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Bounds on F-Index of Tricyclic Graphs with AI Applications

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Abstract. Topological indices, symmetric functions in graph theory, are critical tools for characterizing the structural and topological properties of molecules and networks. The Forgotten index (F-index), defined as the sum of the cubes of vertex degrees in a molecular graph, was introduced by Furtula and Gutman to model the structural dependence of total π-electron energy. Tricyclic graphs, connected graphs of order m and size $m + 2$, are of particular interest due to their intermediate complexity between bicyclic and tetracyclic structures. In this work, we establish sharp upper and lower bounds for the Forgotten index within the class of tricyclic graphs and identify the extremal graphs achieving these bounds. To extend the theoretical contributions, we also propose to integrate artificial intelligence (AI) and machine learning (ML) methodologies, for their utility in three key areas: (1) Predictive modeling via graph neural networks (GNNs) to estimate F-indices for large-scale tricyclic graphs, bypassing combinatorial complexity; (2) Generative design using variational autoencoders (VAEs) to synthesize novel tricyclic graphs with near-optimal F-indices for materials science applications; and (3) AI-driven optimization employing reinforcement learning (RL) to validate extremal graph structures and explore uncharted regions of the tricyclic graph space. We combine mathematical and AI approaches to improve F-index analysis in tricyclic graphs.

AMS (MOS) Subject Classification Codes: 05C92; 05C09; 05C07
Key Words: Tricyclic graphs; Graph transformations; Forgotten chemical invariant.

1. INTRODUCTION

Graph theory [1] is the enormous and ideally disciplined field of mathematics that deals with the modeling of mathematics using graphical representations to create multi-dimensional graphs and describe them under multi-dimension science philosophy simultaneously.

All the graphs related to this paper are simple and strict graph of order m and size q. An undirected connected graph that has no multiple edges or loops is referred to as a strict graph, having $V(\Gamma)$ as vertex set and $E(\Gamma)$ as edge set respectively is known as a molecular graph [2]. The atoms are denoted by $x_i \in V(\Gamma)$, and the covalent bonds between the corresponding atoms are indicated by $x_ix_j \in E(\Gamma)$. Let $\aleph_\Gamma(x)$ stand for the neighbor set of vertex x in Γ, then $d_\Gamma(x) =\mid \aleph_\Gamma(x) \mid$ is the degree of x in Γ. A vertex x of Γ is called a pendent if vertex x has degree 1. A path in Γ is said to be pendent if its one end vertex has degree at least 3, the other vertex has degree one, and the degree of intermediate vertices is 2. An internal path of Γ is described as a walk $x_0, x_1, x_2, \ldots, x_s (s \geq 1)$ such that the vertices $x_0, x_1, x_2, \ldots, x_s$ are distinct, $d_\Gamma(x_0), d_\Gamma(x_s) \geq 2$ and $d_\Gamma(x_i) = 2$, whenever $0 < i < s$. In this paper, we will consider some graph transformations, that involve swapping of edges from one vertex to other and reduction of edges that result in increase or decrease of degree of vertices involved. Moreover we will convert pendent path to internal path and internal path to pendent vertices.

A multigraph is a graph that allows for multiple edges, or edges with identical end nodes. Thus, more than one edge may join two vertices. Let P_m, S_m and C_m be respectively the path, star and cycle with m vertices respectively. A connected graph Γ is called a tree (respectively, unicyclic, bicyclic and tricyclic graph) if $q = m - 1$ (respectively $q = m$, $q = m + 1$ and $q = m + 2$). In this work, family of tricyclic graphs will be considered along with Forgotten topological invariant.

A connectivity index is a numerical value that is linked to a graph Γ and has the property of having the same value for all graphs that are isomorphic to Γ. Topological indices, which are numerical measurements derived from a molecular graph and correlate well with the molecular graph's physicochemical properties, have been shown to be useful in isomer discrimination, QSAR, and QSPR research. Understanding the chemical features of a molecular graph requires examining specific changes in the values of these invariants, see [15]. Assume that Ω_m represent the class of connected graphs of size $m + 2$ and order m. Brace of a tricyclic graph is defined as graph obtained by removing vertices of degree one. All braces set of tricyclic graph represented by Ω_m^0 and are given in Figure 10, Ω_m^1 and Ω_m^2 represent the class of tricyclic graphs given in Figure 9 and 11.

