Molecular descriptors of certain OTIS interconnection networks

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Abstract:

Network theory as an important role in the field of electronic and electrical engineering, for example, in signal processing, networking, communication theory, etc. The branch of mathematics known as Graph theory found remarkable applications in this area of study. A topological index (TI) is a real number attached with graph networks and correlates the chemical networks with many physical and chemical properties and chemical reactivity. The Optical Transpose Interconnection System (OTIS) network has received considerable attention in recent years and has a special place among real world architectures for parallel and distributed systems. In this report, we compute redefined first, second and third Zagreb indices of OTIS swapped and OTIS biswapped networks. We also compute some Zagreb polynomials of understudy Networks.

1. Introduction

Mathematical chemistry is an area of research in chemistry in which mathematical tools are used to solve problems of chemistry. Chemical graph theory is an important area of research in mathematically chemistry which deals with topology of molecular structure such as the mathematical study of isomerism and the development of topological descriptors or indices. Infect, TIs are real numbers attached with graph networks and graph of chemical compounds and has applications in quantitative structure-property relationships. TIs remain invariant upto graph isomorphism and help to predict many properties of chemical compounds, networks and nanomaterials, for example, viscosity, boiling points, radius of gyrations, etc without going to lab [3,5,24].

Other emerging field is Cheminformatics, in which we use QSAR and QSPR relationship to guess biological activity and chemical properties of nanomaterial and networks. In these investigations, some Physico-chemical properties and TIs are utilized to guess the behavior of chemical networks [11]. Like TIs, polynomials also fund considerable applications in network theory and chemistry, for example, Hosoya polynomial, which is also known as Wiener polynomial, introduced in [13] plays an important role in computation of distance-based TIs. M-polynomial [8] was defined in 2015 and plays a similar role in computation of numerous degree-based TIs [1,16,17,18,19]. The M-polynomial contains precious information about degree-based TIs and many TIs can be computed from this simple algebraic polynomial. The first TI was defined in 1947 by Weiner during studying boiling point of alkanes [26]. This index is now known as Weiner index. Thus Weiner established the framework of TIs and the Wiener index is initially the first and most concentrated TI. For details about applications of graph theory and TIs, see [12,15,23,25] and reference therein.

The other oldest TI is Randić index (RI), given by Milan Randi c [20] in 1975. After the success of Randić index, in the year 1988, the generalized version of Randić index was introduced [4,7]. This version attracts both the mathematicians and chemists [2,19].

The RI is a most mainstream regularly connected and most concentrated among all other TIs. Numerous research papers and text books are published in different academic journals on this TI. Two surveys on RI was written by Milan Randić and the reason behind the success of such a simple TI is as yet a puzzle, although some conceivable clarifications were given.

After Randić index, the most studied TIs are 1st Zagreb index (ZI) and

2nd ZI [14]. In this report we aim to study some Zagreb polynomials and redefined Zagreb indices of OTIS (swapped and biswapped) networks.

2. Basic Notions

In mathematical chemistry, precisely speaking, in chemical-graph-theory (CGT), a molecular graph and graph network is a simple and connected graph, in which atoms represents vertices and chemical bonds represents edges. We reserve G for simple connected graph, E for edge set and V for vertex set throughout the thesis. The degree of a vertex u of graph G is the number of vertices that are attached with u and is denoted by d_v. With the help of TIs, many properties of molecular structure can be obtained without going to lab. The reality is, many research paper has been written on computation of degree-based indices and polynomials of different molecular structure and networks but only few work has been done so far on distance based indices and polynomials. Our aim is to compute distance-based as well as degree-based indices of understudy networks. The first and the second ZIs (cf. [14]) are defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

and

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

Considering the ZIs, Fath-Tabar in [10] introduced the following first and the second Zagreb polynomials

$$(2.1) \qquad M_1(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v}$$

and

$$(2.2) \qquad M_2(G, x) = \sum_{uv \in E(G)} x^{d_u \times d_v}.$$

The properties of first and second Zagreb polynomials for some chemical structures have been studied in the literature [21].

