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Original paper

Second Zagreb index for fuzzy graphs and its application in mathematical chemistry

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Abstract

The Zagreb index (ZI) of a crisp graph and also for a fuzzy graph (FG) is a very much useful tool in network theory, spectral graph theory, molecular chemistry and several fields of chemistry and mathematics. The second ZI is studied for FGs here. Bounds of this index are calculated for several FGs: path, star, cycle, complete FG, partial fuzzy subgraph, etc. For isomorphic FGs, it is shown that the value of this index is same. Bounds of this index for the Cartesian product, composition, join and union of two FGs are established. At the end of this article, an application of the index in mathematical chemistry is studied. For this, octane isomers are considered and analyzed the correlation between this index with some physico-chemical properties of octane isomers. This index's correlation coefficient (r) with acentric factor and entropy is determined for the linear curve fittings. Using the value of r, one can conclude that this index can help estimate the acentric factor and entropy with significant accuracy. Also, these outcomes declare the appropriateness of the index in QSPR research.

Keywords: Fuzzy graph, second Zagreb index, topological index, chemical graph.

1 Introduction

1.1 Research background

In the year 1965, the concept of uncertainty in a classical set was firstly introduced by Zadeh [51] and called it fuzzy set. Inspired by this, in 1975, Rosenfeld [45] introduced the concept of the fuzzy graph (FG). Generalized neutrosophic planer graph [31] and link prediction in the neutrosophic graph [33] are studied by Mahapatra et al. A telecommunication system based on FGs [46] and a social network system based on fuzzy graphs [47] is studied by Samanta and Pal. Bipolar FG [1], soft FG [5], m-polar FG [2], generalized m-polar FG [49], bipolar fuzzy soft hypergraph [48] and connectivity in rough FG [6] are investigated by Akram et al. Rashmanlou et al. [44] studied the product of bipolar FGs. Muhiuddin et al. studied cubic planer graphs [38] and cubic Pythagorean fuzzy graphs [37]. Rashmanlou and Borzooei studied domination in vague graphs [11] and product of vague graph [43]. Complex Pythagorean fuzzy threshold graphs [3], $q-$rung orthopair fuzzy graphs [4], complex intuitionistic fuzzy threshold graphs [15], type 2 soft graphs [16], single-valued neutrosophic graphs [27] and hesitant fuzzy graphs [26] are studied by Karaaslan et al. The vertex degree is also studied for an FG in [39] and also discussed strong degree, strong neighbour of an FG. In [2, 24, 34, 36, 39], one can see for more generalization of an FG and related results.

In mathematical chemistry, topological indices are molecular descriptors that are calculated on the molecular graph of a chemical compound. topological indices are numerical quantities of a graph that describe its topology. An atom represents a vertex and a bond between two atoms represents an edge in a molecular graph. In 1947, the Wiener index (WI) was introduced by Wiener [50], which is used to calculate the boiling point of paraffins. Zagreb index (ZI) is degree-based TI established by Gutman and Trinajstic [14] and applied to determine π-electron energy of a conjugate

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system. Javaid et al. [23] studied some bounds for first Zagreb coindex for F-sum graphs. In 2015, Fortula and Gutman defined another degree-based topological index called forgotten topological index (F-index) [13]. Das and Gutman [12] studied some properties of second ZI for crisp graph. Second ZI for molecular graphs are studied by Kazemi [28]. Khalifeh et al. [29] studied the second ZI for some graph operations.

1.2 Motivation

Many results and applications are available for topological indices in crisp graphs. Some circumstances cannot be handled using crisp graphs in many real-life problems. In such cases, to handle the problem, those topological indices are needed to introduce in FGs. In 2019, Binu et al. introduced connectivity index (CI) [7], average CI [7], Wiener index (WI) [8], connectivity status [10] and cyclic CI [9] of an FG. Motivated from these articles, Recently, Islam and Pal also studied WI [17] for an FG and introduced hyper-WI [19], hyper-CI [20], first ZI [18] and F-index [21, 22] for FGs. In [32], Mahapatra et al. studied the RSM index in fuzzy graph. Poulik et al. studied certain index [41], Wiener absolute index [42] and Randic index [40] for bipolar fuzzy graphs. In [25] Kalathian et al. also introduced so many topological indices for fuzzy graphs. Motivated from those articles, in this paper, the second ZI is studied for FGs.

1.3 Significance and objective of the article

topological indices have a vital role in chemical graph, spectral graph, network theory, molecular chemistry, FG theory, etc. ZIs are such topological descriptors which are degree-based topological indices, applied to determine π-electron energy of a conjugate system and established by Gutman and Trinajstic [14] in 1972. The second ZI is studied for FGs here. Main results are arranged in two parts.
(i) In Section 2, some basic definitions are provided. In Section 3, some theoretical development of this index is investigated here i.e. bounds of this index are calculated for several FGs: path, cycle, star, complete FG, PFSG, etc. For an isomorphic FGs, it is shown that the value of this index is same. In Section 4, the bounds of this index for some fuzzy graph operations have been studied.
(ii) In Section 5, an application of the index in chemistry is studied. For this, octane isomers are considered and analyze the correlation of the index with some physico-chemical properties of octane isomers. We have shown that the correlation coefficient (r) of this index with acentric factor and entropy are -0.977966531 and -0.91961647 for the linear fittings respectively. Thus this index can help to estimate the acentric factor and entropy with significant accuracy. Also, these outcomes declare the appropriateness of the index in QSPR analysis.

2 Preliminaries

Some essential definitions and theorems which are needed to develop our results are given, most of them one can be found in [18, 21, 39].

For a universal set X, a fuzzy set is a pair $S = (X, \mu)$ where μ is a called membership function of S whose domain is X and co-domain is [0,1].

Definition 2.1. *An FG is a triplet, $\Gamma = (\Upsilon, \Psi, \Omega)$, where Υ is called vertex set of the fuzzy graph with vertex membership function $\Psi : \Upsilon \to [0,1]$ and membership function of edges $\Omega : \Upsilon \times \Upsilon \to [0,1]$ satisfying $\Omega(u,v) \le \min\{\Psi(u), \Psi(v)\}$. The edge set is defined as $\mathcal{E} = \{(u,v) : \Omega(u,v) > 0\}$.*

Definition 2.2. *For a vertex $v \in V(\Gamma)$, degree is defined as $d(v) = \sum_{u \in \Upsilon} \Omega(uv)$.*

Here, Δ and δ represents the maximum degree and minimum degree of Γ. Throughout this article, the FG, $\Gamma_1 = (\Upsilon_1, \Psi_1, \Omega_1)$ has n_1-vertices, m_1-edges, edge set $\mathcal{E}_1$ and $\Gamma_2 = (\Upsilon_2, \Psi_2, \Omega_2)$ has n_2-vertices, m_2-edges, edge set $\mathcal{E}_2$ and $\Delta_1 = \Delta(\Gamma_1), \Delta_2 = \Delta(\Gamma_2), \delta_1 = \delta(\Gamma_1), \delta_2 = \delta(\Gamma_2)$.

Now, Cartesian product, composition, join and union of two FGs are defined below:

Definition 2.3. [39] *Let $\Gamma_1 = (\Upsilon_1, \Psi_1, \Omega_1), \Gamma_2 = (\Upsilon_2, \Psi_2, \Omega_2)$ be two FGs. Then the Cartesian product of Γ_1 and Γ_2 is an FG $\Gamma_1 \times \Gamma_2 = (\Upsilon, \Psi, \Omega)$, where $\Upsilon = \Upsilon_1 \times \Upsilon_2$, $(u,v), (u_1,v_1), (u_2,v_2) \in \Upsilon, \Psi(u,v) = \wedge\{\Psi_1(u), \Psi_2(v)\}$ and*

$$\Omega((u_1,v_1),(u_2,v_2)) = \begin{cases} \wedge\{\Psi_1(u_1), \Omega_2(v_1,v_2)\} & \text{if } u_1 = u_2, v_1v_2 \in \mathcal{E}_2 \\ \wedge\{\Psi_2(v_1), \Omega_1(u_1,u_2)\} & \text{if } u_1u_2 \in \mathcal{E}_1, v_1 = v_2 \\ 0 & \text{otherwise.} \end{cases}$$