Wiener (1947) established the first distance-based TI, for more information, see [25], when he was working on paraffin. Later, it was identified as the Wiener index, and a great deal of research was done on it. In 1972, Gutman and Trinajstic [14] have shown that the total ϕ energy (ϵ) depends on the sum of squares of vertex degrees in a molecular graph. This term was later called as first Zagreb index and provides a measure of branching of carbon atom skeleton. For any graph Γ, the first and second Zagreb indices are defined as

$$M_1(\Gamma) = \sum_{xy \in E(\Gamma)} d_\Gamma(x) + d_\Gamma(y)$$

$$M_2(\Gamma) = \sum_{xy \in E(\Gamma)} d_\Gamma(x) d_\Gamma(y)$$

Yan *et al.* [30], studied the second Zagreb index of unicyclic graphs with m vertices and k pendant vertices for extremal values. Zhu *et al.* [31], determined the tricyclic graph with cyclomatic number 3, m vertices, and having maximum Merrifield-Simmons index. The total number of independent sets in a graph is its total Merrifield-Simmons index, whereas an independent set of graph is a set of vertices that are not adjacent to one another. Li and Yang [22], identified all tricyclic graphs having less than 1 second largest eigenvalue. Zhu and Yu [32], characterized the smallest number of independent sets for the class of graphs having size $m + 2$. Chen *et al.* [10], described the graphs that attained the upper bound and provided an upper bound for the revised Szeged index for tricyclic graphs. The revised Szeged index is described as

$$S_{z*}(\Gamma) = \sum_{e=xy \in E(\Gamma)} [m_x(e) + \frac{m_0(e)}{2}][m_y(e) + \frac{m_0(e)}{2}]$$

where $m_x(e)$ represents the number of nodes nearer to vertex x, $m_0(e)$ is the number of nodes that are equally spaced from x and y. In [28], for $m \geq 15$ Tomescu and Kanwal established unicyclic graph having minimum degree distance. Ashrafi *et al.* [4], presented the class of all m-vertex tricyclic graphs for first, second, and third maximum atom-bond connectivity index values. The atom-bond connectivity index is described as

$$ABC(\Gamma) = \sum_{xy \in E(\Gamma)} \sqrt{\frac{d_\Gamma(x) + d_\Gamma(y) - 2}{d_\Gamma(x) d_\Gamma(y)}}$$

Akram *et al.* [6], characterized the graphs attaining the largest and smallest values and demonstrated the ordering of the various graphs subfamilies for Forgotten topological invariant in Ω_α^m, where Ω_α^m describes the entire class of graphs having three cycles, having $\alpha \geq 1$ vertices of degree one and order $m \geq 16 + \alpha$. Ali [3], characterized the unique graph with minimal augmented Zagreb index AZI among all classes of connected tricyclic graphs of order m for every $m \geq 6$. The augmented Zagreb index AZI is described as

$$AZI(\Gamma) = \sum_{xy \in E(\Gamma)} (\frac{d_\Gamma(x) d_\Gamma(y)}{d_\Gamma(x) + d_\Gamma(y) - 2})^3$$

Imtiaz *et al.* [18] presented the upper bound for acyclic graph for first Gourava index. Wang *et al.* [29], determined the maximum value of Forgotten topological index using transformations. A degree-based topological index was recently re-evaluated by Furtula and Gutman [13] named it forgotten index ($\mathcal{F}$-index). De *et al.* [11], Milovanovic *et al.* [24] and Basavanagoud *et al.* [8] examined $\mathcal{F}$-index and co-index of $\mathcal{F}$-index for different graphs. Khaksari and Ghorbani [21] determined for $\mathcal{F}$-index the particular product of graphs. In [5, 19] the Forgotten chemical invariant was extensively studied for the graphs having one and two cycles.

Sardar *et al.* [26], determined the extremal values for the Kirchhoff index of line graph of unicyclic graphs and extremal unicyclic graphs by using some graph transformations and techniques derived from electrical networks. Gao [17], explored the extremal graphs

as regular graphs by giving some conditions on the function $f(x, y)$ and using vertex-degree based topological indices. The author also computed the extremal values for the considered indices among c-cyclic graphs, and found the extremal c-cyclic graphs. Su and Tang [27], determined the minimal and the maximal unicyclic graphs with girth k for some exponential vertex degree based topological indices. In this work we use the technique of swapping of edges from one vertex of tricyclic graphs to another vertex. We have observed the increase or decrease in the behavior of $\mathcal{F}$-index under different graph transformations. This helped us to find the extremal values of $\mathcal{F}$-index for tricyclic graphs and the whole work is shown in figure 1.

