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RESEARCH ARTICLE

Machine Learning Driven Exploration of Energies and Generalization of Topological Indices for the Fuzzy Conjugate Graph of Dihedral Group

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ABSTRACT This study introduces a ground-breaking approach to analyzing dihedral groups through the lens of fuzzy graph theory, significantly enhancing computational efficiency in group theory. By extending the fuzzy topological indices to polynomial forms, this research drastically reduces the calculation time for these indices from hours to mere seconds. A notable feature of this work is the innovative use of polynomial regression, a machine learning technique, to generate polynomials for adjacency and degree matrices within the fuzzy conjugate graph of a dihedral group. This method not only simplifies calculations but also incorporates an error analysis component, ensuring accuracy and reliability. The integration of fuzzy graph theory with polynomial regression in this context is a pioneering step, offering valuable insights into the structural attributes of dihedral groups. This research goes beyond traditional methods, highlighting the effectiveness of machine learning in deciphering complex patterns in group theory. The findings and techniques presented hold great promise for future applications in graph theory and group theory, offering a novel perspective for understanding and analyzing intricate graph structures. This study stands as a significant contribution to the field, potentially revolutionizing the way complex mathematical problems are approached and solved.

INDEX TERMS Artificial intelligence, conjugate graph, dihedral group, fuzzy graph, fuzzy topological indices, polynomial regression, topological indices.

I. INTRODUCTION

In the realm of chemical graph theory, where molecules are represented as graphs to simplify the study of their structures, this study marks a significant advancement by introducing a groundbreaking approach to analyzing dihedral groups through fuzzy graph theory. The dihedral group, integral to understanding molecular symmetries in various compounds such as benzene (C_6H_6), is explored with enhanced computational efficiency. By extending fuzzy topological indices to polynomial forms, the research drastically reduces the calculation time of these indices from hours to mere seconds. The incorporation of polynomial regression, a machine learning technique, is a key innovation for generating polynomials for adjacency and degree matrices within the fuzzy conjugate graph of a dihedral group. This method simplifies complex calculations and incorporates error analysis to ensure accuracy and reliability. The integration of fuzzy graph theory with polynomial regression in analyzing dihedral groups' structural attributes is a pioneering step. This research transcends traditional methods, highlighting the effectiveness of machine learning in deciphering complex patterns in group theory. The findings and methodologies presented offer new perspectives in graph theory and group

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theory, potentially revolutionizing the approach to complex mathematical problems in chemistry and beyond.

Conjugate graphs have been the focus of several research papers. They are defined as graphs related to groups, where the vertices represent elements or sets from the groups and the edges represent properties and conditions for the graph [1]. Different properties and matrices associated with conjugate graphs have been studied, such as the conjugate adjacency matrix and the conjugate Laplacian matrix [2]. These matrices have been used to determine various properties of the eigenvalues and eigenvectors of graphs with co-neighbour vertices [3]. Conjugate graphs have also been applied in the field of shape matching, where a novel formalism based on the conjugate product graph has been proposed to find continuous and non-rigid matchings between 2D contours and 3D meshes [1]. Additionally, the conjugate graph has been used to study the isomorphism between nonabelian groups and to compare the conjugate graphs of different groups [4]. Overall, conjugate graphs have been extensively studied in various contexts, including group theory, graph theory, and shape matching.

Different graphs of dihedral groups have been studied in the literature. One type of graph representation is the power graph, which uses the elements of the group as vertices and connects two vertices if their corresponding elements satisfy certain conditions [5]. The conjugacy class graph is another graph related to dihedral groups, where the vertices represent non-central conjugacy classes and two vertices are connected if they have a common prime divisor [6]. Meta-Cayley graphs on dihedral groups have been defined, and their automorphism groups have been fully determined [7]. The conjugacy class graph of a group is a graph with a vertex set represented by the non-central conjugacy classes of the group, and two distinct vertices are connected if they have a common prime divisor [8]. These different graphs provide insights into the properties and topological indices of dihedral groups.

Fuzzy graphs are a significant area of research due to their wide range of applications. They combine the concepts of fuzzy sets and graphs to represent vagueness and uncertainty. Different types of fuzzy graphs have been studied, including fuzzy planar graphs, fuzzy soft graphs, and cubic fuzzy graphs [9]. These graphs have been applied in various fields such as social networks, road networks, traffic management, telecommunication, and brain networks [10]. The properties of fuzzy graphs have been investigated, including graph coloring and the utility value of neutrosophic and intuitionistic structures [11]. The Wiener index, a measure of connectivity, has also been studied in cubic fuzzy graphs. Overall, fuzzy graphs provide a useful framework for dealing with ambiguity and uncertainty in various applications [12]. In [13], the identity graph of a ring is discussed, and its fuzzy and crisp topological indices are presented. Topological indices are numbers that describe specific properties of a graph and are widely used in chemistry. They convert the chemical structure into a numerical value and are helpful in understanding the structure and dynamics of molecules. Various topological indices, such as the Wiener index, Zagreb index, and ABC index, have been computed for different graphs [14]. These indices are algebraic quantities that correlate the chemical structure with physical characteristics and can be used to determine properties like chemical activity, thermodynamic properties, and biological activity [15]. Topological indices are also used in the study of quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR) to correlate molecular structure with different properties and activities [16]. They have been applied in drug design and development to analyze the physical characteristics, chemical reactivity, and biological activity of chemical structures [17]. The energy of a graph in graph theory is a concept that measures the sum of the absolute eigenvalues of the adjacency matrix of the graph [18]. It has applications in various fields, such as chemistry and network analysis [19]. We can use the energy of a graph to determine its properties, including its connectivity and degree. Several theorems and bounds have been established to study the energy of a graph, including upper bounds and bounds based on different graph matrices [20]. The energy of a graph has been compared to the energy of complete graphs and used to classify graphs as hyperenergetic or borderenergetic [21]. Additionally, the energy of a graph can be determined for specific types of graphs, such as regular subdivision graphs and complete graphs [22].

