Topological Indices of Graph Associated to Some Finite Groups

NOR HANIZA SARMIN

Department of Mathematical Sciences, Faculty of Science,
Universiti Teknologi Malaysia, Johor Bahru, Malaysia

6th Biennial International Group Theory Conference

4 March 2021

Presentation Outline

- Introduction
- Literature Review on Zagreb Index
- Motivation of Research
- Preliminaries
- Results : The Zagreb Index of the Non-commuting Graph Associated to Dihedral Groups, D_{2n}
- Results : The Zagreb Index of the Non-commuting Graph Associated to the $G \times D_{2n}$
- Conclusion
- Suggestion for Future Research
- Acknowledgement
- References

Topological Indices

Topological Indices

- A topological index is a numerical value that can be calculated from 2D graph which represents a molecule.
- The information contained in a graph is converted into numerical characteristics in order to link the molecular topology to any molecular property.
- Chemist uses topological indices because it is simpler since it only takes account the degree of vertices and the distance between them.
- Many types of topological indices have been developed by many researchers. For example, Wiener index, Zagreb index, Szeged index, and Harary index.

Wiener Index

- In 1947, Wiener has introduced the Wiener index and computed the Wiener index of some types of alkanes.
- Its formula has been modified by Hosoya(1971) since Wiener does not take account the ring molecule.

Definition 1

Let Γ be a connected graph with a vertex set $V(\Gamma) = \{1, 2, \ldots, m\}$. The Wiener index of Γ, denoted by $W(\Gamma)$, is defined as half of the sum of the distances between every pair of vertices of Γ, written as

$$W(\Gamma) = \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} d(i, j),$$

where $d(i, j)$ is the distance between vertices i and j.

Example 1

Let Γ be a simple connected graph which has vertices, $V(\Gamma) = \{1, 2, 3, 4\}$ and edges $E(\Gamma) = \{e_1, e_2, e_3, e_4, e_5\}$ as shown in Figure 1.

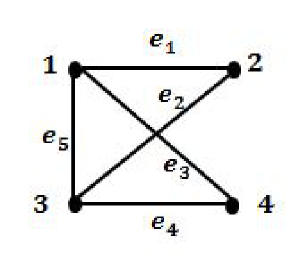


Figure 1: A simple connected graph

Example 1 (Cont.)

Then, the Wiener index of Γ,

$$
\begin{aligned}
W(\Gamma) &= \frac{1}{2}\sum_{i=1}^{4}\sum_{j=1}^{4} d(i,j) \\
&= \frac{1}{2}\sum_{i=1}^{4}[d(i,1)+d(i,2)+d(i,3)+d(i,4))] \\
&= \frac{1}{2}[(d(1,1)+d(1,2)+d(1,3)+d(1,4))+(d(2,1)+d(2,2)+d(2,3)+d(2,4)) \\
&\quad +(d(3,1)+d(3,2)+d(3,3)+d(3,4))+(d(4,1)+d(4,2)+d(4,3)+d(4,4)) \\
&= \frac{1}{2}[(0+1+1+1)+(1+0+1+2)+(1+1+0+1)+(1+2+1+0) \\
&= 7.
\end{aligned}
$$

- The Zagreb index has been developed by Gutman and Trinajsti$\acute{c}$(1972) where the calculation is based on the degree of the vertices in a graph.

Definition 2

Let Γ be a connected graph with a vertex set $V(\Gamma) = \{1, 2, \ldots, n\}$. The first Zagreb index, $M_1(\Gamma)$, is defined as the sum of square of the degree of each vertex in Γ while the second Zagreb index, $M_2(\Gamma)$ is defined as the sum of the product of the degree of two vertices for each edge, respectively, written as

$$M_1(\Gamma) = \sum_{v \in v(\Gamma)} (\deg(v))^2$$

and

$$M_2(\Gamma) = \sum_{\{u,v\} \in E(\Gamma)} \deg(u)\deg(v).$$

Example 2

Let Γ be a simple connected graph which has four vertices and five edges as shown in Figure 1. Then, the first Zagreb index of Γ,

$$
\begin{aligned}
M_1(\Gamma) &= \sum_{i=1}^{4} (\deg(i))^2 \\
&= (\deg(1))^2 + (\deg(2))^2 + (\deg(3))^2 + (\deg(4))^2 \\
&= 3^2 + 2^2 + 3^2 + 2^2 \\
&= 26,
\end{aligned}
$$

and the second Zagreb index of Γ,

$$
\begin{aligned}
M_2(\Gamma) &= \sum_{\{u,v\} \in E(\Gamma)} \deg(u)\deg(v) \\
&= \deg(1)\deg(2) + \deg(2)\deg(3) + \deg(1)\deg(4) + \deg(3)\deg(4) + \\
&\quad \deg(1)\deg(3) \\
&= (3)(2) + (2)(3) + (3)(2) + (3)(2) + (3)(3) \\
&= 33.
\end{aligned}
$$

Szeged Index

- Gutman and Dobrynin(1998) defined the Szeged index, as stated in the following.