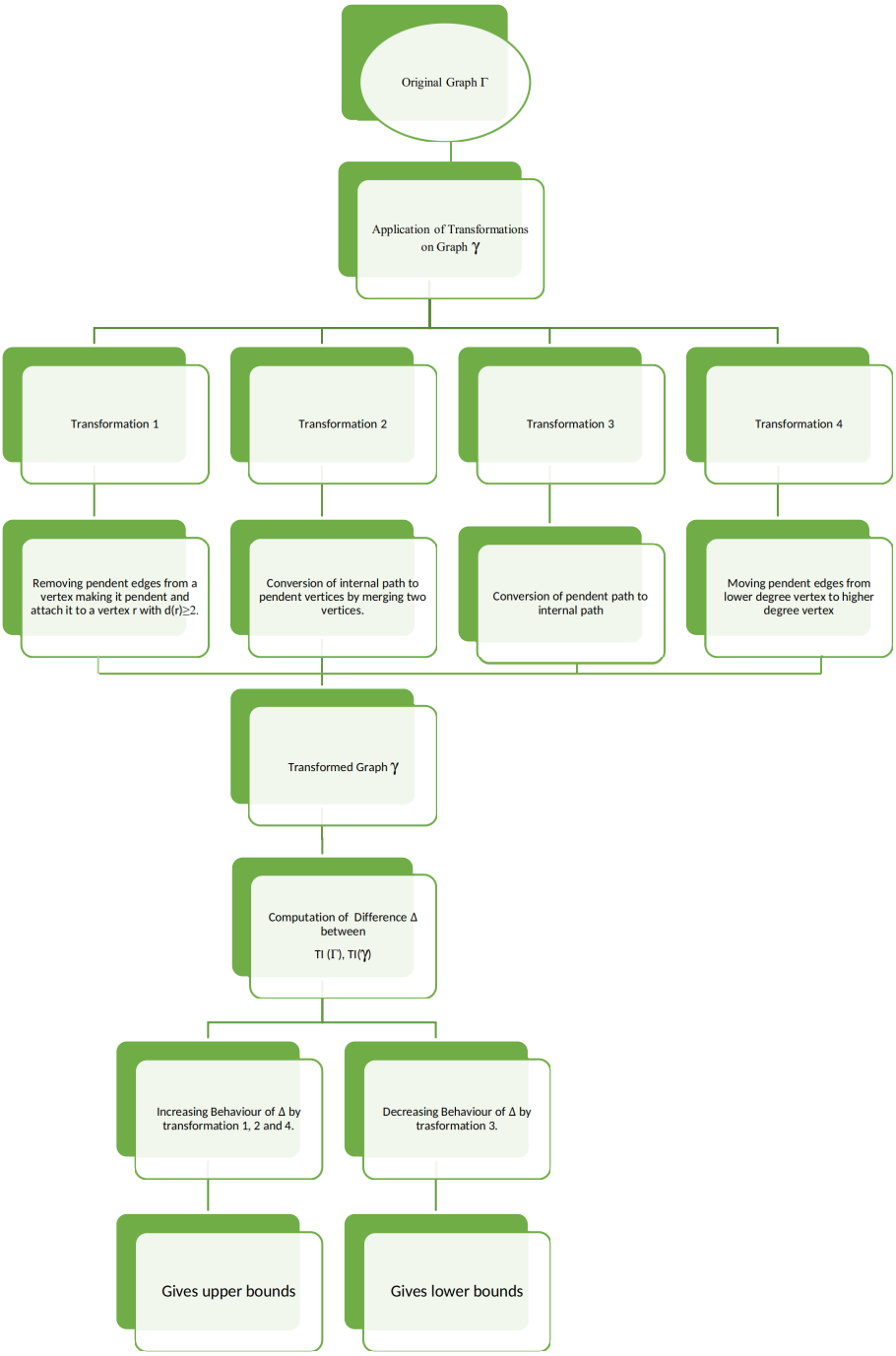

FIGURE 1. Flowchart for finding extremals using transformations

2. EDGE SWAPPING TRANSFORMATIONS

We observe the behavior of $\mathcal{F}$ index under some graph transformations. These transformations involve the swapping of edges from one vertex to another vertex and reduction of edges that result in increase or decrease of degrees of vertices involved, of a tricyclic graph. These transformations are applied to connected graphs (*i.e*, having path from any point to any other point in the graph) and nontrivial (*i.e*, having two or more than two vertices).