Definition 2.4. [39] *Let* $\Gamma_1 = (\Upsilon_1, \Psi_1, \Omega_1), \Gamma_2 = (\Upsilon_2, \Psi_2, \Omega_2)$ *be two FGs. Then the composition of* Γ_1 *and* Γ_2 *is an FG* $\Gamma_1[\Gamma_2] = (\Upsilon, \Psi, \Omega)$*, where* $\Upsilon = \Upsilon_1 \times \Upsilon_2$*,* $(u, v), (u_1, v_1), (u_2, v_2) \in \Upsilon, \Psi(u, v) = \wedge\{\Psi_1(u), \Psi_2(v)\}$ *and*

$$\Omega((u_1, v_1), (u_2, v_2)) = \begin{cases} \wedge\{\Psi_1(u_1), \Omega_2(v_1, v_2)\} \text{ if } u_1 = u_2 \text{ and } v_1v_2 \in \mathcal{E}_2 \\ \wedge\{\Psi_2(v_1), \Psi_2(v_2), \Omega_1(u_1, u_2)\} \text{ if } u_1u_2 \in \mathcal{E}_1 \\ 0 \text{ otherwise.} \end{cases}$$

Join and union of two FGs are defined below:

Definition 2.5. [39] *Let* $\Gamma_1 = (\Upsilon_1, \Psi_1, \Omega_1), \Gamma_2 = (\Upsilon_2, \Psi_2, \Omega_2)$ *be two FGs. Join of* Γ_1 *and* Γ_2 *is* $\Gamma_1 + \Gamma_2 = (\Upsilon, \Psi, \Omega)$*, where* $\Upsilon = \Upsilon_1 \cup \Upsilon_2$*,* $u, v, u_1, v_1 \in \Upsilon$*,*

$$\Psi(u) = \begin{cases} \Psi_1(u), \text{ if } u \in \Upsilon_1 \\ \Psi_2(u), \text{ if } u \in \Upsilon_2 \end{cases}$$

and

$$\Omega(u, v) = \begin{cases} \wedge\{\Psi_1(u), \Psi_2(v)\} \text{ if } u \in \Upsilon_1 \text{ and } v \in \Upsilon_2 \\ \Omega_1(u, v) \text{ if } uv \in \mathcal{E}_1 \\ \Omega_2(u, v) \text{ if } uv \in \mathcal{E}_2 \\ 0 \text{ otherwise.} \end{cases}$$

Definition 2.6. [39] *Suppose two FGs are* $\Gamma_1 = (\Upsilon_1, \Psi_1, \Omega_1)$ *and* $\Gamma_2 = (\Upsilon_2, \Psi_2, \Omega_2)$*. Union of* Γ_1 *and* Γ_2 *is* $\Gamma_1 \cup \Gamma_2 = (\Upsilon, \Psi, \Omega)$*, where* $\Upsilon = \Upsilon_1 \cup \Upsilon_2$*,* $u, v \in \Upsilon$*,*

$$\Psi(u) = \begin{cases} \Psi_1(u), \text{ if } u \in \Upsilon_1 \setminus \Upsilon_2 \\ \Psi_2(u), \text{ if } u \in \Upsilon_2 \setminus \Upsilon_1 \\ \max\{\Psi_1(u), \Psi_2(u)\}, \text{ if } u \in \Upsilon_1 \cap \Upsilon_2 \end{cases}$$

and

$$\Omega(u, v) = \begin{cases} \Omega_1(u, v) \text{ if } uv \in \mathcal{E}_1 \setminus \mathcal{E}_2 \\ \Omega_2(u, v) \text{ if } uv \in \mathcal{E}_2 \setminus \mathcal{E}_1 \\ \vee\{\Psi_1(u, v), \Psi_2(u, v)\} \text{ if } (u, v) \in \mathcal{E}_1 \cap \mathcal{E}_2 \\ 0 \text{ otherwise.} \end{cases}$$

3 Second Zagreb index of fuzzy graphs

Topological indices have an important character in chemical graph, spectral graph theory, network theory, molecular chemistry, FG theory, etc. In 1972, Gutman and Trinajstic [14] introduced the second ZI of a crisp graph as:

Definition 3.1. [14] *Suppose* $\Gamma = (\Upsilon, \mathcal{E})$ *be a crisp graph. The second ZI of* Γ *is defined by:*

$$M_2(\Gamma) = \sum_{uv \in \mathcal{E}} d(u)d(v).$$

Recently, Kalathian et al. [25] introduced second ZI for an FG.

Definition 3.2. [25] *Suppose* $\Gamma = (\Upsilon, \Psi, \Omega)$ *be an FG. The second ZI of* Γ *is defined by:*

$$ZF_2(\Gamma) = \sum_{uv \in \mathcal{E}} \Psi(u)\Psi(v)d(u)d(v).$$

In the next theorem, an upper bound of this index is provided.

Theorem 3.3. *Suppose* Γ *be a fuzzy graph having* n *vertices and* m *edges. Then* $ZF_2(\Gamma) \leq m(n-1)^2$.

Proof. As $\Psi(v) \leq 1$, then,

$$ZF_2(\Gamma) = \sum_{uv \in \mathcal{E}} \Psi(u)d(u)\Psi(v)d(v) \leq \sum_{uv \in \mathcal{E}} \Delta^2 = \Delta^2 m \leq m(n-1)^2.$$

□

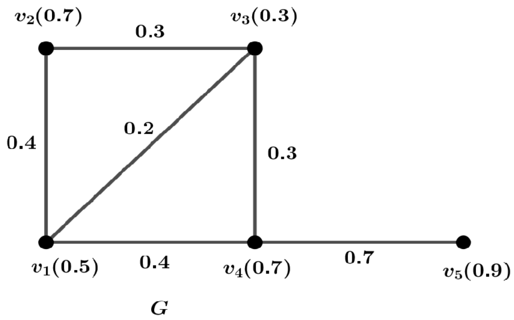

Figure 1: An FG with $ZF_2(G) = 1.8252$.

Example 3.4. *Suppose,* $\Gamma = (\Upsilon, \Psi, \Omega)$ *be an FG shown in Figure 1 where* $\{v_1, v_2, \cdots, v_5\}$ *is vertex set and* $\Psi(v_1) = 0.5, \Psi(v_2) = 0.7, \Psi(v_3) = 0.3, \Psi(v_4) = 0.7, \Psi(v_5) = 0.9, \Omega(v_1, v_2) = 0.4, \Omega(v_1, v_3) = 0.2, \Omega(v_2, v_3) = 0.3, \Omega(v_3v_4) = 0.3, \Omega(v_1v_4) = 0.4, \Omega(v_4, v_5) = 0.7$. *Then* $d(v_1) = 1.0, d(v_2) = 0.7, d(v_3) = 0.8, d(v_4) = 1.4, d(v_5) = 0.7$. *Therefore,*

$$\begin{aligned}
ZF_2(\Gamma) = &\sum_{uv\in\mathcal{E}} \Psi(u)\Psi(v)d(u)d(v)\\
=&[0.5 \times 1.0 \times 0.7 \times 0.7] + [0.5 \times 1.0 \times 0.3 \times 0.8] + [0.5 \times 1.0 \times 0.7 \times 1.4]\\
+&[0.7 \times 0.7 \times 0.3 \times 0.8] + [0.3 \times 0.8 \times 0.7 \times 1.4] + [0.7 \times 1.4 \times 0.9 \times 0.7]\\
=&1.8252 < 96 = m(n-1)^2.
\end{aligned}$$

The Example 3.4 shows the Theorem 3.3 is satisfied for the FG G in Figure 1. Also, the value of this index for an FSG is less than the original FG, as shown in the example below.

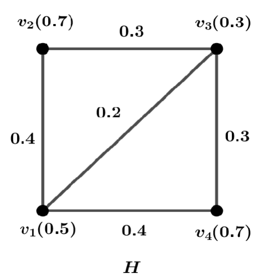

Figure 2: A FSG Γ' of the FG Γ in Figure 1 with $ZF_2(\Gamma') = ZF_2(\Gamma)$.

Example 3.5. *Suppose,* Γ *be an FG and* Γ' *be its FSG (Figure 2) gain by removing* v_5. *Then* $d(v_1) = 1.0, d(v_2) = 0.7, d(v_3) = 0.8, d(v_4) = 0.7$. *Now,*

$$\begin{aligned}
ZF_2(\Gamma') = &\sum_{uv\in\mathcal{E}(\Gamma')} \Psi(u)\Psi(v)d(u)d(v)\\
=&[0.5 \times 1.0 \times 0.7 \times 0.7] + [0.5 \times 1.0 \times 0.3 \times 0.8] + [0.5 \times 1.0 \times 0.7 \times 1.7]\\
+&[0.7 \times 0.7 \times 0.3 \times 0.8] + [0.3 \times 0.8 \times 0.7 \times 0.7]\\
=&0.8452 \leq ZF_2(\Gamma).
\end{aligned}$$

Note that, from Examples 3.4 and 3.5, we get $ZF_2(\Gamma') \leq ZF_2(\Gamma)$. In the next proposition we proved the fact in general.