Definition 3

Let Γ be a connected graph with vertex set $V(\Gamma) = \{1, 2, \ldots, n\}$. The Szeged index, $Sz(\Gamma)$ is given as in the following :

$$Sz(\Gamma) = \sum_{e \in E(\Gamma)} n_1(e|\Gamma) n_2(e|\Gamma),$$

where the summation embraces all edges of Γ,

$$n_1(e|\Gamma) = |\{v | v \in V(\Gamma), d(v, x|\Gamma) < d(v, y|\Gamma)\}|$$

and

$$n_2(e|\Gamma) = |\{v | v \in V(\Gamma), d(v, y|\Gamma) < d(v, x|\Gamma)\}|$$

which means that $n_1(e|\Gamma)$ counts the vertices of Γ lying closer to one endpoint x of the edge e than to its other endpoint y while $n_2(e|\Gamma)$ is vice versa.

Example 3

Let Γ be a simple connected graph which has four vertices and five edges as shown in Figure 1. Note that $N_1(e_i|\Gamma)$ is the vertices of Γ lying closer to one endpoint x of the edge e_i than to its other endpoint y while $N_2(e_i|\Gamma)$ is vice versa. First, $N_1(e_i|\Gamma)$ and $N_2(e_i|\Gamma)$ are calculated for all i.

For $e_1 = \{1, 2\}$,

$$\begin{aligned} N_1(e_1|\Gamma) &= \{x \in V(\Gamma) : d(x,1) < d(x,2)\}, \quad & n_1(e_1|\Gamma) = 2, \\ &= \{1, 4\}, \\ N_2(e_1|\Gamma) &= \{y \in V(\Gamma) : d(y,1) > d(y,2)\}, \quad & n_2(e_1|\Gamma) = 1. \\ &= \{2\}, \end{aligned}$$

For $e_2 = \{2, 3\}$,

$$\begin{aligned} N_1(e_2|\Gamma) &= \{x \in V(\Gamma) : d(x,2) < d(x,3)\}, \quad & n_1(e_2|\Gamma) = 1, \\ &= \{2\}, \\ N_2(e_2|\Gamma) &= \{y \in V(\Gamma) : d(y,2) > d(y,3)\}, \quad & n_2(e_2|\Gamma) = 2. \\ &= \{3, 4\}, \end{aligned}$$

Example 3(Cont.)

For $e_3 = \{1,4\}$,

$$\begin{aligned} N_1(e_3|\Gamma) &= \{x \in V(\Gamma) : d(x,1) < d(x,4)\}, \quad n_1(e_3|\Gamma) = 2, \\ &= \{1,2\}, \\ N_2(e_3|\Gamma) &= \{y \in V(\Gamma) : d(y,1) > d(y,4)\}, \quad n_2(e_3|\Gamma) = 1. \\ &= \{4\}, \end{aligned}$$

For $e_4 = \{3,4\}$,

$$\begin{aligned} N_1(e_4|\Gamma) &= \{x \in V(\Gamma) : d(x,3) < d(x,4)\}, \quad n_1(e_4|\Gamma) = 2, \\ &= \{2,3\}, \\ N_2(e_4|\Gamma) &= \{y \in V(\Gamma) : d(y,3) > d(y,4)\}, \quad n_2(e_4|\Gamma) = 1. \\ &= \{4\}, \end{aligned}$$

Example 3(Cont.)

For $e_5 = \{1, 3\}$,

$$\begin{aligned} N_1(e_5|\Gamma) &= \{x \in V(\Gamma) : d(x,1) < d(x,3)\}, \quad n_1(e_5|\Gamma) = 1, \\ &= \{1\}, \\ N_2(e_5|\Gamma) &= \{y \in V(\Gamma) : d(y,1) > d(y,3)\}, \quad n_2(e_5|\Gamma) = 1. \\ &= \{3\}, \end{aligned}$$

Hence,

$$\begin{aligned} Sz(\Gamma) &= \sum_{i=1}^{5} n_1(e_i|\Gamma)n_2(e_i|\Gamma) \\ &= n_1(e_1|\Gamma)n_2(e_1|\Gamma) + n_1(e_2|\Gamma)n_2(e_2|\Gamma) + n_1(e_3|\Gamma)n_2(e_3|\Gamma) + \\ &\quad n_1(e_4|\Gamma)n_2(e_4|\Gamma) + n_1(e_5|\Gamma)n_2(e_5|\Gamma) \\ &= (2)(1) + (1)(2) + (2)(1) + (2)(1) + (1)(1) \\ &= 9. \end{aligned}$$

Harary Index

- Plavšić *et al.*(1993) introduced the Harary index which involves the reciprocal distance matrix.

Definition 4

Let Γ be a connected graph with vertex set $V = \{1, 2, \ldots, n\}$. The Harary index is defined as a half-sum of the elements in the reciprocal distance matrix, $D^r = D^r(\Gamma)$, written as

$$H = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} D^r(i,j),$$

where

$$D^r(i,j) = \begin{cases} \frac{1}{d(i,j)} & \text{if} \quad i \neq j, \\ 0 & \text{if} \quad i = j, \end{cases}$$

and $d(i,j)$ is the shortest distance between vertex i and j.