II. PRELIMINARIES

The conjugate graph of the dihedral group $D_{2\upsilon}$ is defined as the graph in which the vertex set is the set of elements of the dihedral group $D_{2\upsilon}$ and an edge exists between a pair of vertices if and only if they are conjugate of each other. In this article, we refer to the conjugate graph of the dihedral group $D_{2\upsilon}$ where υ is odd as $G(\dot{D}_{2\upsilon})$ and the conjugate graph of the dihedral group $D_{2\upsilon}$ where υ is even as $G(\ddot{D}_{2\upsilon})$. Based on this definition of conjugate graph, $G(\dot{D}_{14})$ is given in Figure 1 and $G(\ddot{D}_{16})$ in Figure 2.

In this study, we define the fuzzy graph associated with the conjugate graph of a dihedral group, denoted as $D_{2\upsilon}$. This graph is represented by a three-part structure $(\mathfrak{v}, \hbar, \Omega)$. Here, $\mathfrak{v}$ denotes the set of vertices, and $\mathfrak{E}$ signifies the set of edges. Each edge (ψ, Θ) belonging to $\mathfrak{E}$ and each vertex ψ in $\mathfrak{v}$ carry a membership value, noted as $\Omega(\psi, \Theta)$ and $\hbar(\psi)$ respectively, ranging between 0 and 1. These values represent the weights of vertices and edges, termed vertex weight $\hbar$ and edge weight Ω. The specific focus of this article is on the fuzzy conjugate graphs of the dihedral group $D_{2\upsilon}$, differentiated by the parity of υ; the graph for odd υ is expressed as $\maltese(\dot{D}_{2\upsilon})$, and for even υ as $\maltese(\ddot{D}_{2\upsilon})$. We exemplify this with $\maltese(\dot{D}_{14})$ and $\maltese(\ddot{D}_{16})$ in figures 4 and 3, respectively. We propose that the vertex weight $\hbar$ in the fuzzy conjugate graph of any dihedral group $\maltese(D_{2\upsilon})$ is $\frac{1}{\upsilon}$, and the corresponding edge weight Ω is $\frac{1}{2\upsilon}$.

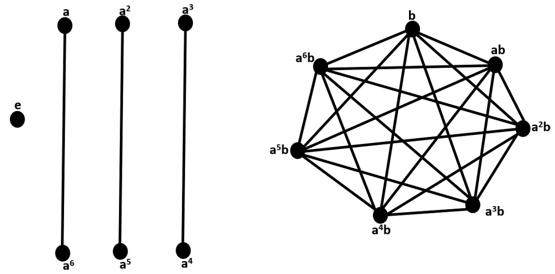

FIGURE 1. Conjugate graph of the dihedral group D_{14}, $G(D_{14})$.

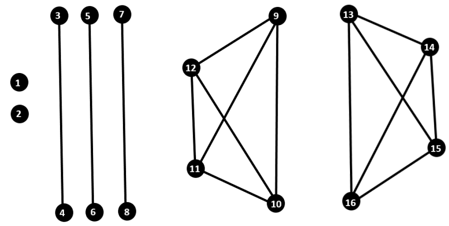

FIGURE 2. Conjugate graph of the dihedral group D_{16}, $G(D_{16})$.

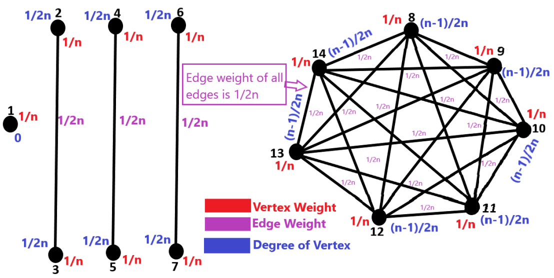

FIGURE 3. Conjugate fuzzy graph of the dihedral group D_{14}, $G(D_{14})$.

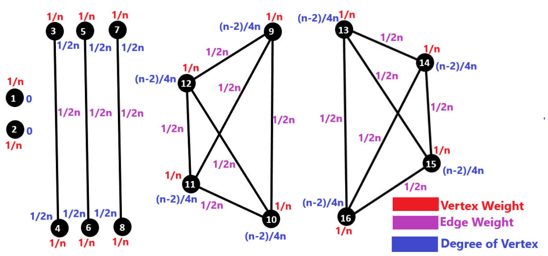

FIGURE 4. Conjugate fuzzy graph of the dihedral group D_{16}, $G(D_{16})$.

Furthermore, we define the fuzzy degree of a vertex $\wp$ in $\maltese(D_{2\upsilon})$ as the aggregate of membership values of all connecting edges. This is mathematically represented by $\wp(\psi) = \sum_{\psi\in\mathfrak{V},(\psi,\Theta)\in\mathfrak{E}} \Omega(\psi,\Theta)$. Additionally, we explore the application of topological indices—numerical descriptors that encapsulate the topological characteristics of graphs—in understanding the chemical and physical attributes of molecules. The computation methods for both crisp and fuzzy topological indices are detailed in Table 1.

III. THE SCOPE OF FUZZY TOPOLOGICAL INDICES FOR $\maltese(D_{2\upsilon})$ BY CREATING υ DEPENDENT POLYNOMIALS

This section is dedicated to introducing generalized υ dependent polynomial expressions for the fuzzy topological indices pertaining to the conjugate graph graph of $\maltese(D_{2\upsilon})$.

TABLE 1. Formulae of fuzzy topological indices.

Index Name	Formula
Fuzzy first Zagreb index [24]	$® = \sum_{\psi\in\mathfrak{V}} \hbar(\psi_i)[\wp(\psi_i)]^2$
Fuzzy second Zagreb index [24]	$¥ = \frac{1}{2}\Big[\sum_{(\psi,\Theta)\in\mathfrak{E}} \hbar(\psi_i)\wp(\psi)\hbar(\Theta)\wp(\psi)\Big]$
Fuzzy harmonic index [25]	$\zeta = 1/2\Big[\sum_{(\psi,\Theta)\in\mathfrak{E}}(\frac{1}{\hbar(\psi)\wp(\psi)+\hbar(\Theta)\wp(\Theta)})\Big]$
Fuzzy Randic index [25]	$\xi = 1/2\Big[\sum_{\psi,\Theta\in\mathfrak{V}} \hbar(\psi)\wp(\Theta)\hbar(\Theta)\wp(\Theta)\Big]^{\frac{-1}{2}}$