After the success of ZIs, the researchers in [9], introduced the following third ZI

$$M_3(G) = \sum_{uv \in E(G)} |d_u - d_v|.$$

and the third Zagreb polynomial

$$(2.3) \qquad M_3(G, x) = \sum_{uv \in E(G)} x^{|d_u + d_v|}.$$

The other Zagreb type polynomials are introduced in [6] in 2016

$$(2.4) \qquad M_4(G, x) = \sum_{uv \in E(G)} x^{d_u(d_u + d_v)},$$

$$(2.5) \qquad M_5(G, x) = \sum_{uv \in E(G)} x^{d_v(d_u + d_v)},$$

$$(2.6) \qquad M_{a,b}(G, x) = \sum_{uv \in E(G)} x^{ad_u + bd_v},$$

$$(2.7) \qquad M'_{a,b}(G, x) = \sum_{uv \in E(G)} x^{(d_u + a)(d_v + b)}.$$

Redefined ZIs are defined in [22] by Ranjini et al.

$$(2.8) \qquad ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u d_v},$$

$$(2.9) \qquad ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v},$$

$$(2.10) \qquad ReZG_3(G) = \sum_{uv \in E(G)} (d_u + d_v)(d_u d_v).$$

3. Methodology

There are three kinds of invariants:
    1) Degree-based TIs
    2) Distance-based TIs
    3) Spectral-based TIs
    In this thesis, we focus on degree-based and distance-based graph invariants. To compute degree-based invariants, we divide the edge set of graph networks into classes based on the degree of the end vertices and compute there cardinality. From this edge partition, we compute our desired results.

4. Computational results

Now we give our main results.

4.1. Topological indices of OR_k OTIS swapped networks

Let R_k be k-regular graph on n vertices and OR_k be OTIS swapped network with basis network R_k. Figure 1 depicts an example of OTIS swapped network OR_5. Now we calculate certain degree based topological indices of OTIS swapped network OR_k.
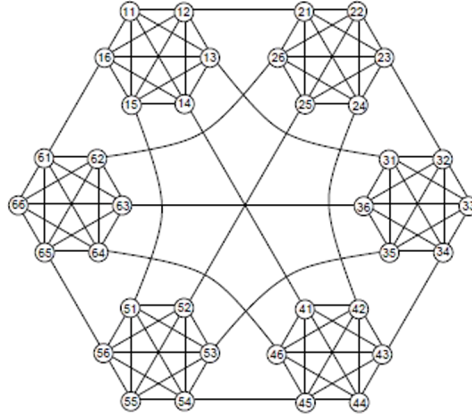

Figure 4.1: OR_5 OTIS swapped network

Theorem 4.2. *Let OR_k be the graph of OTIS swapped network. Then we have*

1. $M_1^-(OR_m, x) = nmx^{2k+1} + \frac{n^2(m+1)-n(1+2m)}{2}x^{2m+2}.$

2. $M_2(OR_m, x) = nmx^{k^2+k} + \frac{n^2(m+1)-n(1+2m)}{2}x^{(m+1)^2}.$

3. $M_3(OR_m, x) = nkx + \frac{n^2(m+1)-n(1+2m)}{2}.$

4. $M_4(OR_m, x) = nmx^{k^2+k} + \frac{n^2(m+1)-n(1+2m)}{2}x^{2(m+1)^2}.$

5. $M_5(OR_m, x) = nkx^{2k^2+3k+1} + \frac{n^2(m+1)-n(1+2m)}{2}x^{2(m+1)^2}.$

6. $M_{a,b}(OR_m, x) = nkx^{am+bm+b} + \frac{n^2(m+1)-n(1+2m)}{2}x^{(a+b)(m+1)}.$

7. $M_{a,b}'(OR_m, x) = nmx^{(m+1)(m+1+b)} + \frac{n^2(m+1)-n(1+2m)}{2}x^{(m+1+a)(m+1+b)}.$