Example 4

Let Γ be a simple connected graph which has five vertices and six edges as shown in Figure 1. The Harary index of Γ,

$$H(\Gamma) = \frac{1}{2}\sum_{i=1}^{4}\sum_{j=1}^{4} D^r(i,j)$$

$$= \frac{1}{2}[(D^r(1,1) + D^r(1,2) + D^r(1,3) + D^r(1,4))+$$
$$(D^r(2,1) + D^r(2,2) + D^r(2,3) + D^r(2,4))+$$
$$(D^r(3,1) + D^r(3,2) + D^r(3,3) + D^r(3,4))+$$
$$(D^r(4,1) + D^r(4,2) + D^r(4,3) + D^r(4,4))]$$

$$= \frac{1}{2}\Bigg[\left(0 + \frac{1}{d(1,2)} + \frac{1}{d(1,3)} + \frac{1}{d(1,4)}\right) + \left(\frac{1}{d(2,1)} + 0 + \frac{1}{d(2,3)} + \frac{1}{d(2,4)}\right) +$$
$$\left(\frac{1}{d(3,1)} + \frac{1}{d(3,2)} + 0 + \frac{1}{d(3,4)}\right) + \left(\frac{1}{d(4,1)} + \frac{1}{d(4,2)} + \frac{1}{d(4,3)} + 0\right)\Bigg]$$

$$= \frac{1}{2}\Bigg[\left(0 + \frac{1}{1} + \frac{1}{1} + \frac{1}{1}\right) + \left(\frac{1}{1} + 0 + \frac{1}{1} + \frac{1}{2}\right) +$$
$$\left(\frac{1}{1} + \frac{1}{1} + 0 + \frac{1}{1}\right) + \left(\frac{1}{1} + \frac{1}{2} + \frac{1}{1} + 0\right)\Bigg] = \frac{11}{2}.$$

Dihedral groups

The dihedral group is a group that consists a set of elements which involves rotations and reflections and is denoted as D_{2n} with order of $2n$. The group presentation of the dihedral groups is as follows (1996) :

$$D_{2n} = \langle a, b | a^n = b^2 = 1, bab = a^{-1} \rangle,$$

where $n \in \mathbb{N}$.

- Through out the presentation, the non-abelian dihedral groups are considered in which $n \geq 3$.

Non-commuting Graph (Abdollahi *et al.*, 2006)

Let G be a finite group. The non-commuting graph of G, denoted as Γ_G^{NC}, is the graph with vertex set $G - Z(G)$ and two distinct vertices x and y are joined by an edge whenever $xy \neq yx$.

Gutman and Das (2004)

Let Γ be a graph with n vertices and m edges, where the average value of the vertex degree is $\frac{2m}{n}$. The average value of the vertex degree is denoted as p. Then, the first Zagreb index is bounded from both below and above by expressions depending solely on the parameters n and m:

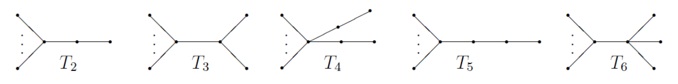
$$2(2p+1)m - p(p+1)n \leq M_1 \leq m\left(\frac{2m}{n-1} + n - 2\right).$$

Muhuo and Bolian (2010)

- Li and Zheng (2005) introduced the concept of first general Zagreb index $M_1^{\alpha}(\Gamma)$:

$$M_1^{\alpha}(\Gamma) = \sum_{v \in V} d(v)^{\alpha}.$$

Let $T_1 = K_{1,n-1}, T_2, T_3, \ldots, T_6$ be the trees on n vertices as shown in the following figure.



Suppose $T \in \mathcal{T}_n - \{T_1, T_2, \ldots, T_6\}$.

1. If $\alpha < 0$ or $\alpha > 1$, then

$$M_1^{\alpha}(T_1) > M_1^{\alpha}(T_2) > M_1^{\alpha}(T_3) > max\{M_1^{\alpha}(T_4), M_1^{\alpha}(T_6)\} > M_1^{\alpha}(T)$$

2. If $0 < \alpha < 1$, then

$$M_1^{\alpha}(T_1) < M_1^{\alpha}(T_2) < M_1^{\alpha}(T_3) < min\{M_1^{\alpha}(T_4), M_1^{\alpha}(T_6)\} < M_1^{\alpha}(T)$$

Das *et al.* (2015)

Let Γ be a graph of order n, m edges with maximum degree $\triangle$. Then

$$M_1(\Gamma) \leq (n+1)m - \triangle(n-\triangle) + \frac{2(m-\triangle)^2}{n-2}.$$

Let Γ be a graph on n vertices with m edges, maximum degree $\triangle$, second maximum degree $\triangle_2$, and maximum degree δ. Then,

$$M_2(\Gamma) \geq 2m^2 - (n-1)m\triangle + \frac{1}{2}(\triangle - 1)\left[\triangle^2 + \frac{(2m-\triangle)^2}{n-1} + \frac{2(n-2)}{(n-1)^2}(\triangle_2 - \delta)^2\right]$$

with equality if and only if Γ is a regular graph.

Motivation of Research

- Many types of topological indices have been developed and widely used by chemists to find the physico-chemical properties of the molecules.
- Some types of topological indices have been generalized for the non-commuting graph associated to a finite group, in terms of the properties of the groups and graphs.
- A graph of larger number of vertices and edges lead to difficulties in computing its topological indices. Same goes to the larger and compact molecules.
- Therefore, the general formulas of the topological indices (Zagreb index - in this presentation) of the non-commuting graph of some groups are determined to simplify the computation.
- The results can help chemists to save their time and cost in determining the physico chemical properties of the molecules.