A. GENERALIZATION OF FUZZY TOPOLOGICAL INDICES FOR $\maltese(\ddot{D}_{2\upsilon})$, WHEN υ IS EVEN

Theorem 1: The first fuzzy Zagreb index ® of conjugate graph $\maltese(D_{2\upsilon})$ where υ is even is given by

$$® = \frac{(\upsilon-2)(\upsilon^2-2\upsilon+4)}{16\upsilon^3} \tag{1}$$

Proof:

$$\begin{aligned}
® &= \sum h(\psi)(w(\psi))^2 \qquad \forall\psi\epsilon\mathfrak{V}\\
&= \frac{1}{\upsilon}(\frac{1}{2\upsilon})^2 + \frac{1}{\upsilon}(\frac{1}{2\upsilon})^2 + \cdots \frac{1}{\upsilon}(\frac{1}{2\upsilon})^2 \ \big((\upsilon-2)\ times\big)\\
&+ \frac{1}{\upsilon}(\frac{\upsilon-2}{4\upsilon})^2 + \frac{1}{\upsilon}(\frac{\upsilon-2}{4\upsilon})^2 + \cdots\\
&+ \frac{1}{\upsilon}(\frac{\upsilon-2}{4\upsilon})^2 \ \big(\upsilon\ times\big) + \frac{1}{\upsilon}(0)^2 + \frac{1}{\upsilon}(0)^2\\
&= \frac{\upsilon-2}{\upsilon}(\frac{1}{2\upsilon})^2 + (\frac{\upsilon-2}{4\upsilon})^2\\
&= \frac{(\upsilon-2)}{4\upsilon^3}(\frac{(\upsilon-2)^2}{16\upsilon^2})\\
&= \frac{4(\upsilon-2)+\upsilon(\upsilon-2)^2}{16\upsilon^3}\\
&= \frac{(\upsilon-2)(4+\upsilon(\upsilon-2))}{16\upsilon^3}\\
&= \frac{(\upsilon-2)(\upsilon^2-2\upsilon+4)}{16\upsilon^3}
\end{aligned}$$

□

Theorem 2: The second fuzzy zegrab index ¥ for conjugate graph $\maltese(D_{2\upsilon})$ where υ is even is given by

$$¥ = \frac{(\upsilon-2)(4+\upsilon^3)}{16\upsilon^5} \tag{2}$$

Proof:

$$\begin{aligned}
¥ &= \sum_{(\psi,\Theta)\epsilon\mathfrak{E}} \hbar(\psi)\wp(\psi)\hbar(\Theta)\wp(\Theta)\\
&= \frac{1}{\upsilon}(\frac{1}{2\upsilon}).\frac{1}{\upsilon}(\frac{1}{2\upsilon}) + \frac{1}{\upsilon}(\frac{1}{2\upsilon}).\frac{1}{\upsilon}(\frac{1}{2\upsilon})\\
&+ \cdots + \frac{1}{\upsilon}(\frac{1}{2\upsilon}).\frac{1}{\upsilon}(\frac{1}{2\upsilon})\ \frac{(\upsilon-2)}{\upsilon}\ times + \frac{1}{\upsilon}(\frac{\upsilon-2}{4\upsilon})\\
&+ \frac{1}{\upsilon}(\frac{\upsilon-2}{4\upsilon}) + \cdots + \frac{1}{\upsilon}(\frac{\upsilon-2}{4\upsilon})\ \frac{\upsilon(\upsilon-2)}{4}\ times\\
&= \frac{1}{4\upsilon^4}(\frac{\upsilon-2}{\upsilon}) + (\frac{\upsilon-2}{16\upsilon^2})
\end{aligned}$$

$$= \frac{\upsilon-2}{4\upsilon^2}\left(\frac{1}{\upsilon^3}+\frac{1}{4}\right)$$
$$= \frac{\upsilon-2}{4\upsilon^2}\left(\frac{4+\upsilon^3}{4\upsilon^3}\right)$$
$$= \frac{(\upsilon-2)(4+\upsilon^3)}{16\upsilon^5} \tag{3}$$

□

Theorem 3: The fuzzy harmonic index ζ of conjugate graph $\maltese(D_{2\upsilon})$ where υ is even is given by

$$\zeta = \frac{\upsilon(\upsilon-2)(\upsilon+1)}{(\upsilon+2)} \tag{4}$$

Proof:

$$\zeta = \frac{1}{2}\Bigg[\sum_{(x,y)\epsilon E}\frac{1}{h(x)w(x)+h(y)w(y)}\Bigg]$$
$$= \frac{1}{2}\Bigg[\frac{1}{(\frac{1}{\upsilon})(\frac{1}{2\upsilon})+(\frac{1}{\upsilon})(\frac{1}{2\upsilon})}+\frac{1}{(\frac{1}{\upsilon})(\frac{1}{2\upsilon})+(\frac{1}{\upsilon})(\frac{1}{2\upsilon})}$$
$$+\ldots..+\frac{1}{(\frac{1}{\upsilon})(\frac{1}{2\upsilon})+(\frac{1}{\upsilon})(\frac{1}{2\upsilon})}\quad\frac{(\upsilon-2)}{\upsilon}\,times+$$
$$+\frac{1}{(\frac{1}{\upsilon})+(\frac{\upsilon-2}{4\upsilon})}+\frac{1}{(\frac{1}{\upsilon})+(\frac{\upsilon-2}{4\upsilon})}$$
$$+\ldots..+\frac{1}{(\frac{1}{\upsilon})+(\frac{\upsilon-2}{4\upsilon})}\quad\frac{\upsilon(\upsilon-2)}{4}\,times\Bigg]$$
$$= \frac{1}{2}\Bigg[\Big(\frac{1}{\frac{2}{2\upsilon^2}}\Big)\Big(\frac{\upsilon-2}{\upsilon}\Big)+\Big(\frac{1}{\frac{4\upsilon+\upsilon^2-2\upsilon}{4\upsilon^2}}\Big)\Big(\frac{\upsilon(\upsilon-2)}{4}\Big)\Bigg]$$
$$= \frac{1}{2}\Bigg[\upsilon\Big(\frac{\upsilon-2}{\upsilon}\Big)+\frac{4\upsilon^2}{4\upsilon+\upsilon^2-2\upsilon}\Big(\frac{\upsilon(\upsilon-2)}{4}\Big)\Bigg]$$
$$= \Big(\frac{\upsilon(\upsilon-2)}{2}\Big)\Bigg[1+\frac{\upsilon^2}{4\upsilon+\upsilon^2-2\upsilon}\Bigg]$$
$$= \Big(\frac{\upsilon(\upsilon-2)}{2}\Big)\Bigg[\frac{\upsilon^2+2\upsilon+\upsilon^2}{\upsilon^2+2\upsilon}\Bigg]$$
$$= \Big(\frac{\upsilon(\upsilon-2)}{2}\Big)\Bigg[\frac{2\upsilon^2+2\upsilon}{\upsilon^2+2\upsilon}\Bigg]$$
$$= \Big(\frac{\upsilon(\upsilon-2)(\upsilon^2+\upsilon)}{\upsilon^2+2\upsilon}\Big)$$
$$= \Big(\frac{\upsilon^2(\upsilon-2)(\upsilon+1)}{\upsilon(\upsilon+2}\Big)$$
$$= \frac{\upsilon(\upsilon-2)(\upsilon+1)}{(\upsilon+2)} \tag{5}$$