Transformation 1: Let xy be such an edge of simple graph Γ with $d_\Gamma(y) \geq 2$. Presumed that $\{y, u_1, u_2, \ldots, u_t\}$ are all adjacent to the vertex x while $u_1, u_2, \ldots, u_t$ are vertices having degree 1. If

$$\Upsilon = \Gamma - \{xu_1, xu_2, \ldots, xu_t\} + \{yu_1, yu_2, \ldots, yu_t\}$$

we say that Υ is obtained from Γ by transformation 1, as given in Figure 2. Transformation

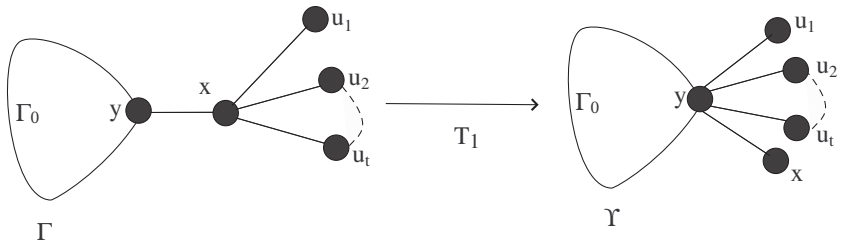

FIGURE 2. Transformation 1

1 increases the $\mathcal{F}$-index as exhibited in Lemma 2.1.

Lemma 2.1. *If* Υ *is derived from* Γ *using transformation* 1*, then*

$$\mathcal{F}(\Gamma) < \mathcal{F}(\Upsilon)$$

Proof. Evidently, $d_\Gamma(y) < d_\Upsilon(y)$ and $d(x) + d(y)$ remains unchanged during transformation 1. Hence,

$$\begin{aligned}
\mathcal{F}(\Upsilon) - \mathcal{F}(\Gamma) &> [d_\Upsilon(y)^2 + d_\Upsilon(x)^2] + \sum_{i=1}^{t}[d_\Upsilon(y)^2 + d_\Upsilon(u_i)^2] \\
&\quad - [d_\Gamma(x)^2 + d_\Gamma(y)^2] - \sum_{i=1}^{t}[d_\Gamma(x)^2 + d_\Gamma(u_i)^2] \\
&= (t+1)[(d_\Gamma(y) + t)^2 + 1] - [d_\Gamma(y)^2 + (t+1)^2] \\
&\quad - t[(t+1)^2 + 1] \\
&= td_\Gamma(y)^2 + 2d_\Gamma(y)t^2 + 2d_\Gamma(y)t - 3t - 2t^2 \\
&= [d_\Gamma(y) - 1][2t^2 + 3t + td_\Gamma(y)] > 0; \;\; d_\Gamma(y) \geq 2
\end{aligned}$$

As a result, the proof is complete. □

Transformation 2: Let Γ be a connected graph and $x, y \in V(\Gamma)$. Let $P_a = (x =)u_1, u_2, \ldots, u_a(= y)$ is a nontrivial path of length "a" of Γ joining vertices x and y. If $w = x + y$, then

$$\Upsilon = \Gamma - \{u_1u_2, u_2u_3, \ldots, u_{a-1}u_a\} + \{wu_1, wu_2, \ldots, wu_{a-1}\}$$

we say that Υ is obtained from Γ, as presented in Figure 3 using transformation 2.