Proof. The edge set of OR_k has following two partitions,

$$E_1(OR_m) = \{e = uv \epsilon E(OR_m) | d_u = k, d_v = k+1\},$$

$$E_2(OR_m) = \{e = uv \epsilon E(OR_m) | d_u = k+1, d_v = k+1\},$$

such that

$$|E_1(OR_m)| = nk,$$

$$|E_2(OR_m)| = \frac{n^2(k+1) - n(1+2k)}{2},$$

1. Using the edge partition and definition 2.1, we have

$$
\begin{aligned}
M_1(OR_m, x) &= \sum_{uv \epsilon E(OR_m)} x^{d_u + d_v} \\
&= \sum_{uv \epsilon E_1(OR_m)(G)} x^{2m+1} + \sum_{uv \epsilon E_2(OR_m)} (OR_m) x^{2m+2} \\
&= |E_1(OR_m)| x^{2m+1} + |E_2(OR_m)| x^{2m+2} \\
&= nm x^{2m+1} + \frac{n^2(m+1) - n(1+2m)}{2} x^{2m+2}.
\end{aligned}
$$

2. Using the edge partition and definition 2.2, we have

$$
\begin{aligned}
M_2(OR_m, x) &= \sum_{uv \epsilon E(OR_m)} x^{d_u . d_v} \\
&= \sum_{uv \epsilon E_1(OR_m)(G)} x^{m^2+m} + \sum_{uv \epsilon M_2(OR_m)} (OR_m) x^{(m+1)^2} \\
&= |E_1(OR_m)| x^{m^2+m} + |E_2(OR_m)| x^{(m+1)^2} \\
&= nm x^{m^2+m} + \frac{n^2(m+1) - n(1+2m)}{2} x^{(m+1)^2}.
\end{aligned}
$$

3. Using the edge partition and definition 2.3, we have

$$
\begin{aligned}
M_3(OR_m, x) &= \sum_{uv \epsilon E(OR_m)} x^{|d_u - d_v|} \\
&= \sum_{uv \epsilon E_1(OR_m)(G)} x + \sum_{uv \epsilon E_2(OR_m)} x^0 \\
&= |E_1(OR_m)| x^1 + |E_2(OR_m)| x^1 \\
&= nm x + \frac{n^2(m+1) - n(1+2m)}{2}.
\end{aligned}
$$

4. Using the edge partition and definition 2.4, we have

$$
\begin{aligned}
M_4(OR_m, x) &= \sum_{uv \epsilon E(OR_m)} x^{d_u(|d_u+d_v|)} \\
&= \sum_{uv \epsilon E_1(OR_m)} x^{m(2m+1)} + \sum_{uv \epsilon E_2(OR_m)} x^{(m+1)(2m+2)} \\
&= |E_1(OR_m)|x^{m^2+m} + |E_2(G)|x^{2(m+1)^2} \\
&= nmx^{m^2+m} + \frac{n^2(m+1) - n(1+2m)}{2}x^{2(m+1)^2}.
\end{aligned}
$$

5. Using the edge partition and definition 2.5, we have

$$
\begin{aligned}
M_5(OR_m, x) &= \sum_{uv \epsilon E(OR_m)} x^{d_v(|d_u+d_v|)} \\
&= \sum_{uv \epsilon E_1(OR_m)} x^{(m+1)(2m+1)} + \sum_{uv \epsilon E_2(OR_m)} x^{(m+1)(2m+2)} \\
&= |E_1(OR_m)|x^{2m^2+3m+1} + |E_2(OR_m)|x^{2(m+1)^2} \\
&= nmx^{2m^2+3m+1} + \frac{n^2(m+1) - n(1+2m)}{2}x^{2(m+1)^2}.
\end{aligned}
$$

6. Using the edge partition and definition 2.6, we have

$$
\begin{aligned}
M_{a,b}(OR_m, x) &= \sum_{uv \epsilon E(OR_m)} x^{(ad_u+bd_v)} \\
&= \sum_{uv \epsilon E_1(OR_m)} x^{am+b(m+1)} + \sum_{uv \epsilon E_2(OR_m)} x^{a(m+1)+b(m+1)} \\
&= |E_1(OR_m)|x^{am+bm+b} + |E_2(OR_m)|x^{(a+b)(m+1)} \\
&= nmx^{am+bm+b} + \frac{n^2(m+1) - n(1+2m)}{2}x^{(a+b)(m+1)}.
\end{aligned}
$$

