph products lies in their ability to decompose intricate graphs into simpler, familiar graphs while simultaneously forming more complex network structures.

Moreover, by addressing and rectifying inaccuracies in specific results of cycle-related graphs, we have enhanced the accuracy and reliability of topological indices, ensuring their precise calculations. Additionally, our investigation into novel cycle-related graphs has expanded our understanding of their properties, offering new insights into their structures.

Finally, by applying our findings to real-world structures such as nanotubes and nanotori structures, we have demonstrated the practical applicability of the derived indices. By unraveling the connections between neighborhood M-polynomials, topological indices, and structural parameters, our work provides valuable insights for future research and applications in the realm of nanostructure analysis.

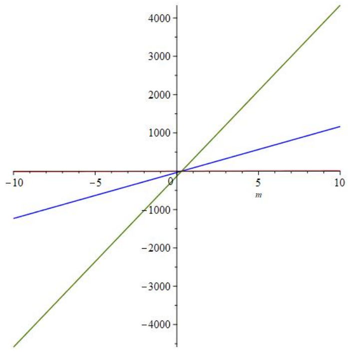

Figure 7: Comparing M_1', H' and M_2' of $VPHX[m,1]$.

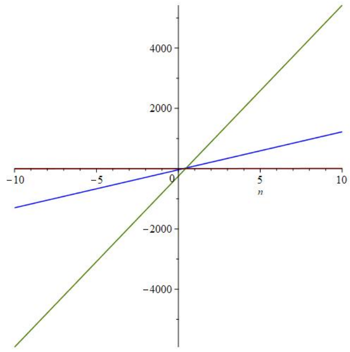

Figure 8: Comparing M_1', H' and M_2' of $VPHX[1,n]$.

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Appendix

In this appendix, we provide a MATLAB code to find neighborhood degree sum of vertices in a graph.

```
function neighborhood_degree_sum(graph)
   num_vertices = size(graph, 1);
    degree_sums = zeros(1, num_vertices);
  for vertex = 1:num_vertices
       neighbors = find(graph(vertex, :));
        degree_sums(vertex) = sum(graph(vertex, neighbors));
    end
    disp('Neighborhood degree sums of all vertices:');
    disp(degree_sums);
end
```