Preliminaries

Proposition 1 (Samaila *et al.*, 2013) Center

Let G be a dihedral group of order $2n$, D_{2n} where $n \geq 3, n \in \mathbb{N}$ and $Z(G)$ is the center of G. Then,

$$Z(G) = \begin{cases} \{1\}, & \text{if} \quad n \text{ is odd}, \\ \{1, a^{\frac{n}{2}}\}, & \text{if} \quad n \text{ is even}. \end{cases}$$

Proposition 2 (Samaila *et al.*, 2013) Conjugacy classes

Let G be a dihedral group, D_{2n} of order $2n$. Then, the conjugacy classes of G are as follows :

- For odd n :
  $\{1\}, \{a, a^{-1}\}, \{a^2, a^{-2}\}, \ldots, \{a^{\frac{n-1}{2}}, a^{-\frac{n-1}{2}}\}$ and $\{a^i b : 0 \leq i \leq n-1\}$.
- For even n :
  $\{1\}, \{a^{\frac{n}{2}}\}, \{a, a^{-1}\}, \{a^2, a^{-2}\}, \ldots, \{a^{\frac{n-2}{2}}, a^{-\frac{n-2}{2}}\}, \{a^{2i} b : 0 \leq i \leq \frac{n-2}{2}\}$ and
  $\{a^{2i+1} b : 0 \leq i \leq \frac{n-2}{2}\}$.

Lemma 1

Let G be a dihedral group, D_{2n} of order $2n$ and the number of the conjugacy classes of G is denoted by $k(G)$. Then,

$$k(G) = \begin{cases} \frac{n+3}{2}, & \text{if} \quad n \text{ is odd,} \\ \frac{n+6}{2}, & \text{if} \quad n \text{ is even.} \end{cases}$$

Proof

From Proposition 2, for n is odd, there are $\frac{n-1}{2}$ conjugacy classes for a^i, where $i = \{1, 2, \ldots, \frac{n-1}{2}\}$. There is a conjugacy class of an identity and a conjugacy class of $a^i b$, where $i = \{1, 2, \ldots, n-1\}$. Thus, the number of conjugacy classes of D_{2n} when n is odd:

$$k(D_{2n}) = \frac{n-1}{2} + 1 + 1 = \frac{n+3}{2}.$$

Proof (Cont.)

For n is even, there are $\frac{n-2}{2}$ conjugacy classes for a^i, where $i = \{1, 2, \ldots, \frac{n-2}{2}\}$. There is a conjugacy class of an identity elements, a conjugacy class of $a^{\frac{n}{2}}$, a conjugacy class of a^{2ib}, where $0 \leq i \leq \frac{n-2}{2}$, and a conjugacy class of a^{2i+1}, where $0 \leq i \leq \frac{n-2}{2}$. Thus, the number of conjugacy classes of D_{2n} when n is even:

$$k(D_{2n}) = \frac{n-2}{2} + 1 + 1 + 1 + 1 = \frac{n+6}{2}.$$

Therefore, the number of conjugacy classes of G,

$$k(G) = \begin{cases} \frac{n+3}{2}, & \text{if} \quad n \text{ is odd,} \\ \frac{n+6}{2}, & \text{if} \quad n \text{ is even.} \end{cases}$$

■

Proposition 3 (Mirzargar and Ashrafi, 2012)

Let G be a finite group and Γ_G^{NC} be the non-commuting graph of G. Then, the first Zagreb index of the non-commuting graph of G,

$$M_1(\Gamma_G^{\mathrm{NC}}) = |G|^2(|G| + |Z(G)| - 2k(G)) - \sum_{x \in G - Z(G)} |C_G(x)|^2.$$

Proposition 4 (Mirzargar and Ashrafi, 2012)

Let G be a finite group and Γ_G^{NC} be the non-commuting graph. Then, the second Zagreb index of the non-commuting graph of G,

$$M_2(\Gamma_G^{\mathrm{NC}}) = -|G|^2|E(\Gamma_G^{\mathrm{NC}})| + |G|M_1(\Gamma_G^{\mathrm{NC}}) + \sum_{x,y \in E(\Gamma_G^{\mathrm{NC}})} |C_G(x)||C_G(y)|.$$

Proposition 5 (Abdollahi *et al.*, 2006)

Let G be a finite group and Γ_G^{NC} be the non-commuting graph of G. Then,

$$2|E(\Gamma_G^{\mathrm{NC}})| = |G|^2 - k(G)|G|,$$

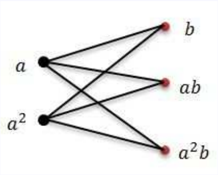
where $k(G)$ is the number of conjugacy classes of G.