7. Using the edge partition and definition 2.7, we have

$$
\begin{aligned}
M'_{a,b}(OR_m, x) &= \sum_{uv \epsilon E(OR_m)} x^{(d_u+a)(d_v+b)} \\
&= \sum_{uv \epsilon E_1(OR_m)} x^{(m+a)(m+1+b)} + \sum_{uv \epsilon E_2(OR_m)} x^{(m+1+a)+(m+1+b)} \\
&= |E_1(OR_m)|x^{(m+a)(m+1+b)} + |E_2(OR_m)|x^{(m+1+a)(m+1+b)} \\
&= nmx^{(m+a)+(m+1+b)} + \frac{n^2(m+1) - n(1+2m)}{2}x^{(m+1+a)(k+1+b)}.
\end{aligned}
$$

Theorem 4.3. *Let OR_m be the graph of OTIS swapped network. Then we have*

1. $ReZG_1(OR_m) = n^2$.

2. $ReZG_2(OR_m) = (nm)\frac{m^2+m}{2m+1} - \left(\frac{n^2(m+1)-n(1+2m)}{2}\right)\frac{m+1}{2}$.

3. $ReZG_3(OR_m) = (nm)\left(2m^3 + 3m^2m\right) + n^2(m+1) - n(1+2m)(m+1)^3$.

Proof.

1. Using the edge partition given in Theorem 4.2 and definition 2.8, we have

$$
\begin{aligned}
ReZG_1(OR_m) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{d_u.d_v} \\
&= \sum_{uv\in E_1(OR_m)} \frac{m+m+1}{m(m+1)} + \sum_{uv\in E_2(OR_m)} \frac{m+1+m+1}{(m+1)(m+1)} \\
&= |E_1(OR_m)|\frac{2m+1}{m^2+m} + |E_2(OR_m)|\frac{2}{m+1} \\
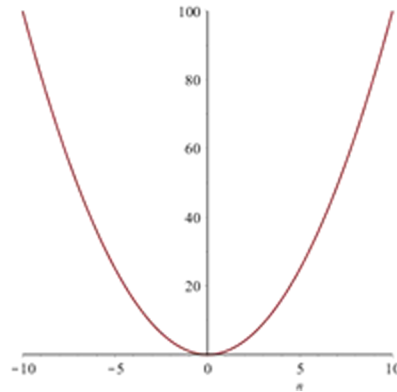&= n^2.
\end{aligned}
$$

Figure 4.2: Plot of first redefined Zagreb index

2. Using the edge partition given in Theorem 4.2 and definition 2.9, we have

$$
\begin{aligned}
ReZG_2(OR_m) &= \sum_{uv \epsilon E(OR_m)} \frac{d_u.d_v}{d_u + d_v} \\
&= \sum_{uv \epsilon E_1(OR_m)} \frac{m(m+1)}{m+m+1} + \sum_{uv \epsilon E_2(OR_m)} \frac{(m+1)(m+1)}{m+1+m+1} \\
&= |E_1(OR_m)| \frac{m^2+m}{2m+1} + |E_2(OR_m)| \frac{m+1}{2} \\
&= nm.\frac{m^2+m}{2m+1} - \left(\frac{n^2(m+1) - n(1+2m)}{2} \right) \frac{m+1}{2}.
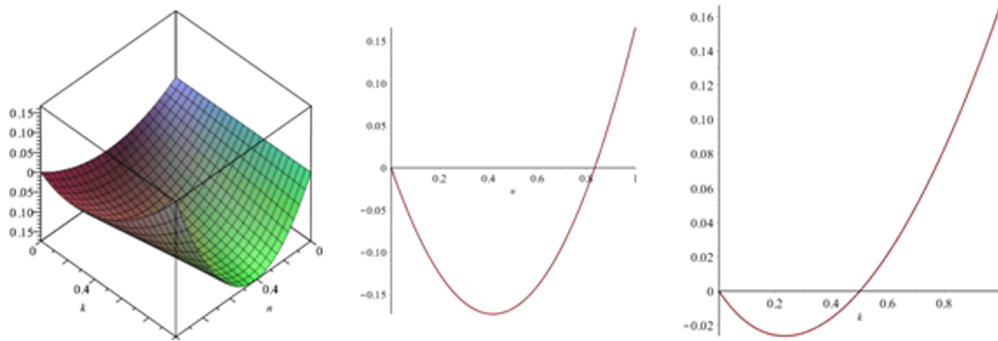\end{aligned}
$$