Proposition 3.6. *Let* $\Gamma' = (\Upsilon', \Psi', \Omega')$ *be a PFSG of an FG* $\Gamma = (\Upsilon, \Psi, \Omega)$. *Then* $ZF_2(\Gamma') \leq ZF_2(\Gamma)$.

Proof. If $u, v \in \Upsilon'$, then $\Psi'(u) \leq \Psi(u)$ and $\Omega'(uv) \leq \Omega(uv)$. So, $d'_\Gamma(u) \leq \sum_{v\in\Upsilon'} \Omega(u, v) \leq d_\Gamma(u)$. Therefore,

$$ZF_2(\Gamma') = \sum_{uv\in\mathcal{E}'} \Psi'(u)\Psi'(v)d_{\Gamma'}(u)d_{\Gamma'}(v) \leq \sum_{uv\in\mathcal{E}} \Psi(u)d_\Gamma(u)\Psi(v)d_\Gamma(v) = ZF_2(\Gamma).$$

Hence, $ZF_2(\Gamma') \leq ZF_2(\Gamma)$. □

Let $0 \leq p \leq 1$, the FG $\Gamma^p = (\Upsilon', \Psi', \Omega')$ is a FSG of the FG $\Gamma = (\Upsilon, \Psi, \Omega)$ and is defined as $\Upsilon' = \{v \in \Upsilon : \Psi(v) \leq p\}$ and $\Psi'(v) = \Psi(v), \Omega'(uv) = \Omega(uv)$ for $u, v \in \Upsilon'$.

Theorem 3.7. *Suppose $\Gamma = (\Upsilon, \Psi, \Omega)$ be an FG and let $0 \leq p_1 \leq p_2 \leq 1$. Then $MF_2(\Gamma^{p_2}) \leq MF_2(\Gamma^{p_1})$.*

Corollary 3.8. *Let $\Gamma = (\Upsilon, \Psi, \Omega)$ be an FG and let $0 \leq p_1 \leq p_2 \leq \cdots \leq p_n \leq 1$. Then*

$$ZF_2(\Gamma^{p_n}) \leq ZF_2(\Gamma^{p_{n-1}}) \leq \cdots \leq ZF_2(\Gamma^{p_2}) \leq ZF_2(\Gamma^{p_1}).$$

In the next theorem, second ZI of a path is discussed.

Theorem 3.9. *Suppose P is a path having n vertices. Then $ZF_2(P) \leq 4(n-2)$.*

Proof. As $P(v_1, \cdots, v_n)$ is an n-vertex path, then $d(v_1) = \Omega_1, d(v_n) = \Omega_n$ and $d(v_i) = \Omega_i + \Omega_{i-1}$ for $i = 2, 3, \cdots, n-1$. Therefore,

$$\begin{aligned} ZF_2(P) = &\sum_{uv\in\mathcal{E}} \Psi(u)d(u)\Psi(v)d(v) \\ =&\Psi_1\Psi_2\Omega_1(\Omega_1 + \Omega_2) + \Psi_{n-1}\Psi_n\Omega_n(\Omega_{n-1} + \Omega_n) + \sum_{i=2}^{n-2} \Psi_i\Psi_{i+1}(\Omega_i + \Omega_{i+1})(\Omega_{i+1} + \Omega_{i+2}) \\ \leq&2 + 2 + \sum_{i=2}^{n-2} 4 \\ =&4(n-2). \end{aligned}$$

This completes the proof. □

Now second ZI of a cycle is studied here.

Theorem 3.10. *Suppose C is a cycle having n vertices. Then $ZF_2(C) \leq 4(n-1)$.*

Proof. As $C(v_1, \cdots, v_n)$ is a n-vertex cycle, then $d(v_1) = \Omega_1 + \Omega_n$ and $d(v_i) = \Omega_{i-1} + \Omega_i$ for $i = 2, \cdots, n$. Therefore,

$$\begin{aligned} ZF_2(C) = &\sum_{uv\in\mathcal{E}} \Psi(u)d(u)\Psi(v)d(v) \\ =&\Psi_1\Psi_2(\Omega_1 + \Omega_2)(\Omega_1 + \Omega_n) + \Psi_1\Psi_n(\Omega_1 + \Omega_n)(\Omega_{n-1} + \Omega_n) \\ &+ \sum_{i=2}^{n-2} \Psi_i\Psi_{i+1}(\Omega_{i-1} + \Omega_i)(\Omega_i + \Omega_{i+1}) \\ \leq&4 + 4 + \sum_{i=2}^{n-2} 4 \\ =&4(n-1). \end{aligned}$$

This completes the proof. □

Theorem 3.11. *Suppose S is a star having n vertices. Then $ZF_2(S) \leq (n-1)^2$.*

Proof. As $S(v_0 : v_1, \cdots, v_n)$ is a star having $(n + 1)$ vertices, then $d(v_0) = \sum_{i=1}^n \Omega_i$ and $d(v_i) = \Omega_i$ for $i = 1, 2, \cdots, n$. Therefore,

$$ZF_2(S) = \sum_{uv\in\mathcal{E}} \Psi(u)d(u)\Psi(v)d(v) = \Psi_0(\sum_{i=1}^n \Omega_i)(\sum_{i=1}^n \Psi_i\Omega_i) \leq n^2.$$

□

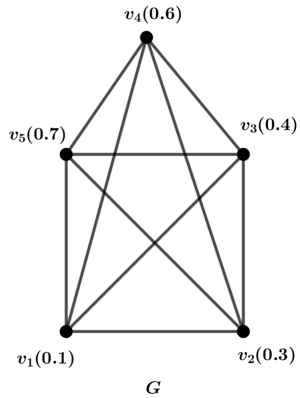

Figure 3: A complete FG with $ZF_2(\Gamma) = 2.4908$.

Second ZI of the complete FG depicted in Figure 3 is evaluated below.

Example 3.12. *Suppose Γ is a complete FG depicted in Figure 3 with $\Upsilon = \{v_1, v_2, \cdots, v_5\}$ is a vertex set and $\Psi(v_1) = 0.1, \Psi(v_2) = 0.3, \Psi(v_3) = 0.4, \Psi(v_4) = 0.6, \Psi(v_5) = 0.7$. Then the degree of the vertices are $d(v_1) = 0.4, d(v_2) = 1, d(v_3) = 1.2, d(v_4) = 1.4, d(v_5) = 1.4$. Therefore, the second ZI of the FG Γ is*

$$\begin{aligned}
ZF_2(\Gamma) = &\sum_{uv\in\mathcal{E}} \Psi(u)\Psi(v)d(u)d(v)\\
=&[0.1\times 0.4\times 0.3\times 1] + [0.1\times 0.4\times 0.4\times 1.2] + [0.1\times 0.4\times 0.6\times 1.4]\\
+&[0.1\times 0.4\times 0.7\times 1.4] + [0.3\times 1\times 0.4\times 1.2] + [0.3\times 1\times 0.6\times 1.4]\\
+&[0.3\times 1\times 0.7\times 1.4] + [0.4\times 1.2\times 0.6\times 1.4] + [0.4\times 1.2\times 0.7\times 1.4]\\
+&[0.6\times 1.4\times 0.7\times 1.4]\\
=&2.4908.
\end{aligned}$$

Theorem 3.13. *Suppose Γ is a complete FG with vertex set $V = \{v_1, v_2, \cdots, v_n\}$. Then*

$$0 \le \frac{n(n-1)^3}{2}\Psi_0^4 \le ZF_2(\Gamma) \le \frac{n(n-1)^3}{2}\Psi_n^4 \le \frac{n(n-1)^3}{2},$$

where $\Psi(v_i) = \Psi_i$ and $\Psi_1 \le \Psi_2 \le \cdots \le \Psi_n$ for $i = 1, 2, \cdots, n$.

Proof. As Γ is a complete FG, and $\Psi(v_i) = \Psi_i$ and $\Psi_1 \le \Psi_2 \le \cdots \le \Psi_n$ for $i = 1, 2, \cdots, n$, so $d(v_i) = (n-i)\Psi_i + \sum_{j=1}^{i-1}\Psi_j$. Therefore,

$$\begin{aligned}
ZF_2(\Gamma) &= \sum_{uv\in E} \Psi(u)d(u)\Psi(v)d(v)\\
&= \sum_{1\le i<j\le n} \Psi_i\Psi_j\{[(n-i)\Psi_i + \sum_{k=1}^{i-1}\Psi_k][(n-j)\Psi_j + \sum_{k=1}^{j-1}\Psi_k]\}\\
&\le \sum_{1\le i<j\le n} \Psi_n^2\{[(n-i)\Psi_n + \sum_{k=1}^{i-1}\Psi_n][(n-j)\Psi_n + \sum_{k=1}^{j-1}\Psi_n]\}\\
&= \Psi_n^4 \sum_{1\le i<j\le n} [(n-i)+i-1][(n-j)+j-1]\\
&= \frac{n(n-1)^3}{2}\Psi_n^4.
\end{aligned}$$

Other inequalities follows similarly. □

An FG $C[\Gamma] = (\Upsilon, \Psi, \Omega^c)$ is constructed from the FG $\Gamma = (\Upsilon, \Psi, \Omega)$ as $\Omega^c(uv) = \wedge\{\Psi(u), \Psi(v)\}$. This FG is called completion FG of Γ.