Proposition 6 (Mahmoud, 2018)

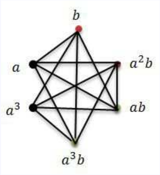
Let G be the dihedral groups of order $2n$ where $n \geq 3, n \in \mathbb{N}$ and let Γ_G^{NC} be the non-commuting graph of G. Then,

$$\Gamma_G^{NC} = \begin{cases} K_{\underbrace{1,1,\ldots,1}_{\text{n times}},n-1}, & \text{if} \quad n \text{ is odd,} \\ K_{\underbrace{2,2,\ldots,2}_{\frac{n}{2} \text{ times}},n-2}, & \text{if} \quad n \text{ is even.} \end{cases}$$

If $n = 3$, the non-commuting graph of D_6 is $K_{1,1,1,2}$. If $n = 4$, the non-commuting graph of D_8 is $K_{2,2,2}$.



$K_{1,1,1,2}$



$K_{2,2,2}$

The Zagreb Index of the Non-commuting Graph of Dihedral Group

The First Zagreb Index of the Non-commuting Graph of Dihedral Group

Lemma 2

Let G be the dihedral group, D_{2n} where $n \geq 3$ and $C_G(x)$ is the centralizer of an element $x \in G$. Then,

$$\sum_{x \in G - Z(G)} |C_G(x)|^2 = \begin{cases} n^3 - n^2 + 4n, & \text{if} \quad n \text{ is odd,} \\ n^3 - 2n^2 + 16n, & \text{if} \quad n \text{ is even.} \end{cases}$$

Proof.

For n is odd, there are n elements that have $|C_G(x)| = 2$ since $a^i b^j$ does not commute with $b^j a^i$ where $i = 0, 1, \ldots, n-1$ and $j = 0, 1$. There are also $n-1$ elements which have $|C_G(x)| = n$ since all a^i commute each other where $i = 0, 1, \ldots, n-1$ and $|Z(G)| = 1$. Then,

$$\sum_{x \in G - Z(G)} |C_G(x)|^2 = n^3 - n^2 + 4n.$$

For n is even, there are n elements that have $|C_G(x)| = 4$ since it has two central elements which lead to having four elements that commute with x. There are $n-2$ elements that have $|C_G(x)| = n$ since all a^i commute among each other where $i = 0, 1, \ldots, n-1$ and $|Z(G)| = 2$. Then,

$$\sum_{x \in G - Z(G)} |C_G(x)|^2 = n^3 - 2n^2 + 16n.$$

Therefore,

$$\sum_{x \in G - Z(G)} |C_G(x)|^2 = \begin{cases} n^3 - n^2 + 4n, & \text{if} \quad n \text{ is odd}, \\ n^3 - 2n^2 + 16n, & \text{if} \quad n \text{ is even}. \end{cases}$$

Theorem 1

Let G be the dihedral groups, D_{2n} where $n \geq 3, n \in \mathbb{N}$. Then, the first Zagreb index of the non-commuting graph of G is stated as follows :

$$M_1(\Gamma_G^{NC}) = \begin{cases} n(5n-4)(n-1), & \text{if} \quad n \text{ is odd}, \\ n(5n-8)(n-2), & \text{if} \quad n \text{ is even}. \end{cases}$$

Proof

By Proposition 1, Proposition 2, Lemma 1 and Lemma 2, the first Zagreb index of the non-commuting graph for D_{2n} is as follows :
For n is odd,

$$
\begin{aligned}
M_1(\Gamma_G^{\mathrm{NC}}) &= |G|^2\left(|G| + |Z(G)| - 2k(G)\right) - \sum_{x \in G - Z(G)} |C_G(x)|^2 \\
&= 4n^2\left[2n + 1 - 2\left(\frac{n+3}{2}\right)\right] - 2^2 n + n^2(n-1) \\
&= n\left(5n-4\right)\left(n-1\right).
\end{aligned}
$$

Proof (Cont.)

For n is even,

$$M_1(\Gamma_G^{\mathrm{NC}}) = |G|^2\left(|G| + |Z(G)| - 2k(G)\right) - \sum_{x\in G-Z(G)} |C_G(x)|^2$$
$$= 4n^2\left[2n+1-2\left(\frac{n+6}{2}\right)\right] - 4^2n + n^2(n-2)$$
$$= n\left(5n-8\right)\left(n-2\right).$$

Therefore, the first Zagreb index of the non-commuting graph for D_{2n}, where $n \geq 3$,

$$M_1(\Gamma_G^{\mathrm{NC}}) = \begin{cases} n(5n-4)(n-1), & \text{if} \quad n \text{ is odd,} \\ n(5n-8)(n-2), & \text{if} \quad n \text{ is even.} \end{cases}$$

■

The Second Zagreb Index of the Non-commuting Graph of Dihedral Group

Lemma 3

Let G be the dihedral group, D_{2n} where $n \geq 3$ and $C_G(x)$ is the centralizer of an element $x \in G$. Then,

$$\sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)| = \begin{cases} 2n(n^2-1), & \text{if} \quad n \, \text{is odd}, \\ 4n(n^2-4), & \text{if} \quad n \, \text{is even}. \end{cases}$$