Figure 4.3: Plot of second redefined Zagreb index (3D (left), for k=1 (middle), for n=1 (right)

3. Using the edge partition given in Theorem 4.2 and definition 2.10, we have

$$
\begin{aligned}
ReZG_3(OR_m) &= \sum_{uv \epsilon E(OR_m)} (d_u.d_v)(d_u + d_v) \\
&= \sum_{uv \epsilon E_1(OR_m)} (m(m+1)(m+m+1) \\
&\quad + \sum_{uv \epsilon E_2(OR_m)} ((m+1).(m+1))(m+1+m+1)
\end{aligned}
$$

$$
\begin{aligned}
&= &|E_1(OR_m)|(2m^3 + 3m^2 m) + 2|E_2(OR_m)|(m+1)^3 \\
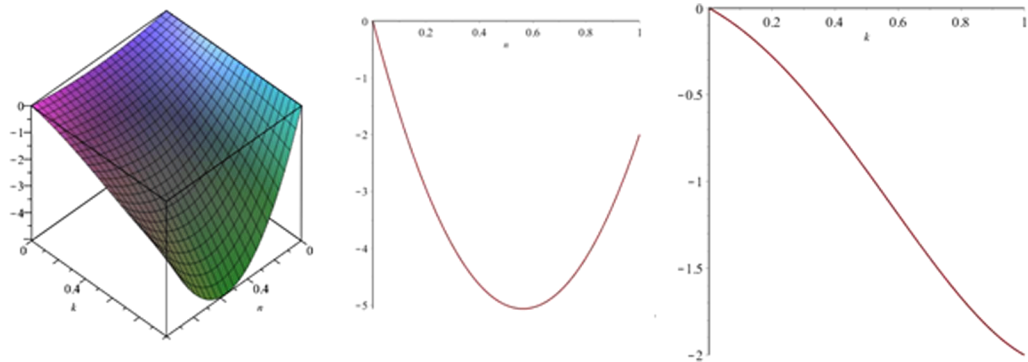&= &nm.(2m^3 + 3m^2 m) + n^2(m+1) - n(1+2m)(m+1)^3.
\end{aligned}
$$

Figure 4.4: Plot of third redefined Zagreb index (3D (left), for k=1 (middle), for n=1 (right)

4.4. Topological induces of OP_n OTIS swapped Networks

Let P_n be path on n vertices and OP_n be OTIS swapped network with basis network P_n. An OTIS swapped network with the basis network OP_6 is shown in Figure 5.
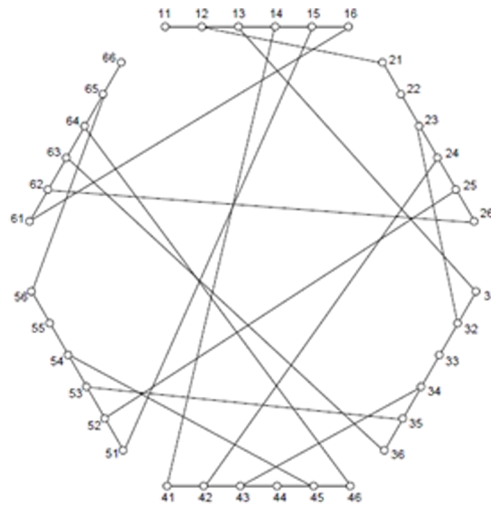

Figure 4.5: OP_6 OTIS swapped network

Theorem 4.5. *Let OP_n be the graph of OTIS swapped network. Then we have*

1. $M_1(OP_n, x) = 5x^4 + (6n - 14)x^5 + \frac{3(n-2)(n-3)}{2}x^6.$

2. $M_2(OP_n, x) = 2x^3 + 3x^4 + (6n - 14)x^6 + \frac{3(n-2)(n-3)}{2}x^9.$

3. $M_3(OP_n, x) = 2x^2 + (6n - 14)x + \frac{9(n-2)(n-3)}{2}x^6.$

4. $M_4(OP_n, x) = 2x^4 + 3x^8 + (6n - 14)x^10 + \frac{3(n-2)(n-3)}{2}x^{18}.$

5. $M_5(OP_n, x) = 3x^8 + (6n - 12)x^12 + \frac{3(n-2)(n-3)}{2}x^{18}.$

6. $M_{a,b}(OP_n, x) = 2x^{a+3b} + 3x^{2a+2b} + (6n-14)x^{2a+3b} + \frac{3(n-2)(n-3)}{2}x^{3a+3b}.$