Theorem 3.14. *For any FG Γ, $ZF_2(\Gamma) \leq ZF_2(C[\Gamma])$.*

Proof. As $C[\Gamma]$ is completion FG of Γ, then $\forall (u,v) \in \mathcal{E}, \Omega(u,v) \leq \Omega^c(u,v)$. So, Γ is partial fuzzy subgraph of $C[\Gamma]$. Therefore, the result follows by Proposition 3.6. □

Corollary 3.15. *Suppose an FG Γ has n vertices. Then $ZF_2(\Gamma) \leq \frac{n(n-1)^3}{2}$.*

Second ZI is discussed for isomorphic FGs in the next theorem.

Theorem 3.16. *Suppose Γ_1 and Γ_2 are isomorphic FGs. Then $ZF_2(\Gamma_1) = ZF_2(\Gamma_2)$.*

Proof. There exists a bijective mapping $\Phi : \Upsilon_1 \to \Upsilon_2$ and $\forall u, v \in V_1, \Psi_1(v) = \Psi_2(\Phi(v))$ and $\Omega_1(u,v) = \Omega_2(\Phi(u), \Phi(v))$, as Γ_1 and Γ_2 be isomorphic FGs. Then

$$d_{\Gamma_1}(v) = \sum_{u\in\Upsilon_1} \Omega_1(u,v) = \sum_{u\in\Upsilon_1} \Omega_2(\Phi(u),\Phi(v)) = \sum_{\phi(u)\in\Upsilon_2} \Omega_2(\Phi(u),\Phi(v)) = d_{\Gamma_2}(\Phi(v)).$$

Therefore,

$$\begin{aligned} ZF_2(\Gamma_1) &= \sum_{uv\in\mathcal{E}_1} \Psi_1(u)d_{\Gamma_1}(u)\Psi_1(v)d_{\Gamma_1}(v) = \sum_{uv\in\mathcal{E}_1} \Psi_2(\Phi(u))d_{\Gamma_2}(\Phi(u))\Psi_2(\Phi(v))d_{\Gamma_2}(\Phi(v)) \\ &= \sum_{\Phi(u)\Phi(v)\in\mathcal{E}_2} \Psi_2(\Phi(u))d_{\Gamma_2}(\Phi(u))\Psi_2(\Phi(v))d_{\Gamma_2}(\Phi(v)) = ZF_2(\Gamma_2). \end{aligned}$$

This completes the proof. □

One can see Theorem 1 of [25] for another proof of the above Theorem 3.16. Bounds for the second ZI is provided below.

Theorem 3.17. *Suppose Γ be an FG having n vertices and m edges. Then $\frac{\delta^4}{m} \leq ZF_2(\Gamma) \leq m\Delta^2$.*

Proof. For $v \in \Upsilon, \delta \leq d(v) \leq m\Psi(v)$. Therefore, $\Psi(v) \geq \frac{\delta}{m}$. Now,

$$ZF_2(\Gamma) = \sum_{uv\in\mathcal{E}} \Psi(u)d(u)\Psi(v)d(v) \leq \Delta^2 \sum_{uv\in\mathcal{E}} [\Psi(u)\Psi(v)] \leq m\Delta^2.$$

Again,

$$ZF_2(\Gamma) = \sum_{uv\in\mathcal{E}} \Psi(u)d(u)\Psi(v)d(v) \geq \delta^2 \sum_{uv\in\mathcal{E}} [\Psi(u)\Psi(v)] \geq \delta^2 \sum_{1}^{m} (\frac{\delta}{m})^2 = \frac{\delta^4}{m}.$$

□

4 Bounds of second Zagreb indices for fuzzy graphs during operations

Some relations of second ZI are discussed during some FG operations here.

Theorem 4.1. $ZF_2(\Gamma_1 \times \Gamma_2) \leq m_2 ZF_1(\Gamma_1) + m_1 ZF_1(\Gamma_2) + n_2 ZF_2(\Gamma_1) + n_1 ZF_2(\Gamma_2) + 2\Delta_1\Delta_2(n_1m_2 + n_2m_1)$.

Proof. As $\Gamma_1 \times \Gamma_2$ is Cartesian product of Γ_1 and Γ_2, then for $(u,v), (u_1,v_1) \in \Upsilon, \Psi(u,v) = \wedge\{\Psi_1(u), \Psi_2(v)\}$ and

$$\Omega((u,v),(u_1,v_1)) = \begin{cases} \wedge\{\Psi_1(u), \Omega_2(v,v_1)\} & \text{if } u = u_1 \text{ and } vv_1 \in \mathcal{E}_2 \\ \wedge\{\Psi_2(v), \Omega_1(u,u_1)\} & \text{if } uu_1 \in \mathcal{E}_1 \text{ and } v = v_1 \\ 0 & \text{otherwise.} \end{cases}$$

Then

$$\begin{aligned} d_{\Gamma_1\times\Gamma_2}(u,v) &= \sum_{v_iv\in\mathcal{E}_2}\Omega\{(u,v),(u,v_i)\}+\sum_{u_iu\in\mathcal{E}_1}\Omega\{(u,v),(u_i,v)\} \\ &= \sum_{v_iv\in\mathcal{E}_2}\wedge\{\Psi_1(u),\Omega_2(v,v_i)\}+\sum_{u_iu\in\mathcal{E}_1}\wedge\{\Psi_2(v),\Omega_1(u,u_i)\} \\ &\le \sum_{v_iv\in\mathcal{E}_2}\Omega_2(v,v_i)+\sum_{u_iu\in\mathcal{E}_1}\Omega_1(u,u_i) \\ &= d_{\Gamma_1}(u)+d_{\Gamma_2}(v). \end{aligned}$$

Then second ZI of $\Gamma_1\times\Gamma_2$ is:

$$\begin{aligned} ZF_2(\Gamma_1\times\Gamma_2) &= \sum_{(u_1,v_1)(u_2,v_2)\in\mathcal{E}(\Gamma_1\times\Gamma_2)}\Psi(u_1,v_1)\Psi(u_2,v_2)d_{\Gamma_1\times\Gamma_2}(u_1,v_1)d_{\Gamma_1\times\Gamma_2}(u_2,v_2) \\ &= \sum_{u\in\Upsilon_1,v_1v_2\in\mathcal{E}_2}\Psi(u,v_1)\Psi(u,v_2)d_{\Gamma_1\times\Gamma_2}(u,v_1)d_{\Gamma_1\times\Gamma_2}(u,v_2) \\ &+ \sum_{v\in\Upsilon_2,u_1u_2\in\mathcal{E}_1}\Psi(u_1,v)\Psi(u_2,v)d_{\Gamma_1\times\Gamma_2}(u_1,v)d_{\Gamma_1\times\Gamma_2}(u_2,v) \\ &= K_1+K_2, \end{aligned}$$

where $K_1=\sum_{u\in\Upsilon_1,v_1v_2\in\mathcal{E}_2}\Psi(u,v_1)\Psi(u,v_2)d_{\Gamma_1\times\Gamma_2}(u,v_1)d_{\Gamma_1\times\Gamma_2}(u,v_2)$ and

$$K_2=\sum_{v\in\Upsilon_2,u_1u_2\in\mathcal{E}_1}\Psi(u_1,v)\Psi(u_2,v)d_{\Gamma_1\times\Gamma_2}(u_1,v)d_{\Gamma_1\times\Gamma_2}(u_2,v).$$