Proof

By definition of the non-commuting graph, the vertices in the non-commuting graph of the dihedral group are connected by an edge if and only if $a^i b^j \neq b^j a^i$ where $i = 0, 1, \ldots, n-1$ and $j = 0, 1$.
For n is odd, two vertices x and y which have $|C_G(x)| = 2$ and $|C_G(y)| = n$ where there are $n(n-1)$ edges connecting them while another $|E(\Gamma_G)| - n(n-2)$ edges connect two distinct vertices x and y which have $|C_G(x)| = |C_G(y)| = 2$. Then,

$$\begin{aligned}
\sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)| &= n(n-1)(2)(n) + \left[|E(\Gamma_G)| - n(n-1)\right](2)(2) \\
&= n(n-1)(2)(n) + \left[\frac{|G|^2 - k(G)|G|}{2} - n(n-1)\right](2)(2) \\
&= n(n-1)(2)(n) + \left[4n^2 - \frac{n+3}{2}(2n) - 2n(n-1)\right](2) \\
&= 2n(n^2-1).
\end{aligned}$$

For n is even, there are $n(n-2)$ edges which connect two vertices x and y that have $|C_G(x)| = 4$ and $|C_G(y)| = n$ while the rest of edges connect two distinct vertices that have $|C_G(x)| = |C_G(y)| = 4$. Then,

Theorem 2

Let G be the dihedral groups, D_{2n} where $n \geq 3, n \in \mathbb{N}$. Then, the second Zagreb index of the non-commuting graph of G is stated as follows :

$$M_2(\Gamma_G^{\mathrm{NC}}) = \begin{cases} 2n(2n-1)(n-1)^2, & \text{if} \quad n \, \text{is odd}, \\ 4n(n-1)(n-2)^2, & \text{if} \quad n \, \text{is even}. \end{cases}$$

Proof

By Proposition 1, Proposition 4, Proposition 5, Lemma 1 and Lemma 3, the second Zagreb index of the non-commuting graph for D_{2n} is as follows :
For n is odd,

$$\begin{aligned} M_2(\Gamma_G^{\mathrm{NC}}) &= -|G|^2|E\left(\Gamma_G^{\mathrm{NC}}\right)| + |G|M_1\left(\Gamma_G^{\mathrm{NC}}\right) + \sum_{x,y\in E(\Gamma_G^{\mathrm{NC}})} |C_G(x)||C_G(y)| \\ &= -2n^2\left[4n^2 - \frac{n+3}{2}(2n)\right] + 2n^2(5n-4)(n-1) + \\ &\quad 2n^2(n-1) + 2n(n-1) \\ &= 2n(n-1)^2(2n-1). \end{aligned}$$

Proof (Cont.)

For n is even,

$$M_2(\Gamma_G^{NC}) = -|G|^2|E\left(\Gamma_G^{NC}\right)| + |G|M_1\left(\Gamma_G^{NC}\right) + \sum_{x,y\in E(\Gamma_G^{NC})} |C_G(x)||C_G(y)|$$

$$= -2n^2\left[4n^2 - \frac{n+6}{2}(2n)\right] + 2n^2(5n-8)(n-2) + 4n^2(n-2) + 8n(n-2)$$

$$= 4n(n-2)^2(n-1).$$

Therefore, the second Zagreb index of the non-commuting graph for D_{2n}, where $n \geq 3$,

$$M_2(\Gamma_G^{NC}) = \begin{cases} 2n(n-1)^2(2n-1), & \text{if} \quad n \text{ is odd}, \\ 4n(n-2)^2(n-1), & \text{if} \quad n \text{ is even}. \end{cases}$$

■

The Zagreb Index of the Non-commuting Graph of $G \times D_{2n}$

The Non-commuting Graph of $G \times D_{2n}$

Lemma 1

Let $\Gamma^{\mathrm{NC}}_{G\times D_{2n}}$ be the non-commuting graph of the direct products of an abelian group, G, and the dihedral groups, D_{2n}, which is denoted as $G \times D_{2n}$. Then,

$$\Gamma^{\mathrm{NC}}_{G\times D_{2n}} = \begin{cases} K_{\underbrace{|G|,|G|,\ldots,|G|}_{\text{n times}},(n-1)|G|}, & \text{if} \quad n \text{ is odd,} \\ K_{\underbrace{2|G|,2|G|,\ldots,2|G|}_{\frac{n}{2}\text{ times}},(n-2)|G|}, & \text{if} \quad n \text{ is even.} \end{cases}$$

Proof

The vertices of the non-commuting graph for $G \times D_{2n}$ is,

$$\begin{aligned} V\left(\Gamma^{\mathrm{NC}}_{G\times D_{2n}}\right) &= (G \times D_{2n}) \setminus Z\left(G \times D_{2n}\right) \\ &= (G \times D_{2n}) \setminus (G \times Z(D_{2n})) . \end{aligned}$$

By Proposition 6, there are two cases of the non-commuting graph of dihedral groups, which are n is odd and n is even. By Proposition 1, there is a center of D_{2n} when n is odd and two centers of D_{2n} when n is even.

For n is odd, there are $|G| \times (n-1)$ elements that do not commute to each other and there are n sets of $|G|$ elements which do not commute to each other. Then,

$$K_{\underbrace{|G|, |G|, \ldots, |G|}_{n \text{ times}}, (n-1)|G|} .$$

For n is even, there are $|G| \times (n-2)$ elements that do not commute to each other and there $\frac{n}{2}$ sets of $2|G|$ elements that do not commute to each other. Then,

$$K_{\underbrace{2|G|, 2|G|, \ldots, 2|G|}_{\frac{n}{2} \text{ times}}, (n-2)|G|} .$$

Proof (Cont.)