□

Theorem 4: The fuzzy Randic index ξ for conjugate graph $\maltese(D_{2\upsilon})$ where υ is even is given by

$$\xi = \frac{1}{2}\Bigg[\frac{(\upsilon-2)(4+\upsilon^3)}{16\upsilon^5}+\frac{(\upsilon-2)(\upsilon-3)}{8\upsilon^4}+\frac{\upsilon^2(\upsilon-2)^2}{64\upsilon^4}$$
$$+\frac{\upsilon(\upsilon-2)^2}{8\upsilon^4}\Bigg]^{\frac{-1}{2}} \tag{6}$$

Proof:

$$\zeta = \frac{1}{2}\Bigg[\sum_{(\psi,\Theta)\epsilon\mathfrak{V}}\hbar(\psi)\wp(\psi)\hbar(\Theta)\wp(\Theta)\Bigg]^{\frac{-1}{2}}$$
$$= \frac{1}{2}\Bigg[\sum_{(\psi,\Theta)\epsilon\mathfrak{V}}\hbar(\psi)\wp(\psi)\hbar(\Theta)\wp(\Theta)$$
$$+\sum_{(\psi,\Theta)\epsilon\acute{\mathfrak{V}}}h(\psi)w(\psi)h(\Theta)w(\Theta)\Bigg]^{\frac{-1}{2}}$$
$$= \frac{1}{2}\Bigg[\frac{(\upsilon-2)(4+\upsilon^3)}{16\upsilon^5}+\Big(\frac{1}{\upsilon}\Big)\Big(\frac{1}{2\upsilon}\Big)\Big(\frac{1}{\upsilon}\Big)\Big(\frac{1}{2\upsilon}\Big)+$$
$$+\Big(\frac{1}{\upsilon}\Big)\Big(\frac{1}{2\upsilon}\Big)\Big(\frac{1}{\upsilon}\Big)\Big(\frac{1}{2\upsilon}\Big)+\cdots\Big(\frac{1}{\upsilon}\Big)\Big(\frac{1}{2\upsilon}\Big)\Big(\frac{1}{\upsilon}\Big)\Big(\frac{1}{2\upsilon}\Big)$$
$$\frac{(\upsilon-2)(\upsilon-3)}{2}\;times$$
$$+\Big(\frac{1}{\upsilon}\Big)\Big(\frac{(\upsilon-2)}{4\upsilon}\Big)\Big(\frac{1}{\upsilon}\Big)\Big(\frac{(\upsilon-2)}{4\upsilon}\Big)$$
$$+\cdots+\Big(\frac{1}{\upsilon}\Big)\Big(\frac{(\upsilon-2)}{4\upsilon}\Big)\Big(\frac{1}{\upsilon}\Big)\Big(\frac{(\upsilon-2)}{4\upsilon}\Big)\;\frac{\upsilon^2}{4}\;times$$
$$+\Big(\frac{1}{\upsilon}\Big)\Big(\frac{1}{2\upsilon}\Big)\Big(\frac{1}{\upsilon}\Big)\Big(\frac{1}{2\upsilon}\Big)+\ldots.$$
$$+\Big(\frac{1}{\upsilon}\Big)\Big(\frac{1}{2\upsilon}\Big)\Big(\frac{1}{\upsilon}\Big)\Big(\frac{1}{2\upsilon}\Big)\;\big(\upsilon(\upsilon-2)\;times\big)\Bigg]^{\frac{-1}{2}}$$
$$= \frac{1}{2}\Bigg[\frac{(\upsilon-2)(4+\upsilon^3)}{16\upsilon^5}+\frac{(\upsilon-2)(\upsilon-3)}{8\upsilon^4}$$
$$+\frac{\upsilon^2(\upsilon-2)^2}{64\upsilon^4}+\frac{\upsilon(\upsilon-2)^2}{8\upsilon^4}\Bigg]^{\frac{-1}{2}} \tag{7}$$

□

Figure 5 shows the comparison of fuzzy topological indices for different values of υ

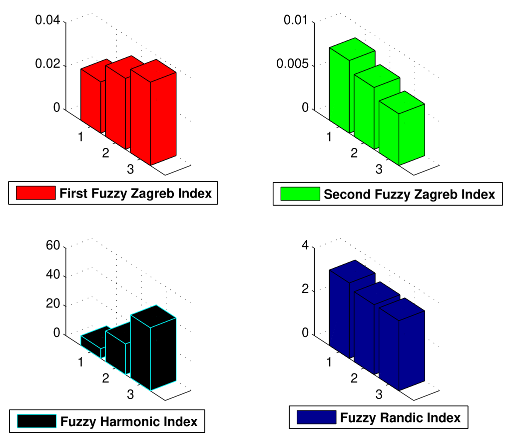

FIGURE 5. Fuzzy topological indices for $\upsilon = 4, 6, 8$.