Now

$$\begin{aligned} K_1 &= \sum_{u\in\Upsilon_1,v_1v_2\in\mathcal{E}_2}\Psi(u,v_1)\Psi(u,v_2)d_{\Gamma_1\times\Gamma_2}(u,v_1)d_{\Gamma_1\times\Gamma_2}(u,v_2) \\ &\le \sum_{u\in\Upsilon_1,v_1v_2\in\mathcal{E}_2}[\Psi_1(u)d_{\Gamma_1}(u)+\Psi_2(v_1)d_{\Gamma_2}(v_1)][\Psi_1(u)d_{\Gamma_1}(u)+\Psi_2(v_2)d_{\Gamma_2}(v_2)] \\ &= \sum_{u\in\Upsilon_1,v_1v_2\in\mathcal{E}_2}\{\Psi_1(u)d_{\Gamma_1}(u)\}^2+\sum_{u\in\Upsilon_1,v_1v_2\in\mathcal{E}_2}\Psi_2(v_1)d_{\Gamma_2}(v_1)\Psi_2(v_2)d_{\Gamma_2}(v_2) \\ &+ \sum_{u\in\Upsilon_1,v_1v_2\in\mathcal{E}_2}\Psi_1(u)d_{\Gamma_1}(u)\{\Psi_2(v_1)d_{\Gamma_2}(v_1)+\Psi_2(v_2)d_{\Gamma_2}(v_2)\} \\ &\le \sum_{v_1v_2\in\mathcal{E}_2}ZF_1(\Gamma_1)+\sum_{u\in\Upsilon_1}ZF_2(\Gamma_2)+2\Delta_1\Delta_2\sum_{u\in\Upsilon_1,v_1v_2\in\mathcal{E}_2}1 \\ &= m_2ZF_1(\Gamma_1)+n_1ZF_2(\Gamma_2)+2n_1m_2\Delta_1\Delta_2. \end{aligned}$$

So, $K_1\le m_2ZF_1(\Gamma_1)+n_1ZF_2(\Gamma_2)+2n_1m_2\Delta_1\Delta_2$.
Similarly one can get $K_2\le m_1ZF_1(\Gamma_2)+n_2ZF_2(\Gamma_1)+2n_2m_1\Delta_1\Delta_2$.
Therefore,

$$\begin{aligned} ZF_2(\Gamma_1\times G_2) &\le K_1+K_2 \\ &\le m_2ZF_1(\Gamma_1)+m_1ZF_1(\Gamma_2)+n_2ZF_2(\Gamma_1)+n_1ZF_2(\Gamma_2)+2\Delta_1\Delta_2(n_1m_2+n_2m_1). \end{aligned}$$

Hence the result. □

Corollary 4.2. *(i)* $ZF_2(\Gamma_1\times\Gamma_2)\le(n_1m_2+n_2m_1)(\Delta_1+\Delta_2)^2$,
(ii) $ZF_2(\Gamma_1\times\Gamma_2)\le(n_1m_2+n_2m_1)(n_1+n_2-2)^2$ *and*
(iii) $ZF_2(\Gamma_1\times\Gamma_2)\le 4m_1^2n_1^2m_2+4m_2^2n_2^2m_1+m_1n_2(n_1-1)^2+m_2n_1(n_2-1)^2+2(n_1-1)(n_2-1)(n_1m_2+n_2m_1)$.

Theorem 4.3. $ZF_2(\Gamma_1[\Gamma_2]) \leq n_2^2 m_2 ZF_1(\Gamma_1) + n_2^4 ZF_2(\Gamma_1) + (m_1+n_1)ZF_2(\Gamma_2) + 2n_2(n_1 m_2 + m_1 n_2^2)\Delta_1\Delta_2 + m_1(n_2^2 - m_2)\Delta_2^2$.

Proof. As $\Gamma_1[\Gamma_2]$ is composition graph of Γ_1 and Γ_2, then for $(u,v),(u_1,v_1) \in \Upsilon, \Psi(u,v) = \wedge\{\Psi_1(u),\Psi_2(v)\}$ and

$$\Omega((u,v),(u_1,v_1)) = \begin{cases} \wedge\{\Psi_1(u),\Omega_2(v,v_1)\} & \text{if } u=u_1 \text{ and } vv_1 \in \mathcal{E}_2 \\ \wedge\{\Psi_2(v),\Psi_2(v_1),\Omega_1(u,u_1)\} & \text{if } uu_1 \in \mathcal{E}_1 \\ 0 & \text{otherwise.} \end{cases}$$

Then,

$$\begin{aligned} d_{\Gamma_1[\Gamma_2]}(u,v) &= \sum_{v_i v \in \mathcal{E}_2} \Omega\{(u,v),(u,v_i)\} + \sum_{u_i u \in \mathcal{E}_1, v_j \in \Upsilon_2} \Omega\{(u,v),(u_i,v_j)\} \\ &= \sum_{v_i v \in \mathcal{E}_2} \wedge\{\Psi_1(u),\Omega_2(v,v_i)\} + \sum_{u_i u \in \mathcal{E}_1, v_j \in \Upsilon_2} \wedge\{\Psi_2(v),\Psi_2(v_j)\Omega_1(u,u_i)\} \\ &\leq \sum_{v_i v \in \mathcal{E}_2} \Omega_2(v,v_i) + \sum_{u_i u \in \mathcal{E}_1, v_j \in \Upsilon_2} \Omega_1(u,u_i) \\ &= n_2 d_{\Gamma_1}(u) + d_{\Gamma_2}(v). \end{aligned}$$

Then second ZI of $\Gamma_1[\Gamma_2]$ is:

$$\begin{aligned} ZF_2(\Gamma_1[\Gamma_2]) &= \sum_{(u_1,v_1)(u_2,v_2) \in E(\Gamma_1[\Gamma_2])} \Psi(u_1,v_1)\Psi(u_2,v_2) d_{\Gamma_1[\Gamma_2]}(u_1,v_1) d_{\Gamma_1[\Gamma_2]}(u_2,v_2) \\ &= \sum_{u \in \Upsilon_1, v_1 v_2 \in \mathcal{E}_2} \Psi(u,v_1)\Psi(u,v_2) d_{\Gamma_1[\Gamma_2]}(u,v_1) d_{\Gamma_1[\Gamma_2]}(u,v_2) \\ &+ \sum_{v_1,v_2 \in \Upsilon_2, u_1 u_2 \in \mathcal{E}_2} \Psi(u_1,v_1)\Psi(u_2,v_2) d_{\Gamma_1[\Gamma_2]}(u_1,v_1) d_{\Gamma_1[\Gamma_2]}(u_2,v_2) \\ &= K_1 + K_2, \end{aligned}$$

where $K_1 = \sum_{u \in \Upsilon_1, v_1 v_2 \in \mathcal{E}_2} \Psi(u,v_1)\Psi(u,v_2) d_{\Gamma_1[\Gamma_2]}(u,v_1) d_{\Gamma_1[\Gamma_2]}(u,v_2)$ and

$$K_2 = \sum_{v_1,v_2 \in \Upsilon_2, u_1 u_2 \in \mathcal{E}_1} \Psi(u_1,v_1)\Psi(u_2,v_2) d_{\Gamma_1[\Gamma_2]}(u_1,v_1) d_{\Gamma_1[\Gamma_2]}(u_2,v_2).$$

Now

$$\begin{aligned} K_1 &= \sum_{u \in \Upsilon_1, v_1 v_2 \in \mathcal{E}_2} \Psi(u,v_1)\Psi(u,v_2) d_{\Gamma_1[\Gamma_2]}(u,v_1) d_{\Gamma_1[\Gamma_2]}(u,v_2) \\ &\leq \sum_{u \in \Upsilon_1, v_1 v_2 \in \mathcal{E}_2} [n_2\Psi_1(u) d_{\Gamma_1}(u) + \Psi_2(v_1) d_{\Gamma_2}(v_1)][n_2\Psi_1(u) d_{\Gamma_1}(u) + \Psi_2(v_2) d_{\Gamma_2}(v_2)] \\ &= n_2^2 \sum_{u \in \Upsilon_1, v_1 v_2 \in \mathcal{E}_2} \{\Psi_1(u) d_{\Gamma_1}(u)\}^2 + \sum_{u \in \Upsilon_1, v_1 v_2 \in \mathcal{E}_2} \Psi_2(v_1) d_{\Gamma_2}(v_1)\Psi_2(v_2) d_{\Gamma_2}(v_2) \\ &+ n_2 \sum_{u \in \Upsilon_1, v_1 v_2 \in \mathcal{E}_2} \Psi_1(u) d_{\Gamma_1}(u)\{\Psi_2(v_1) d_{\Gamma_2}(v_1) + \Psi_2(v_2) d_{\Gamma_2}(v_2)\} \\ &\leq n_2^2 \sum_{v_1 v_2 \in \mathcal{E}_2} ZF_1(\Gamma_1) + \sum_{u \in \Upsilon_1} ZF_2(\Gamma_2) + 2n_2\Delta_1\Delta_2 \sum_{u \in \Upsilon_1, v_1 v_2 \in \mathcal{E}_2} 1 \\ &= n_2^2 m_2 ZF_1(\Gamma_1) + n_1 ZF_2(\Gamma_2) + 2n_1 n_2 m_2 \Delta_1\Delta_2. \end{aligned}$$

So, $K_1 \leq n_2^2 m_2 ZF_1(\Gamma_1) + n_1 ZF_2(\Gamma_2) + 2n_1 n_2 m_2 \Delta_1\Delta_2$.