Therefore,

$$\Gamma^{NC}_{G\times D_{2n}} = \begin{cases} K_{\underbrace{|G|,|G|,\ldots,|G|}_{\text{n times}},(n-1)|G|}, & \text{if} \quad n \text{ is odd}, \\ K_{\underbrace{2|G|,2|G|,\ldots,2|G|}_{\frac{n}{2}\text{ times}},(n-2)|G|}, & \text{if} \quad n \text{ is even}. \end{cases}$$

∎

The First Zagreb Index of the Non-commuting Graph of $G \times D_{2n}$

Theorem 3

Let $G \times D_{2n}$ be the direct product of an abelian group with dihedral groups. Then, the first Zagreb index of the non-commuting graph for $G \times D_{2n}$,

$$M_1\left(\Gamma^{\mathrm{NC}}_{G\times D_{2n}}\right) = |G|^3 M_1\left(\Gamma^{\mathrm{NC}}_{D_{2n}}\right).$$

Proof.

Let X be the elements in G and Y be the elements in D_{2n}. Then, $X = \{x_1, x_2, \ldots, x_m\}$, where m is the total number of elements in X and $Y = \{y_1, y_2, \ldots, y_n\}$, where n is the total number of vertices in Y. For $G \times D_{2n}$, where G is abelian, based on the definition of Zagreb index,

$$
\begin{aligned}
M_1\left(\Gamma^{\mathrm{NC}}_{G\times D_{2n}}\right) &= \sum_{(x,y)\in V(\Gamma^{\mathrm{NC}}_{G\times D_{2n}})} \deg^2(x,y) \\
&= \deg^2(x_1,y_1) + \deg^2(x_1,y_2) + \ldots + \deg^2(x_1,y_n) + \\
&\quad \deg^2(x_2,y_1) + \deg^2(x_2,y_1) + \ldots + \deg^2(x_2,y_n) + \\
&\quad \ldots + \deg^2(x_m,y_1) + \deg^2(x_m,y_2) + \ldots + \deg^2(x_m,y_n) \\
&= \left[|G|\deg_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_1)\right]^2 + \left[|G|\deg_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_2)\right]^2 + \ldots + \left[|G|\deg_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_n)\right]^2 + \\
&\quad \ldots + \left[|G|\deg_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_1)\right]^2 + \left[|G|\deg_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_2)\right]^2 + \ldots + \left[|G|\deg_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_n)\right]^2 \\
&= |G|^2\sum_{i=1}^{n}\deg^2_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_i) + |G|^2\sum_{i=1}^{n}\deg^2_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_i) + \ldots + |G|^2\sum_{i=1}^{n}\deg^2_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_i) \\
&= \left[|G|^2 + |G|^2 + \ldots |G|^2\right]|G|^2\sum_{i=1}^{n}\deg^2_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_i) \\
&= m|G|^2\sum_{i=1}^{n}\deg^2_{\Gamma^{\mathrm{NC}}_{D_{2n}}}(y_i) = |G|^3 M_1(\Gamma^{\mathrm{NC}}_{D_{2n}}).
\end{aligned}
$$

The Second Zagreb Index of the Non-commuting Graph of $G \times D_{2n}$

Theorem 4

Let $G \times D_{2n}$ be the direct product of an abelian group with dihedral groups. Then, the second Zagreb index of the non-commuting graph for $G \times D_{2n}$,

$$M_2\left(\Gamma^{\mathrm{NC}}_{G\times D_{2n}}\right) = |G|^4 M_2\left(\Gamma^{\mathrm{NC}}_{D_{2n}}\right).$$

Proof.

Let X be the elements in G and Y be the elements in D_{2n}. $X = \{x_1, x_2, \ldots, x_m\}$, where m is the total number of elements in X and $Y = \{y_1, y_2, \ldots, y_n\}$, where n is the total number of vertices in Y.

For $G \times D_{2n}$, where G is abelian, based on definition of Zagreb index,

$$\begin{aligned}
M_2\left(\Gamma^{\mathrm{NC}}_{G\times D_{2n}}\right) &= \sum_{((x_i,y_j),(x_k,y_l))\in E(\Gamma^{\mathrm{NC}}_{G\times D_{2n}})} \deg(x_i, y_j)\deg(x_k, y_l) \\
&= \deg(x_1, y_1)\deg(x_1, y_1) + \deg(x_1, y_1)\deg(x_1, y_2) + \ldots \\
&\quad + \deg(x_1, y_1)\deg(x_1, y_n) + \deg(x_1, y_2)\deg(x_1, y_2) + \\
&\quad \deg(x_1, y_2)\deg(x_1, y_3) + \ldots + \deg(x_1, y_2)\deg(x_1, y_n) + \ldots + \\
&\quad \deg(x_1, y_1)\deg(x_1, y_n) + \ldots + \deg(x_2, y_1)\deg(x_2, y_1) + \\
&\quad \deg(x_2, y_1)\deg(x_2, y_2) + \ldots + \deg(x_2, y_1)\deg(x_2, y_n) + \\
&\quad \deg(x_2, y_2)\deg(x_2, y_2) + \deg(x_2, y_2)\deg(x_2, y_3) + \ldots + \\
&\quad \deg(x_2, y_2)\deg(x_2, y_n) + \ldots + \deg(x_2, y_n)\deg(x_2, y_n) + \ldots + \\
&\quad \deg(x_m, y_1)\deg(x_m, y_1) + \deg(x_m, y_1)\deg(x_m, y_2) + \ldots + \\
&\quad \deg(x_m, y_1)\deg(x_m, y_n) + \deg(x_m, y_2)\deg(x_m, y_2) + \\
&\quad \deg(x_m, y_2)\deg(x_m, y_3) + \ldots + \deg(x_m, y_n)\deg(x_m, y_n)
\end{aligned}$$