B. GENERALIZATION OF FUZZY TOPOLOGICAL INDICES FOR $\maltese(\dot{D}_{2\upsilon})$, WHEN υ IS ODD

Theorem 5: The first fuzzy Zagreb index of conjugate graph $\maltese(D_{2\upsilon})$ where υ is odd is given by

$$\circledR = \frac{(\upsilon-1)}{4\upsilon^3} + \frac{\upsilon(\upsilon-1)}{2\upsilon^2} \tag{8}$$

Proof:

$$\begin{aligned}
\circledR &= \sum h(\psi)(w(\psi))^2 \qquad \forall \psi \epsilon \mathfrak{V} \\
&= \frac{1}{\upsilon}(\frac{1}{2\upsilon})^2 + \frac{1}{\upsilon}(\frac{1}{2\upsilon})^2 + \ldots\ldots\frac{1}{\upsilon}(\frac{1}{2\upsilon})^2 \quad (\upsilon-1)times \\
&\quad + \frac{1}{\upsilon}(\frac{\upsilon-1}{2\upsilon}) + \frac{1}{\upsilon}(\frac{\upsilon-1}{2\upsilon}) + \ldots\ldots \\
&\quad + \frac{1}{\upsilon}(\frac{\upsilon-1}{2\upsilon}) \quad \upsilon \ times \\
&= (\frac{1}{\upsilon}\frac{1}{4\upsilon^2})(\upsilon-1) + \upsilon(\frac{\upsilon-1}{2\upsilon^2}) \\
&= \frac{\upsilon-1}{4\upsilon^3} + \upsilon(\frac{\upsilon-1}{2\upsilon^2})
\end{aligned} \tag{9}$$

□

Theorem 6: The second fuzzy Zagreb index ¥ for conjugate graph $\maltese(D_{2\upsilon})$ where υ is odd is given by

$$\yen = \frac{(\upsilon-1)(\upsilon^2-\upsilon+1)}{8\upsilon^4} \tag{10}$$

Proof:

$$\begin{aligned}
\yen &= \sum_{(\psi,\Theta)\epsilon E} h(\psi)w(\psi)h(\Theta)w(\Theta) \\
&= \frac{1}{\upsilon}(\frac{1}{2\upsilon}).\frac{1}{\upsilon}(\frac{1}{2\upsilon}) + \frac{1}{\upsilon}(\frac{1}{2\upsilon}).\frac{1}{\upsilon}(\frac{1}{2\upsilon}) \\
&\quad + \cdots + \frac{1}{\upsilon}(\frac{1}{2\upsilon}).\frac{1}{\upsilon}(\frac{1}{2\upsilon}) \quad \frac{(\upsilon-1)}{2} times \\
&\quad + \frac{1}{\upsilon}(\frac{\upsilon-1}{2\upsilon})\frac{1}{\upsilon}(\frac{\upsilon-1}{2\upsilon}) + \cdots \\
&\quad + \frac{1}{\upsilon}(\frac{\upsilon-1}{2\upsilon})\frac{1}{\upsilon}(\frac{\upsilon-1}{2\upsilon}) \ \frac{\upsilon(\upsilon-2)}{4} \ times \\
&= \frac{\upsilon-1}{4\upsilon^4}(\frac{\upsilon(\upsilon-1)}{2}) + (\frac{\upsilon-1}{8\upsilon^4}) \\
&= \frac{\upsilon(\upsilon-1)^2}{8\upsilon^4} + \frac{\upsilon-1}{8\upsilon^4}) \\
&= \frac{(\upsilon-1)}{8\upsilon^4}(\upsilon(\upsilon-1)+1) \\
&= \frac{(\upsilon-1)}{8\upsilon^4}(\upsilon^2-\upsilon+1) \\
&= \frac{(\upsilon-1)(\upsilon^2-\upsilon+1)}{8\upsilon^4}
\end{aligned} \tag{11}$$

□

Theorem 7: The fuzzy harmonic index ζ of conjugate graph $\maltese(D_{2\upsilon})$ where υ is odd is given by

$$\zeta = \frac{\upsilon^2(2(\upsilon-1)+\upsilon}{4} \tag{12}$$

Proof:

$$\begin{aligned}
\zeta &= \frac{1}{2}\Bigg[\sum_{(\psi,\Theta)\epsilon E} \frac{1}{h(\psi)w(\psi)+h(\Theta)w(\Theta)}\Bigg] \\
&= \frac{1}{2}\Bigg[\frac{1}{(\frac{1}{\upsilon})(\frac{1}{2\upsilon})+(\frac{1}{\upsilon})(\frac{1}{2\upsilon})} + \frac{1}{(\frac{1}{\upsilon})(\frac{1}{2\upsilon})+(\frac{1}{\upsilon})(\frac{1}{2\upsilon})} \\
&\quad + \ldots\ldots + \frac{1}{(\frac{1}{\upsilon})(\frac{1}{2\upsilon})+(\frac{1}{\upsilon})(\frac{1}{2\upsilon})} \quad (\upsilon-1)times+ \\
&\quad + \frac{1}{(\frac{1}{\upsilon})(\frac{\upsilon-1}{2\upsilon})+(\frac{1}{\upsilon})(\frac{\upsilon-1}{2\upsilon})} + \frac{1}{(\frac{1}{\upsilon})(\frac{\upsilon-1}{2\upsilon})+(\frac{1}{\upsilon})(\frac{\upsilon-1}{2\upsilon})} \\
&\quad + \ldots\ldots + \frac{1}{(\frac{1}{\upsilon})(\frac{\upsilon-1}{2\upsilon})+(\frac{1}{\upsilon})(\frac{\upsilon-1}{2\upsilon})} \quad \frac{\upsilon(\upsilon-1)}{2} times\Bigg] \\
&= \frac{1}{2}\Bigg[(\frac{1}{\frac{2}{2\upsilon^2}})(\upsilon-1) + (\frac{1}{\frac{2(\upsilon-1)}{2\upsilon^2}})(\frac{\upsilon(\upsilon-1)}{2})\Bigg] \\
&= \frac{1}{2}\Bigg[\upsilon^2(\upsilon-1) + (\frac{\upsilon^2-\upsilon)}{2})\Bigg] \\
&= \frac{1}{2}\Bigg[\upsilon^2(\upsilon-1) + (\frac{\upsilon^3)}{2})\Bigg] \\
&= \frac{1}{4}\Bigg[2\upsilon^2(\upsilon-1) + \upsilon^3\Bigg] \\
&= \frac{\upsilon^2(2(\upsilon-1)+\upsilon}{4}
\end{aligned} \tag{13}$$

□

Theorem 8: The fuzzy Randic index ξ of conjugate graph $\maltese(D_{2\upsilon})$ where υ is odd is given by

$$\begin{aligned}
\xi = \frac{1}{2}\Bigg[&\frac{(\upsilon-1)(\upsilon^2-\upsilon+1)}{8\upsilon^4} + \frac{(\upsilon-1)(\upsilon-3)}{8\upsilon^4} \\
&+ \frac{\upsilon(\upsilon-1)^2}{4\upsilon^4}\Bigg]^{\frac{-1}{2}}
\end{aligned} \tag{14}$$