7. $M'_{a,b}(OP_n, x) = 2x^{(1+a)(3+b)} + 3x^{(2+a)(2+b)} + (6n - 14)x^{(2+a)(3+b)}$
   $+ \frac{3(n-2)(n-3)}{2}x^{(3+a)(3+b)}.$

Proof.   The edge set of OP_n has following two partitions,

$$E_{1(OP_n)} = [e = uv \epsilon E(OP_n)|d_u = 1, d_v = 3],$$

$$E_{2(OP_n)} = [e = uv \epsilon E(OP_n)|d_u = 2, d_v = 2],$$

$$E_{3(OP_n)} = [e = uv \epsilon E(OP_n)|d_u = 2, d_v = 3],$$

$$E_{4(OP_n)} = [e = uv \epsilon E(OP_n)|d_u = 3, d_v = 3],$$

such that

$$|E_1(OP_n)| = 2,$$

$$|E_2(OP_n)| = 3,$$

$$|E_3(OP_n)| = 6n - 14,$$

$$|E_4(OP_n)| = \frac{3(n - 2)(n - 3)}{2},$$

1. Using the edge partition and definition 2.1, we have

$$
\begin{aligned}
M_1(OP_n, x) &= \sum_{uv \epsilon E(OP_n)} x^{d_u + d_v} \\
&= \sum_{uv \epsilon E_1(OP_n)(G)} x^4 + \sum_{uv \epsilon E_2(OP_n)} x^4 + \sum_{uv \epsilon E_3(OP_n)} x^5 + \sum_{uv \epsilon E_4(OP_n)} x^6 \\
&= |E_1(OP_n)|x^4 + |E_2(OP_n)|x^4 + |E_3(OP_n)|x^5 + |E_4(OP_n)|x^6 \\
&= 5x^4 + (6n - 14)x^5 + \frac{3(n - 2)(n - 3)}{2}x^6.
\end{aligned}
$$

2. Using the edge partition and definition 2.2, we have

$$
\begin{aligned}
M_2(OP_n, x) &= \sum_{uv \in E(OP_n)} x^{d_u.d_v} \\
&= \sum_{uv \in E_1(OP_n)(OP_n)} x^3 + \sum_{uv \in E_2(OP_n)} x^4 + \sum_{uv \in E_3(OP_n)} x^6 + \sum_{uv \in E_4(OP_n)} x^9 \\
&= |E_1(OP_n)|x^3 + |E_2(OP_n)|x^4 + |E_3(OP_n)|x^6 + |E_4(OP_n)|x^9 \\
&= 2x^3 + 3x^4 + (6n-14)x^6 + \frac{3(n-2)(n-3)}{2}x^9.
\end{aligned}
$$

3. Using the edge partition and definition 2.3, we have

$$
\begin{aligned}
M_3(OP_n, x) &= \sum_{uv \in E(OP_n)} x^{|d_u-d_v|} \\
&= \sum_{uv \in E_1(OP_n)} x^2 + \sum_{uv \in E_2(OP_n)} x^0 + \sum_{uv \in E_3(OP_n)} x^1 + \sum_{uv \in E_4(OP_n)} x^0 \\
&= |E_1(OP_n)|x^2 + |E_2(OP_n)| + |E_3(OP_n)|x + |E_4(OP_n)| \\
&= 2x^2 + (6n-14)x + \frac{9(n-2)(n-3)}{2}.
\end{aligned}
$$

4. Using the edge partition and definition 2.4, we have

$$
\begin{aligned}
M_4(OP_n, x) &= \sum_{uv \in E(OP_n)} x^{d_u(|d_u+d_v|)} \\
&= \sum_{uv \in E_1(OP_n)} x^4 + \sum_{uv \in E_2(OP_n)} x^8 + \sum_{uv \in E_3(OP_n)} x^{10} + \sum_{uv \in E_4(OP_n)} x^{18} \\
&= |E_1(OP_n)|x^4 + |E_2(OP_n)|x^8 + |E_3(OP_n)|x^{10} + |E_4(OP_n)|x^{18} \\
&= 2x^4 + 3x^8 + (6n-14)x^{10} + \frac{3(n-2)(n-3)}{2}x^{18}.
\end{aligned}
$$