Now

$$\begin{aligned}
K_2 &= \sum_{v_1,v_2\in\Upsilon_2,u_1u_2\in\mathcal{E}_1} \Psi(u_1,v_1)\Psi(u_2,v_2)d_{\Gamma_1[\Gamma_2]}(u_1,v_1)d_{\Gamma_1[\Gamma_2]}(u_2,v_2)\\
&\le \sum_{v_1,v_2\in V_2,u_1u_2\in\mathcal{E}_1} [n_2\Psi_1(u_1)d_{\Gamma_1}(u_1)+\Psi_2(v_1)d_{\Gamma_2}(v_1)][n_2\Psi_1(u_2)d_{\Gamma_1}(u_2)+\Psi_2(v_2)d_{\Gamma_2}(v_2)]\\
&= n_2^2\sum_{v_1,v_2\in\Upsilon_2,u_1u_2\in\mathcal{E}_1} \Psi_1(u_1)d_{\Gamma_1}(u_1)\Psi_1(u_2)d_{\Gamma_1}(u_2)+\sum_{v_1,v_2\in\Upsilon_2,u_1u_2\in\mathcal{E}_1}\Psi_2(v_1)d_{\Gamma_2}(v_1)\Psi_2(v_2)d_{\Gamma_2}(v_2)\\
&+n_2\sum_{v_1,v_2\in\Upsilon_2,u_1u_2\in\mathcal{E}_1}[\Psi_1(u_1)d_{\Gamma_1}(u_1)\Psi_2(v_2)d_{\Gamma_2}(v_2)+\Psi_1(u_2)d_{\Gamma_1}(u_2)\Psi_2(v_1)d_{\Gamma_2}(v_1)]\\
&= n_2^2\sum_{v_1,v_2\in\Upsilon_2,u_1u_2\in\mathcal{E}_1} \Psi_1(u_1)d_{\Gamma_1}(u_1)\Psi_1(u_2)d_{\Gamma_1}(u_2)+\sum_{v_1v_2\in\mathcal{E}_2,u_1u_2\in\mathcal{E}_1}\Psi_2(v_1)d_{\Gamma_2}(v_1)\Psi_2(v_2)d_{\Gamma_2}(v_2)\\
&+\sum_{(v_1,v_2)\in\Upsilon_2\times\Upsilon_2\setminus\mathcal{E}_2,u_1u_2\in\mathcal{E}_1}\Psi_2(v_1)d_{\Gamma_2}(v_1)\Psi_2(v_2)d_{\Gamma_2}(v_2)\\
&+n_2\sum_{v_1,v_2\in\Upsilon_2,u_1u_2\in\mathcal{E}_1}[\Psi_1(u_1)d_{\Gamma_1}(u_1)\Psi_2(v_2)d_{\Gamma_2}(v_2)+\Psi_1(u_2)d_{\Gamma_1}(u_2)\Psi_2(v_1)d_{\Gamma_2}(v_1)]\\
&\le n_2^2\sum_{v_1,v_2\in\Upsilon_2}ZF_2(\Gamma_1)+\sum_{u_1u_2\in\mathcal{E}_1}ZF_2(\Gamma_2)+\sum_{(v_1,v_2)\in\Upsilon_2\times\Upsilon_2\setminus\mathcal{E}_2,u_1u_2\in\mathcal{E}_1}\Delta_2^2+n_2\sum_{v_1,v_2\in\Upsilon_2,u_1u_2\in\mathcal{E}_1}2\Delta_1\Delta_2\\
&= n_2^4ZF_2(\Gamma_1)+m_1ZF_2(\Gamma_2)+m_1(n_2^2-m_2)\Delta_2^2+2n_2^3m_1\Delta_1\Delta_2.
\end{aligned}$$

So, $K_1 \le n_2^4ZF_2(\Gamma_1)+m_1ZF_2(\Gamma_2)+m_1(n_2^2-m_2)\Delta_2^2+2n_2^3m_1\Delta_1\Delta_2$.
Therefore,

$$\begin{aligned}
ZF_2(\Gamma_1[\Gamma_2]) &\le K_1+K_2\\
&\le n_2^2m_2ZF_1(\Gamma_1)+n_2^4ZF_2(\Gamma_1)+(m_1+n_1)ZF_2(\Gamma_2)\\
&+2n_2(n_1m_2+m_1n_2^2)\Delta_1\Delta_2+m_1(n_2^2-m_2)\Delta_2^2.
\end{aligned}$$

Hence the result. □

Corollary 4.4. *(i)* $ZF_2(\Gamma_1[\Gamma_2]) \le n_2^2(n_1+1)^2(n_1m_2+m_1n_2^2)$ *and*
(ii) $ZF_2(\Gamma_1[\Gamma_2]) \le 4m_1^2n-1^2n_2^2m_2+m_1n_2^4(n_1-1)^2+m_2(m_1+n_1)(n_2-1)^2+2n_2(n_1-1)(n_2-1)(n_1m_2+m_1n_2^2)+m_1(n_2-1)^2(n_2^2-m_2)$.

Theorem 4.5. $ZF_2(\Gamma_1)+ZF_2(\Gamma_2) \le ZF_2(\Gamma_1+\Gamma_2) \le ZF_2(\Gamma_1)+ZF_2(\Gamma_2)+m_1n_2(2\Delta_1+n_2)+n_1m_2(2\Delta_2+n_1)+n_1n_2(\Delta_1+n_2)(\Delta_2+n_1)$.

Proof. As $\Gamma_1+\Gamma_2$ is join graph of Γ_1 and Γ_2, then for $u,v,u_1,v_1\in\Upsilon$,

$$\Psi(u)=\begin{cases}\Psi_1(u), & u\in\Upsilon_1\\ \Psi_2(u), & u\in\Upsilon_2\end{cases}$$

and

$$\Omega(u,v)=\begin{cases}\wedge\{\Psi_1(u),\Psi_2(v)\} & u\in\Upsilon_1 \text{ and } v\in\Upsilon_2\\ \Omega_1(u,v) & uv\in\mathcal{E}_1\\ \Omega_2(u,v) & uv\in\mathcal{E}_2\\ 0 & \text{otherwise.}\end{cases}$$

Then,

$$\begin{aligned}
d_{\Gamma_1+\Gamma_2}(u) &= \begin{cases}d_{\Gamma_1}(u)+\sum_{v\in\Upsilon_2}\wedge\{\Psi_1(u),\Psi_2(v)\}, & u\in\Upsilon_1\\ d_{\Gamma_2}(u)+\sum_{v\in\Upsilon_1}\wedge\{\Psi_2(u),\Psi_1(v)\}, & u\in\Upsilon_2\end{cases} \qquad (1)\\
&\ge \begin{cases}d_{\Gamma_1}(u), & u\in\Upsilon_1\\ d_{\Gamma_2}(u), & u\in\Upsilon_2.\end{cases} \qquad (2)
\end{aligned}$$

Also, from equation (1), we get

$$d_{\Gamma_1+\Gamma_2}(u) \le \begin{cases} d_{\Gamma_1}(u) + \sum_{v\in\Upsilon_2} \Psi_1(u), & u \in \Upsilon_1 \\ d_{\Gamma_2}(u) + \sum_{v\in\Upsilon_1} \Psi_2(u), & u \in \Upsilon_2 \end{cases} \tag{3}$$

$$\le \begin{cases} d_{\Gamma_1}(u) + n_2\Psi_1(u), & u \in \Upsilon_1 \\ d_{\Gamma_2}(u) + n_1\Psi_2(u), & u \in \Upsilon_2 \end{cases} \tag{4}$$

Then second ZI of $\Gamma_1 + \Gamma_2$ is:

$$\begin{aligned} ZF_2(\Gamma_1+\Gamma_2) &= \sum_{uv\in E(\Gamma_1+\Gamma_2)} \Psi(u)\Psi(v)d_{\Gamma_1+\Gamma_2}(u)d_{\Gamma_1+\Gamma_2}(v) \\ &= \sum_{uv\in\mathcal{E}_1} \Psi(u)\Psi(v)d_{\Gamma_1+\Gamma_2}(u)d_{\Gamma_1+\Gamma_2}(v) + \sum_{uv\in\mathcal{E}_2} \Psi(u)\Psi(v)d_{\Gamma_1+\Gamma_2}(u)d_{\Gamma_1+\Gamma_2}(v) \\ &+ \sum_{u\in\Upsilon_1, v\in\Upsilon_2} \Psi(u)\Psi(v)d_{\Gamma_1+\Gamma_2}(u)d_{\Gamma_1+\Gamma_2}(v) \\ &\ge \sum_{uv\in\mathcal{E}_1} \Psi_1(u)\Psi_1(v)d_{\Gamma_1}(u)d_{\Gamma_1}(v) + \sum_{uv\in\mathcal{E}_2} \Psi_2(u)\Psi_2(v)d_{\Gamma_2}(u)d_{\Gamma_2}(v) \\ &\ge ZF_2(\Gamma_1) + ZF_2(\Gamma_2). \end{aligned}$$