Proof:

$$\begin{aligned}
\xi &= \frac{1}{2}\Bigg[\sum_{(\psi,\Theta)\epsilon\mathfrak{V}} h(\psi)w(\psi)h(\Theta)w(\Theta)\Bigg]^{\frac{-1}{2}} \\
&= \frac{1}{2}\Bigg[\sum_{(\psi,\Theta)\epsilon\mathfrak{V}} h(\psi)w(\psi)h(\Theta)w(\Theta) \\
&\quad + \sum_{(\psi,\Theta)\epsilon\acute{\mathfrak{V}}} h(\psi)w(\psi)h(\Theta)w(\Theta)\Bigg]^{\frac{-1}{2}}
\end{aligned} \tag{15}$$

$$\begin{aligned}
&= \frac{1}{2}\Bigg[\frac{(\upsilon-1)(\upsilon^2-\upsilon+1}{8\upsilon^4}) + \frac{1}{\upsilon}(\frac{1}{2\upsilon}).\frac{1}{\upsilon}(\frac{1}{2\upsilon}) \\
&\quad + \frac{1}{\upsilon}(\frac{1}{2\upsilon}).\frac{1}{\upsilon}(\frac{1}{2\upsilon}) \\
&\quad + \cdots + \frac{1}{\upsilon}(\frac{1}{2\upsilon}).\frac{1}{\upsilon}(\frac{1}{2\upsilon}) \ (\frac{(\upsilon-1)(\upsilon-3)}{2} \ times) \\
&\quad + \frac{1}{\upsilon}(\frac{1}{2\upsilon})\frac{1}{\upsilon}(\frac{\upsilon-1}{2\upsilon}) + \frac{1}{\upsilon}(\frac{1}{2\upsilon})\frac{1}{\upsilon}(\frac{\upsilon-1}{2\upsilon}) \\
&\quad + \cdots + \frac{1}{\upsilon}(\frac{1}{2\upsilon})\frac{1}{\upsilon}(\frac{\upsilon-1}{2\upsilon}) \ \big(\upsilon(\upsilon-1) \ times\big)\Bigg]^{\frac{-1}{2}} \\
&= \frac{1}{2}\Bigg[\frac{(\upsilon-1)(\upsilon^2-\upsilon+1)}{8\upsilon^4} + \frac{1}{4\upsilon^4}\frac{(\upsilon-1)(\upsilon-3)}{2}
\end{aligned}$$

$$
\begin{aligned}
&+ \frac{(\upsilon-1)}{4\upsilon^4}\upsilon(\upsilon-1)\Bigg]^{\frac{-1}{2}} \\
&= \frac{1}{2}\Bigg[\frac{(\upsilon-1)(\upsilon^2-\upsilon+1)}{8\upsilon^4} + \frac{(\upsilon-1)(\upsilon-3)}{8\upsilon^4} \\
&\quad + \frac{\upsilon(\upsilon-1)^2}{4\upsilon^4}\Bigg]^{\frac{-1}{2}} \qquad (16)
\end{aligned}
$$

□

Figure 6 show the comparison of fuzzy topological indices for different values of υ

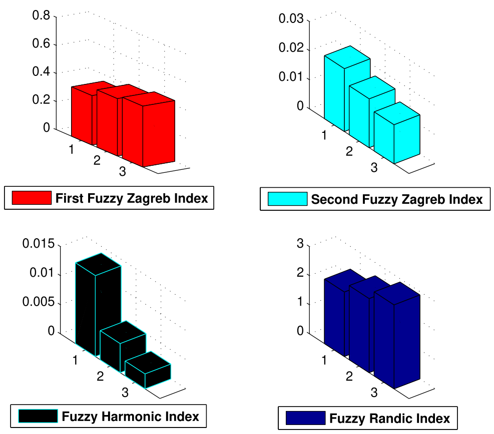

FIGURE 6. Fuzzy topological indices for $\upsilon = 3, 5, 7$.

IV. APPLICATION OF MACHINE LEARNING TO GENERATE POLYNOMIALS FOR THE ENERGIES OF $\maltese(\ddot{D}_{2\upsilon})$

We use polynomial regression in this machine learning section to generate polynomials for fuzzy energies of adjacency and degree matrices. Table 2 shows the computed energies. We used the MATLAB software for computation purposes. Python uses ''pandas'' and ''numpy'' to compute the energies for polnomial regression.

TABLE 2. Computed energies of adjacency and degree matrices.

υ	Energies of degree matrix	Energies of adjacency matrix	υ	Energies of adjacency matrix	Energies of adjacency matrix
3	1	1.3333	2	0.75	0.75
5	1.2	2.4	4	1	1.3333
7	1.2857	3.4286	6	1.125	1.875
9	1.3333	4.4444	8	1.2	2.4
11	1.3636	5.4545	10	1.25	2.9167
13	1.3846	6.4615	12	1.2857	3.4286
15	1.4	7.4667	14	1.3125	3.9375
17	1.4118	8.4706	16	1.3333	4.4444
19	1.4211	9.4737	18	1.35	4.95
21	1.4286	10.4762	20	1.3636	5.4545
23	1.4348	11.4783	22	1.375	5.9583
25	1.44	12.48	24	1.3846	6.4615
27	1.4444	13.4815	26	1.3929	6.9643
29	1.4483	14.4828	28	1.4	7.4667
31	1.4516	15.4839	30	1.4063	7.9688
33	1.4545	16.4848	32	1.4118	8.4706
35	1.4571	17.4857	34	1.4167	8.9722
37	1.4595	18.4865	36	1.4211	9.4737
39	1.4615	19.4872	38	1.425	9.975
41	1.4634	20.4878	40	1.4286	10.4762

A. FUZZY ADJACENCY MATRIX ENERGY $\ddot{\Phi}$ OF $\maltese(\ddot{D}_{2\upsilon})$, WHERE υ IS EVEN

The relation between fuzzy adjacency matrix energy $\ddot{\Phi}$ for $\maltese(\ddot{D}_{2\upsilon})$ and the values of υ in $\maltese(\ddot{D}_{2\upsilon})$ is given in equation (17) which is generated by polynomial regression.

$$
\begin{aligned}
\ddot{\Phi} = &-\frac{4047653480013547\,\upsilon^6}{604462909807314587353088} \\
&+\frac{4940584157399497\,\upsilon^5}{4722366482869645213696} \\
&-\frac{607046617967185\,\upsilon^4}{9223372036854775808} \\
&+\frac{4924605032620321\,\upsilon^3}{2305843009213693952} \\
&-\frac{5482776509751437\,\upsilon^2}{144115188075855872} \\
&+\frac{3292057333465955\,\upsilon}{9007199254740992} \\
&-\frac{1973197593104899}{9007199254740992} \qquad (17)
\end{aligned}
$$

The absolute error between precise adjacency matrix energies and approximated adjacency matrix energies by equation (17) obtained with the help of polynomial regression is shown in Figure 7.