5. Using the edge partition and definition 2.5, we have

$$
\begin{aligned}
M_5(OP_n, x) &= \sum_{uv \in E(OP_n)} x^{d_v(|d_u+d_v|)} \\
&= \sum_{uv \in E_1(OP_n)} x^{12} + \sum_{uv \in E_2(OP_n)} x^8 + \sum_{uv \in E_3(OP_n)} x^{15} + \sum_{uv \in E_4(OP_n)} x^{18} \\
&= |E_1(OP_n)|x^{12} + |E_2(OP_n)|x^8 + |E_3(OP_n)|x^{15} + |E_4(OP_n)|x^{18} \\
&= 2x^{12} + 3x^8 + (6n-14)x^{15} + \frac{3(n-2)(n-3)}{2}x^{18}.
\end{aligned}
$$

6. Using the edge partition and definition 2.6, we have

$$
\begin{aligned}
M_{(a,b)}(OP_n, x) &= \sum_{uv \in E(OP_n)} x^{(ad_u + bd_v)} \\
&= \sum_{uv \in E_1(OP_n)} x^{a+3b} + \sum_{uv \in E_2(OP_n)} x^{2a+2b} \\
&\quad + \sum_{uv \in E_3(OP_n)} x^{2a+3b} + \sum_{uv \in E_4(OP_n)} x^{3a+3b} \\
&= |E_1(OP_n)| x^{a+3b} + |E_2(OP_n)| x^{2a+2b} \\
&\quad + |E_3(OP_n)| x^{2a+3b} + |E_4(OP_n)| x^{3a+3b} \\
&= 2x^{a+3b} + 3x^{2a+2b} + (6n-14)x^{2a+3b} + \frac{3(n-2)(n-3)}{2} x^{3a+3b}.
\end{aligned}
$$

7. Using the edge partition and definition 2.7, we have

$$
\begin{aligned}
M'_{(a,b)}(OP_n, x) &= \sum_{uv \in E(OP_n)} x^{(d_u + a)(d_v + b)} \\
&= \sum_{uv \in E_1(OP_n)} x^{(1+a)(3+b)} + \sum_{uv \in E_2(OP_n)} x^{(2+a)(2+b)} \\
&\quad + \sum_{uv \in E_3(OP_n)} x^{(2+a)(3+b)} + \sum_{uv \in E_4(OP_n)} x^{(3+a)(3+b)} \\
&= |E_1(OP_n)| x^{(1+a)(3+b)} + |E_2(OP_n)| x^{(2+a)(2+b)} \\
&\quad + |E_3(OP_n)| x^{(2+a)(3+b)} + |E_4(OP_n)| x^{(3+a)(3+b)} \\
&= 2x^{(1+a)(3+b)} + 3x^{(2+a)(2+b)} + (6n-14)x^{(2+a)(3+b)} \\
&\quad + \frac{3(n-2)(n-3)}{2} x^{(3+a)(3+b)}.
\end{aligned}
$$

Theorem 4.6. *Let OP_n be the graph of OTIS swapped network. Then we have*

1. $ReZG_1(OP_n) = n^2.$

2. $ReZG_2(OP_n) = \frac{6}{5} - \frac{81}{20}n + \frac{9}{4}n^2.$

3. $ReZG_3(OP_n) = 78n^2 - 210n + 120.$

Proof.