Again,

$$\begin{aligned} ZF_2(\Gamma_1+\Gamma_2) &= \sum_{uv\in\mathcal{E}(\Gamma_1+\Gamma_2)} \Psi(u)\Psi(v)d_{\Gamma_1+\Gamma_2}(u)d_{\Gamma_1+\Gamma_2}(v) \\ &= \sum_{uv\in\mathcal{E}_1} \Psi(u)\Psi(v)d_{\Gamma_1+\Gamma_2}(u)d_{\Gamma_1+\Gamma_2}(v) + \sum_{uv\in\mathcal{E}_2} \Psi(u)\Psi(v)d_{\Gamma_1+\Gamma_2}(u)d_{\Gamma_1+\Gamma_2}(v) \\ &+ \sum_{u\in\Upsilon_1, v\in\Upsilon_2} \Psi(u)\Psi(v)d_{\Gamma_1+\Gamma_2}(u)d_{\Gamma_1+\Gamma_2}(v) \end{aligned}$$

$$\begin{aligned} &\le \sum_{uv\in\mathcal{E}_1} \Psi_1(u)\Psi_1(v)\{d_{\Gamma_1}(u) + n_2\Psi_1(u)\}\{d_{\Gamma_1}(v) + n_2\Psi_1(v)\} \\ &+ \sum_{uv\in\mathcal{E}_2} \Psi_2(u)\Psi_2(v)\{d_{\Gamma_2}(u) + n_1\Psi_2(u)\}\{d_{\Gamma_2}(v) + n_1\Psi_2(v)\} \qquad \text{[by (4)]} \\ &+ \sum_{u\in\Upsilon_1, v\in\Upsilon_2} \Psi_1(u)\Psi_2(v)\{d_{\Gamma_1}(u) + n_2\Psi_1(u)\}\{d_{\Gamma_1}(v) + n_1\Psi_1(v)\} \\ &= K_1 + K_2 + K_3, \end{aligned}$$

where $K_1 = \sum_{uv\in\mathcal{E}_1} \Psi_1(u)\Psi_1(v)\{d_{\Gamma_1}(u) + n_2\Psi_1(u)\}\{d_{\Gamma_1}(v) + n_2\Psi_1(v)\}$,

$$K_2 = \sum_{uv\in\mathcal{E}_2} \Psi_2(u)\Psi_2(v)\{d_{\Gamma_2}(u) + n_1\Psi_2(u)\}\{d_{\Gamma_2}(v) + n_1\Psi_2(v)\}$$

and

$$K_3 = \sum_{u\in\Upsilon_1, v\in\Upsilon_2} \Psi_1(u)\Psi_2(v)\{d_{\Gamma_1}(u) + n_2\Psi_1(u)\}\{d_{\Gamma_1}(v) + n_1\Psi_1(v)\}.$$

Now

$$\begin{aligned} K_1 &= \sum_{uv\in\mathcal{E}_1} \Psi_1(u)\Psi_1(v)\{d_{\Gamma_1}(u) + n_2\Psi_1(u)\}\{d_{\Gamma_1}(v) + n_2\Psi_1(v)\} \\ &= \sum_{uv\in\mathcal{E}_1} \Psi_1(u)\Psi_1(v)[d_{\Gamma_1}(u)d_{\Gamma_1}(v) + n_2\{\Psi_1(u)d_{\Gamma_1}(v) + \Psi_1(v)d_{\Gamma_1}(u)\} + n_2^2\Psi_1(u)\Psi_1(v)] \\ &\le ZF_2(\Gamma_1) + 2m_1n_2\Delta_1 + m_1n_2^2. \end{aligned}$$

So, $K_1 \leq ZF_2(\Gamma_1)+2m_1n_2\Delta_1+m_1n_2^2$. Similarly, $K_2 \leq ZF_2(\Gamma_2)+2m_2n_1\Delta_2+m_2n_1^2$ and $K_3 \leq n_1n_2(\Delta_1+n_2)(\Delta_2+n_1)$. Therefore,

$$\begin{aligned} ZF_2(\Gamma_1+\Gamma_2) &\leq K_1+K_2+K_3 \\ &\leq ZF_2(\Gamma_1)+ZF_2(\Gamma_2)+m_1n_2(2\Delta_1+n_2)+n_1m_2(2\Delta_2+n_1)+n_1n_2(\Delta_1+n_2)(\Delta_2+n_1). \end{aligned}$$

Hence the result. □

Corollary 4.6. *(i)* $ZF_2(\Gamma_1+\Gamma_2) \leq (m_1+m_2+n_1n_2)(n_1+n_2-1)^2$ *and*
(ii) $ZF_2(\Gamma_1+\Gamma_2) \leq m_1(n_1-1)^2+m_2(n_2-1)^2+m_1n_2(2n_1+n_2-1)+m_2n_1(n_1+2n_2-1)+n_1n_2(n_1+n_2-1)^2$.

Theorem 4.7. $ZF_2(\Gamma_1 \cup \Gamma_2) \geq ZF_2(\Gamma_1)+ZF_2(\Gamma_2)-k\Delta^2$ *where* $p=|E_1 \cap E_2|, \Delta=\max\{\Delta_1,\Delta_2\}$.

Proof. As $\Gamma_1 \cup \Gamma_2$ is union FG of Γ_1 and Γ_2, then

$$d_{\Gamma_1\cup\Gamma_2}(u)=\begin{cases} d_{\Gamma_1}(u) \text{ if } u \in V_1 \setminus V_2 \\ d_{\Gamma_2}(u) \text{ if } u \in V_2 \setminus V_1 \\ \max\{d_{\Gamma_1}(u), d_{\Gamma_1}(u)\} \text{ if } u \in V_1 \cap V_2 \end{cases}$$

Then

$$\begin{aligned} ZF_2(\Gamma_1 \cup \Gamma_2) &= \sum_{uv\in E} \Psi(u)\Psi(v)d(u)d(v) \\ &= \sum_{uv\in E_1} \Psi(u)\Psi(v)d(u)d(v)+\sum_{uv\in E_2} \Psi(u)\Psi(v)d(u)d(v)-\sum_{uv\in E_1\cap E_2} \Psi(u)\Psi(v)d(u)d(v) \\ &\geq ZF_2(\Gamma_1)+ZF_2(\Gamma_2)-p\Delta^2. \end{aligned}$$

□

5 Application of second Zagreb index for chemical compounds

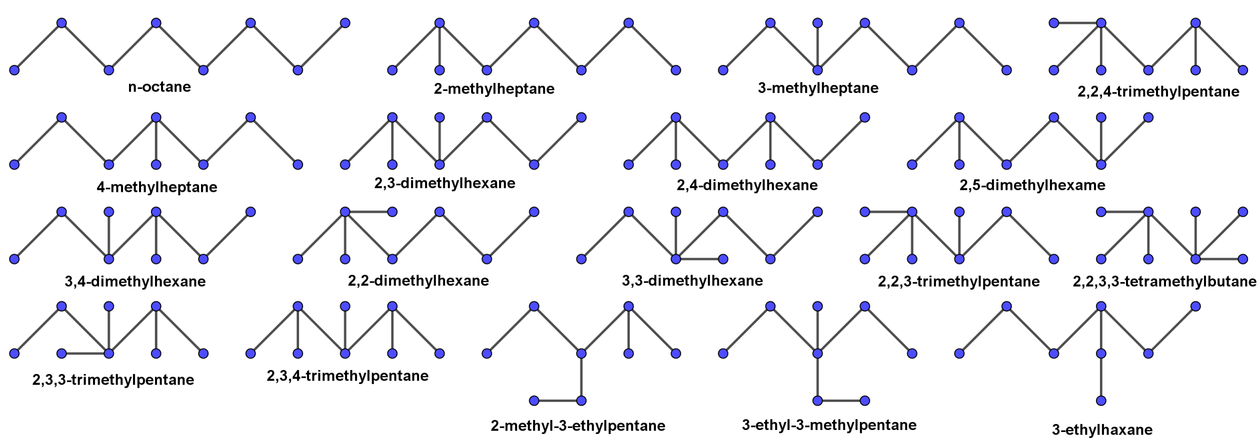

Figure 4: Simple representation of octane isomers.