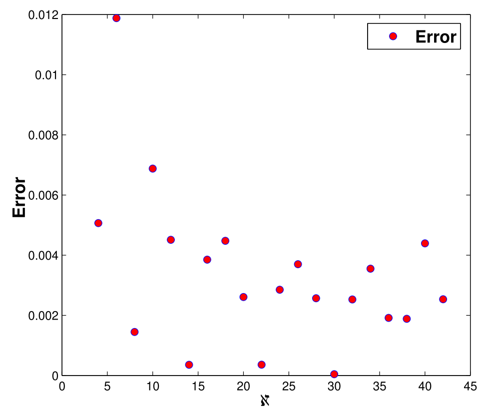

FIGURE 7. Absolute error between exact adjacency energies and approximated adjacency energies by with equation (17).

B. FUZZY DEGREE MATRIX ENERGY $\ddot{\Psi}$ OF $\maltese(\ddot{D}_{2\upsilon})$, WHERE υ IS EVEN

The relation between fuzzy degree matrix energy $\ddot{\Phi}$ for $\maltese(\ddot{D}_{2\upsilon})$ and the values of υ in $\maltese(\ddot{D}_{2\upsilon})$ is given in equation (18), which is generated by polynomial regression.

$$
\ddot{\Psi} = \frac{4574178239290795\,x}{18014398509481984} - \frac{175917086628555}{1125899906842624} \qquad (18)
$$

The absolute error between precise degree matrix energies and approximated degree matrix energies by equation (18) obtained with the help of polynomial regression is shown in Figure 8.

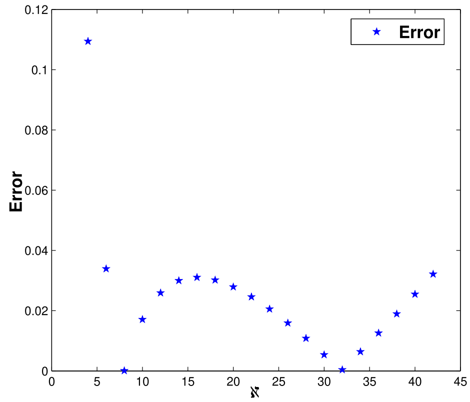

FIGURE 8. Absolute error between exact adjacency energies and approximated adjacency energies by with equation (18).

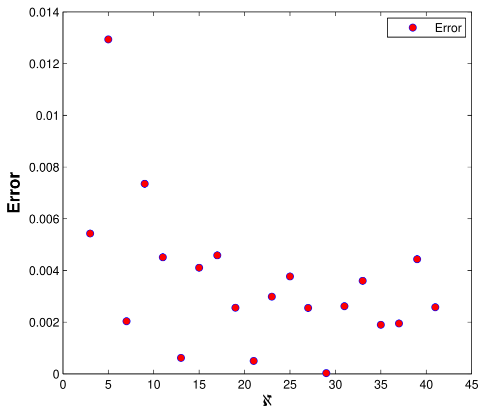

FIGURE 9. Absolute error between exact adjacency energies and approximated adjacency energies by with equation (19).

C. FUZZY ADJACENCY MATRIX ENERGY $\dot{\Phi}$ OF $\maltese(\dot{D}_{2\upsilon})$, WHERE υ IS ODD

The relation between fuzzy adjacency matrix energy $\dot{\Phi}$ for $\maltese(\dot{D}_{2\upsilon})$ and the values of υ in $\maltese(\dot{D}_{2\upsilon})$ is given in equation (19), which is generated by polynomial regression.

$$\begin{aligned}\dot{\Phi} = &-\frac{7789955364297077\,\upsilon^6}{1208925819614629174706176} \\ &+\frac{2264999464565113\,\upsilon^5}{2361183241434822606848} \\ &-\frac{8428646944186213\,\upsilon^4}{147573952589676412928} \\ &+\frac{4006096819602223\,\upsilon^3}{2305843009213693952} \\ &-\frac{2061371430098643\,\upsilon^2}{72057594037927936} \\ &+\frac{2240482132713677\,\upsilon}{9007199254740992} \\ &+\frac{2135402885199973}{4503599627370496}\end{aligned} \tag{19}$$

The absolute error between precise adjacency matrix energies and approximated adjacency matrix energies by equation (19) obtained with the help of polynomial regression is shown in Figure 9.

D. FUZZY DEGREE MATRIX ENERGY $\dot{\Psi}$ OF $\maltese(\dot{D}_{2\upsilon})$, WHERE υ IS ODD

The relation between fuzzy adjacency matrix energy $\dot{\Phi}$ for $\maltese(\dot{D}_{2\upsilon})$ and the values of υ in $\maltese(\dot{D}_{2\upsilon})$ is given in equation (20) which is generated by polynomial regression.

$$\dot{\Psi} = \frac{4525761030488853\,\upsilon}{9007199254740992} - \frac{6609891379687135}{72057594037927936} \tag{20}$$

The absolute error between precise degree matrix energies and approximated degree matrix energies by equation (20) obtained with the help of polynomial regression is shown in Figure 10.

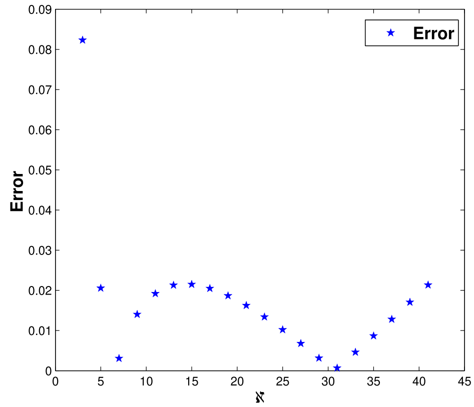

FIGURE 10. Absolute error between exact adjacency energies and approximated adjacency energies by with equation (20).