Proof (Cont.)

$$
\begin{aligned}
&= |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_1)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_1) + |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_1)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_2) + \ldots \\
&\quad + |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_1)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_n) + |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_2)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_2) + \\
&\quad |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_2)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_3) + \ldots + |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_2)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_n) + \\
&\quad \ldots + |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_n)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_n) + \ldots + \\
&\quad |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_1)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_1) + |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_1)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_2) + \ldots \\
&\quad + |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_1)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_n) + |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_2)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_2) + \\
&\quad |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_2)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_3) + \ldots + |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_2)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_n) + \\
&\quad \ldots + |G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_n)|G|\deg_{\Gamma^{NC}_{D_{2n}}}(y_n) \\
&= \sum_{(y_i, y_l) \in E(\Gamma^{NC}_{D_{2n}})} \deg(y_i)\deg(y_j) \left[|G|^2 + |G|^2 + \ldots + |G|^2\right] \times m \\
&= m \times m \times |G|^2 \sum_{(y_i, y_l) \in E(\Gamma^{NC}_{D_{2n}})} \deg(y_i)\deg(y_j) \\
&= |G|^4 M_2\left(\Gamma^{NC}_{G \times D_{2n}}\right).
\end{aligned}
$$

Conclusion

- The general formulas of the first and second Zagreb indices of the non-commuting graph associated to the dihedral groups are found, in terms of n.
- The general formulas of the first and second Zagreb indices of the non-commuting graph associated to the larger group which is direct product of an abelian group G and the dihedral groups, D_{2n} are determined.

Suggestions for Future Research

- The research can be extended in finding the other types of topological indices i.e. Degree-distance index and Randić index.
- The direct product of arbitrary number of dihedral groups, $D_{n_1} \times D_{n_2} \times \ldots \times D_{n_m}$ can be considered.
- The upper and lower bound of the topological indices can be determined.

Acknowledgement

The authors would like to acknowledge **MoHE** through **Fundamental Research Grant Scheme (FRGS1/2020/STG06/UTM/01/2)** and **UTM** for funding the research through **UTM Fundamental Research Grant (UTMFR) Vote Number 20H70.**

References

1. Wiener, H. Structural determination of paraffin boiling points. *Journal of the American Chemical Society.* 1947. 69(1): 17-20.
2. Hosoya, H. Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. *Bulletin of the Chemical Society of Japan.* 1971. 44(9): 2332-2339.
3. Gutman, I. and Trinajstic, N. Graph theory and molecular orbitals. Total $\pi-$ electron energy of alternant hydrocarbons. *Chemical Physics Letters.* 1972. 17(4): 535-538.
4. Gutman, I. and Dobrynin, A. A. The Szeged index-a success story. *Graph Theory Notes NY.* 1998. 34: 37-44.
5. Plavsic, D., Nikolic, S., Trinajstic, N. and Mihalic, Z. On the Harary index for the characterization of chemical graphs. *Journal of Mathematical Chemistry.* 1993. 12(1): 235-250.
6. Humphreys, J. *A course in group theory.* vol. 6. Oxford University Press on Demand. 1996.

References (Cont.)

8. Abdollahi, A., Akbari, S. and Maimani, H. Non-commuting graph of a group. *Journal of Algebra.* 2006. 298(2): 468-492.
9. Gutman, I. and Das, K. C. The first Zagreb index 30 years after. *MATCH Commun. Math. Comput. Chem.* 2004. 50: 83-92.
10. Muhuo, L. and Bolian, L. Some properties of the first general Zagreb index. *Australas. J. Comb.* 2010. 47: 285-294.
11. Das, K. C., Xu, K. and Nam, J. Zagreb indices of graphs. *Frontiers of Mathematics in China.* 2015. 10(3): 567-582.
12. Samaila, D., Abba, B. I. and Pur, M. P. On the conjugacy classes, centers and representation of the groups S_n and D_n. *Int. J. Pure Appl. Sci. Technol.* 2013. 15(1): 87-95.
13. Mirzargar, M. and Ashrafi, A. Some distance-based topological indices of a noncommuting graph. *Hacettepe Journal of Mathematics and Statistics.* 2012. 41(4): 515-526.
14. Mahmoud, R. B. Energy and Laplacian Energy of Graphs Related to a Family of Finite Groups. Universiti Teknologi Malaysia: Ph.D. Thesis. 2018.

Thank you

THANK YOU!