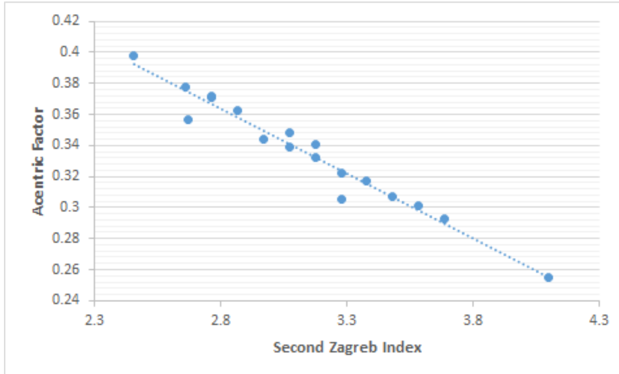

Figure 5: Linear fitting of second Zagreb index with acentric factor for octane isomer.

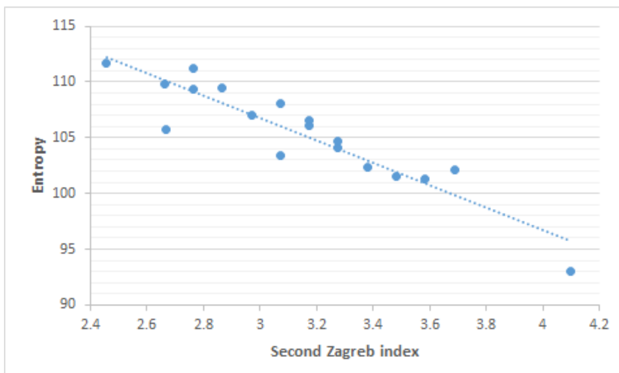

Figure 6: Linear fitting of second Zagreb index with entropy for octane isomer.

Table 1: The acentric factor (AF), entropy(S) and second ZI for octane isomers.

Octane isomers	Acentric factor	Entropy	Second Zagreb index
n-octane	0.397898	111.67	2.4576
2-methyl heptane	0.377916	109.84	2.6624
3-methyl heptane	0.371002	111.26	2.7648
4-methyl heptane	0.371504	109.32	2.7648
3-ethyl hexane	0.362472	109.43	2.8672
2,2-dimethyl hexane	0.339426	103.42	3.072
2,3-dimethyl hexane	0.348247	108.02	3.072
2,4-dimethyl hexane	0.344223	106.98	2.9696
2,5-dimethyl hexane	0.35683	105.72	2.6692
3,3-dimethyl hexane	0.322569	104.74	3.2768
3,4-dimethyl hexane	0.340345	106.59	3.1744
2-methyl-3-ethyl pentane	0.332433	106.06	3.1744
3-methyl-3-ethyl pentane	0.306899	101.48	3.4816
2,2,3-trimethyl pentane	0.300816	101.31	3.584
2,2,4-trimethyl pentane	0.30537	104.09	3.2768
2,3,3-trimethyl pentane	0.293177	102.06	3.6864
2,3,4-trimethyl pentane	0.317422	102.39	3.3792
2,2,3,3-tetramethyl butane	0.255294	93.06	4.096

To study the fruitfulness of a topological index, we have to correlate this index with at least one physico-chemical characteristic of a chemical compound. Due to the instruction of International Academy of Mathematical Chemistry, we studied regression analysis of that index with physico-chemical properties of chemical compounds. As octane isomers are a large, diverse group of alkanes for the preliminary testing of indices, they are helpful for such a type of investigation. Different chemical compounds with the same molecular crisp graph structure have a different value of entropy/acentric factor, so entropy/acentric factor not only depends on the molecular crisp graph structure but also on atomic energy, bond energy, etc. Therefore, studying the topological indices in molecular crisp graph structure is not realistic to determine the entropy/acentric factor for octane isomers or other isomers. Also, it is very difficult to find out a specific relation between atomic energy and bond energy with entropy/acentric factor, i.e. finding of specific energy is not possible! Hence, for each octane isomer, we have constructed a fuzzy graph using atomic energy, bond energy and then correlated second Zagreb index with entropy and acentric factor. The vertex set of the fuzzy graph is the carbon atoms and the carbon-carbon bond represents the edge set. As there are no crisp relations between atomic energy, bond energy with entropy/acentric factor of an octane isomer, we have defined vertex and edge membership values as:

$$\Psi(v) = \frac{\text{Atomic energy of the vertex } v}{\text{Maximum atomic energy among all vertices}},$$
$$\text{and } \Omega(uv) = \frac{\text{Bond energy of the edge } uv}{\text{Maximum of atomic energy of } u,\, v}.$$

Clearly, $\Psi(v) \in [0,1], \forall v \in \Upsilon$. Also, bond energy of the edge uv is always less than atomic energy of end vertices, hence, $\Omega(uv) \in [0,1], \forall uv \in \mathcal{E}$ and $\Omega(uv) \leq \min\{\Psi(u), \Psi(v)\}, \forall uv \in \mathcal{E}$. As the triplet (Γ, Ψ, Ω) satisfies all the criteria of a fuzzy graph, (Γ, Ψ, Ω) forms a fuzzy graph. The simple structure of the octane isomers (C_8H_{18}) are shown in Figure 4, where each vertex represents the carbon atom and edge represents the C-C bond. Note that the atomic energy of Carbon is 1086.5 kJ/mol and the bond energy of C-C is 345 kJ/mol. Using the above two formulae, we get $\Psi(C) = 1.00$ and $\Omega(C - C) = 0.32$. The value of the acentric factor, entropy and second ZI of octane isomers are listed in Table 1. The value of acentric factor and entropy for octane isomers are taken from [35]. Here, one can calculate the correlation coefficient of second ZI with acentric factor is -0.977966531 and the correlation coefficient of second ZI with entropy is -0.91961647. Thus second ZI can help estimate the acentric factor ($r = -0.977966531$) and entropy ($r = -0.91961647$) with significant accuracy. These outcomes declare the appropriateness of the index "Second Zagreb index". The following equation represents the linear regression model between second ZI with an acentric factor:

$$\text{Acentric factor } = (-0.0835) \times \text{ Second ZI } + 0.5975, \text{ where } r = -0.977966531$$

and the linear regression model between second ZI with entropy is represented by the equation:

$$\text{Entropy } = (-10.003) \times \text{ Second ZI } + 136.77, \text{ where } r = -0.91961647.$$

The linear fitting of this index with acentric factor and entropy for octane isomers is shown in Figure 5 and 6 respectively. In both figures, the regression line is represented by the blue line. Figure 5 and 6 shows the strength of the structure-property relationship for second ZI with acentric factor and entropy respectively. From the value of r, it is clear that the data point in Figure 5 is closer than the data point in Figure 6 to the best fitting line. Hence, the linear fitting model between the second ZI and the acentric factor is more accurate than the linear fitting model between the second ZI and entropy.

Also, topological indices are applied for isomer discrimination. The discrimination ability of an index has amazing significance for the coding theory. Konstantinova [30] proposed the sensitivity, formulated as

$$S_T = \frac{N - N_T}{N},$$

Table 2: Sensitivity of different topological indices.

Topological indices	**Sensitivity (S_T)**
First ZI	0.333
Second ZI	**0.722**
F-index	0.389

where N represents the total number of isomer, N_T represents the total number of isomers that cannot be discriminated by the TI T. Sensitivity of an index is directly proportional to the isomer discrimination ability. Mondal et al. provide the values of S_T for different topological indices in [35]. The value of S_T is listed in Table 2 for first ZI, second ZI and F-index for octane isomers. From Table 2, second ZI exhibits better response compared to first ZI and F-index.

6 Conclusion

topological indices have an vital role in chemical graph, coding theory, spectral graph, etc. The second ZI has studied for FGs here. Bounds of this index are calculated for several FGs: path, star, cycle, complete FG, partial fuzzy subgraph, etc. For an isomorphic FGs, it is shown that the value of this index is the same. Bounds of this index for the Cartesian product, composition, join, and union of two FGs are established. At the end of this article, an application of the index in chemistry is studied. We have shown that the correlation coefficient of this index with acentric factor and entropy are -0.977966531 and -0.91961647 for the linear fittings respectively. Thus this index can help estimate the acentric factor and entropy with significance accuracy. These outcomes declare the appropriateness of the index in QSPR research. Also there are many problem related to second ZIs on FGs which are unsolved till now. Some of the problems are:
(i) Find the minimal n-vertex FG with respect to second ZI.
(ii) Find the maximal n-vertex tree (fuzzy) with respect to second ZI.
(iii) Find the minimal n-vertex tree (fuzzy) with respect to second ZI.

Data availability:

All the data are collected from http://www.moleculardescriptors.eu and https://pubchem.ncbi.nlm.nih.gov.

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Compliance with ethical standards

Disclosure statement

No potential conflict of interest was reported by the authors.

Ethical approval

This article does not contain any studies with human participants or animals performed by any of the authors.

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