V. POTENTIAL APPLICATIONS

The application of dihedral groups in the study of molecular symmetry within the field of chemistry is a critical aspect of molecular modeling and analysis. Here are the key applications.

A. SYMMETRY OF MOLECULES

Dihedral groups are pivotal in the field of chemistry, offering profound insights into the symmetry of molecules, which is essential for comprehending their three-dimensional shape and structure. This understanding is exemplified in molecules like benzene (C_6H_6), where dihedral symmetry elucidates its stable, planar hexagonal structure. Beyond molecular geometry, the symmetry of reactants and products, as dictated by dihedral groups, plays a critical role in determining the outcomes of chemical reactions, influencing both the feasibility and nature of the products formed.

In the realm of spectroscopy, particularly when analyzing vibrational and rotational spectra, the symmetry of molecules, as characterized by these groups, is crucial. It aids in predicting the activity of various vibrational modes using techniques like infrared and Raman spectroscopy. Similarly, in quantum chemistry, dihedral groups assist in deciphering the electronic structure of molecules, enabling predictions about the behavior of molecular orbitals under different symmetry operations.

The role of dihedral groups extends to stereochemistry, where they are instrumental in understanding the spatial arrangement of atoms in both chiral and achiral molecules. This knowledge is fundamental in determining properties such as optical activity in organic compounds. In material science, understanding molecular symmetry, including dihedral symmetry, is key to predicting and explaining the properties of materials, particularly in crystalline structures.

Furthermore, in the field of drug design and pharmacology, the symmetry of drug molecules, as influenced by dihedral groups, can significantly impact their interaction with biological targets, affecting both their binding affinity and efficacy.Â

In conclusion, dihedral groups serve as a cornerstone in the study of molecular symmetry, with broad implications across various chemical disciplines. Their application is critical to accurately predicting and comprehending the physical and chemical properties of molecules based on their symmetrical characteristics.

B. CHIRALITY AND OPTICAL ACTIVITY

Chirality and optical activity are key concepts in chemistry, particularly relevant in stereochemistry, where dihedral groups play a significant role in their understanding. Chirality in molecules, defined by the inability to be superimposed on their mirror images, akin to human hands, is critical in various chemical and biological processes. Dihedral groups aid in identifying chirality by analyzing a molecule's symmetry elements. For example, a molecule with certain dihedral symmetries, like a rotation axis, can be achiral, whereas the absence of these symmetrical elements often signifies chirality.

In achiral molecules, dihedral symmetry elements, such as a rotation-reflection axis (S_n), are typically present and associated with dihedral groups, indicating a lack of chirality. In contrast, chiral molecules lack these dihedral symmetry elements, and understanding the presence or absence of such symmetries is crucial in determining a molecule's chirality.

Optical activity is another fascinating aspect, where chiral molecules uniquely rotate the plane of polarized light. This property is particularly significant in pharmacology, as the chirality of drug molecules can greatly influence their effectiveness. Dihedral groups provide insights into how different chiral molecules (enantiomers) interact with polarized light, with each enantiomer rotating the plane of polarized light to an equal degree but in opposite directions.

In practical applications, such as drug design, many drugs are chiral, and their therapeutic effect often hinges on their chirality. Understanding dihedral symmetries is key to designing and synthesizing the correct enantiomer. In material science, the chirality of molecules can impact the properties of various materials, including polymers and liquid crystals.

Finally, advanced analytical techniques like circular dichroism spectroscopy, which rely on the principles of chirality and optical activity, benefit from the understanding of dihedral groups. This knowledge aids in interpreting spectroscopic data to determine the absolute configuration of chiral molecules, illustrating the widespread implications of dihedral groups in the field of chemistry.

VI. CONCLUSION AND OPPORTUNITIES FOR FUTURE WORK

In this article, we have explored the application of fuzzy graph theory to the dihedral group's conjugate graph, presenting a significant enhancement in the computational approach to group theory analysis. By generalizing the fuzzy first Zagreb index, fuzzy second Zagreb index, fuzzy harmonic index, and fuzzy Randic index in polynomial form, we offer a transformative approach that simplifies and accelerates the calculation process. This advancement is crucial as it shifts the computational timeframe from hours to mere seconds, representing a substantial improvement in efficiency.

The core innovation in our research is the integration of machine learning, particularly polynomial regression, into the study of group theory. Polynomial regression, a technique commonly used in various fields for pattern recognition and prediction, is applied here to derive polynomials for the energies of adjacency and degree matrices in the fuzzy conjugate graph of a dihedral group. This application is ground-breaking in its approach, as it allows for a more nuanced and accurate analysis of the graph's properties. Furthermore, the inclusion of error analysis adds a layer of rigor and precision, ensuring the reliability of the results.

Our research serves as a testament to the potential of interdisciplinary approaches to solving complex mathematical problems. By bridging fuzzy graph theory with machine learning, we not only enhance the computational methods in group theory but also provide deeper insights into the structural and functional properties of dihedral groups. The polynomial forms of the indices facilitate a more accessible and quicker computation, which is invaluable for extensive studies involving large and complex graphs.

Moreover, the implications of this research extend beyond the realm of dihedral groups. The methodologies and findings presented here open up new possibilities for the application of these techniques to other complicated graph structures. This is particularly significant in the broader field of graph theory, where unraveling the intricate properties of various graph types is crucial.

In conclusion, our work stands as a pivotal contribution to both fuzzy graph theory and group theory. The incorporation of polynomial regression as a machine learning strategy in this context not only simplifies the computational process but also provides a novel perspective on the analysis of group structures. It paves the way for further research in this area, promising advancements in our understanding of complex graph structures and their applications. As such, the methodologies and findings of this study hold substantial promise for future explorations in group theory, graph theory, and related fields, potentially revolutionizing the way these disciplines approach and solve complex problems.

USE OF AI TOOLS DECLARATION

The authors declare they have not used artificial intelligence. (AI) tools in the creation of this article.

CONFLICT OF INTEREST

The authors state that there is no conflict of interest.

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