1. Using the edge partition given in Theorem 4.5 and definition 2.8, we have

$$
\begin{aligned}
ReZG_1(OP_n) &= \sum_{uv\epsilon E(OP_n)} \frac{d_u + d_v}{d_u.d_v}\\
&= \sum_{uv\epsilon E_1(OP_n)} \frac{4}{3} + \sum_{uv\epsilon E_2(OP_n)} \frac{4}{4} + \sum_{uv\epsilon E_3(OP_n)} \frac{5}{6} + \sum_{uv\epsilon E_4(OP_n)} \frac{6}{9}\\
&= |E_1(OP_n)|\frac{4}{3} + |E_2(OP_n)| + |E_3(OP_n)|\frac{5}{6} + |E_4(OP_n)|\frac{2}{3}\\
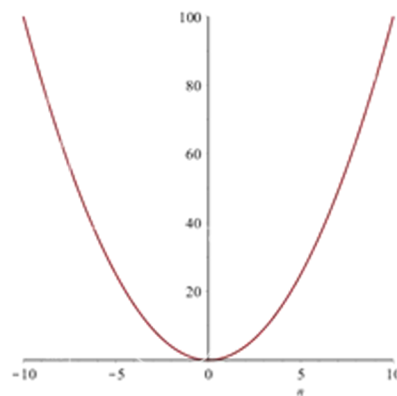&= n^2.
\end{aligned}
$$

Figure 4.6: Plot of first redefined Zagreb index

2. Using the edge partition given in Theorem 4.5 and definition 2.9, we have

$$
\begin{aligned}
ReZG_2(OP_n) &= \sum_{uv\epsilon E(OP_n)} \frac{d_u.d_v}{d_u + d_v}\\
&= \sum_{uv\epsilon E_1(OP_n)} \frac{3}{4} + \sum_{uv\epsilon E_2(OP_n)} \frac{4}{4} + \sum_{uv\epsilon E_3(OP_n)} \frac{6}{5} + \sum_{uv\epsilon E_4(OP_n)} \frac{9}{6}\\
&= |E_1(OP_n)|\frac{3}{4} + |E_2(OP_n)| + |E_3(OP_n)|\frac{6}{5} + |E_4(OP_n)|\frac{3}{2}\\
&= \frac{6}{5} - \frac{81}{20}n + \frac{9}{4}n^2.
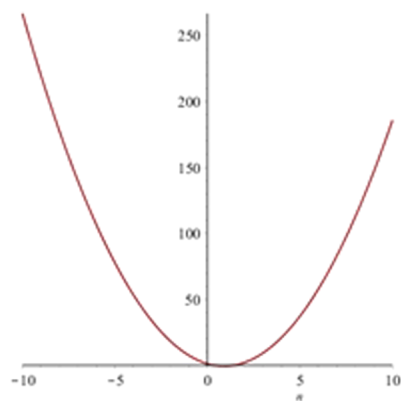\end{aligned}
$$

Figure 4.7: Plot of second redefined Zagreb index

3. Using the edge partition given in Theorem 4.5 and definition 2.10, we have

$$
\begin{aligned}
ReZG_3(OP_n) &= \sum_{uv \epsilon E(OP_n)} (d_u . d_v)(d_u + d_v) \\
&= \sum_{uv \epsilon E_1(OP_n)} 12 + \sum_{uv \epsilon E_2(OP_n)} 16 + \sum_{uv \epsilon E_3(OP_n)} 30 + \sum_{uv \epsilon E_4(OP_n)} 54 \\
&= |E_1(OP_n)|12 + |E_2(OP_n)|16 + |E_3(OP_n)|30 + |E_4(OP_n)|54 \\
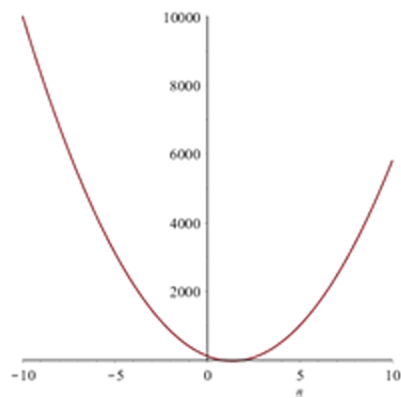&= 78n^2 - 210n + 120.
\end{aligned}
$$

□

Figure 4.8: Plot of third redefined Zagreb index

Conclusion

It is important to calculate topological indices of networks, because it is proved fact that topological indices help to predict many properties without going to the wet lab. There are more than 148 topological indices but none of them can completely describe all properties of a chemical compound. Therefore there is always room to define and study new topological indices. Redefined Zagreb indices are one step in this direction and are very close to Zagreb indices. Zagreb indices are very well studied by chemists and mathematician due to its huge applications in chemistry. It is an interesting problem for researchers to study chemical properties and bonds of redefined Zagreb indices.

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