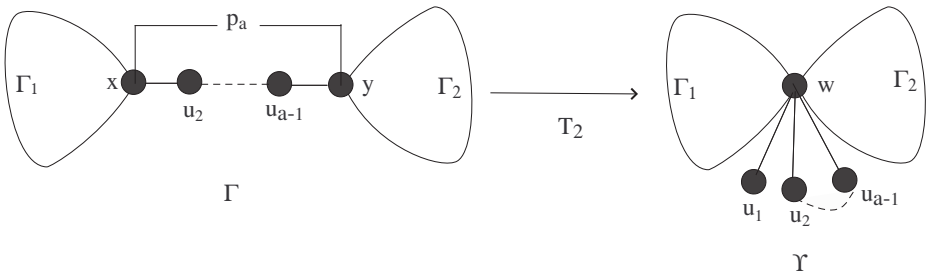

FIGURE 3. Transformation 2

Lemma 2.2. *If Υ is derived from Γ using transformation 2, as illustrated in Figure 3, then*

$$\mathcal{F}(\Gamma) < \mathcal{F}(\Upsilon)$$

Proof. From transformation 2 we discern that, let $d_{\Gamma_1}(x) = u$ and $d_{\Gamma_2}(y) = v$ while $w = x + y$ (fusing x and y to attain w) with $d_\Upsilon(w) = u + v + a - 1$, where $a \geq 2$. If $a = 2$,

$$\begin{aligned}\mathcal{F}(\Upsilon) - \mathcal{F}(\Gamma) &> [d_\Upsilon(w)^2 + d_\Upsilon(u_1)^2] - [d_\Gamma(x)^2 + d_\Gamma(y)^2] \\ &= (u + v + 2 - 1)^2 + 1 - (u + 1)^2 - (v + 1)^2 \\ &= 2uv > 0; \;\; (u, v) \geq 1\end{aligned}$$

If $a \geq 3$

$$\begin{aligned}\mathcal{F}(\Upsilon) - \mathcal{F}(\Gamma) > \sum_{i=1}^{a-1}&[d_\Upsilon(w)^2 + d_\Upsilon(u_i)^2] - [d_\Gamma(x)^2 + d_\Gamma(u_2)^2] \\ &- [d_\Gamma(y)^2 + d_\Gamma(u_{a-1})^2] - (a - 3)(8) \\ &= (a - 1)[(u + v + a - 1)^2 + 1] - [(u + 1)^2 + 4] \\ &- [(v + 1)^2 + 4] - 8(a - 3) \\ &= u^2(a - 2) + v^2(a - 2) + 2uv(a - 1) + 2ua^2 - 4ua \\ &+ 2va^a - 4va + a^3 - 3a^2 - 4a + 12 \\ &= u^2(a - 2) + v^2(a - 2) + 2ua(a - 2) + 2va(a - 2) \\ &+ 2uv(a - 1) + (a^2 - 4)(a - 3) > 0; \;\; (u, v) \geq 1\end{aligned}$$

As a result, the proof is complete. □

Transformation 3: Let K be a acyclic subgraph of Γ with $V(\mid K \mid) = t$ that is affixed to u_1 in graph Γ and x, y being two neighbors of u_1 other than that in K. If

$$\Upsilon = \Gamma - \{K - u_1\} + \{u_1u_2, u_2u_3, \ldots, u_ty\}$$

we claim that Υ is derived from Γ, as presented in Figure 4.

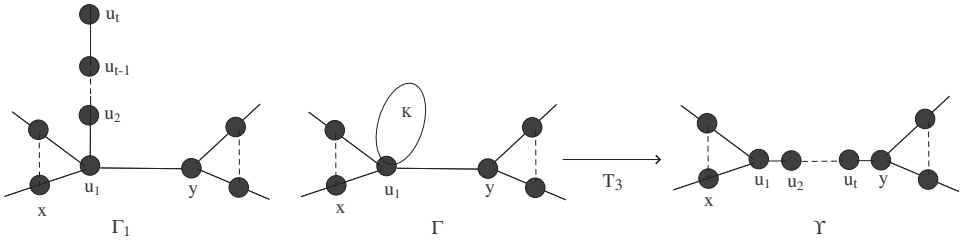

FIGURE 4. Transformation 3

Lemma 2.3. *If* Υ *is derived from* Γ *using transformation* 3*, then*

$$\mathcal{F}(\Gamma) > \mathcal{F}(\Upsilon)$$

Proof. From Lemma 2.1 we discern $\mathcal{F}(\Gamma) \geq \mathcal{F}(\Gamma_1)$. So we simply prove the following inequality,

$$F(\Gamma_1) > \mathcal{F}(\Upsilon)$$

By definition of Forgotten invariant,

$$\begin{aligned}
\mathcal{F}(\Gamma_1) - \mathcal{F}(\Upsilon) &= [d_{\Gamma_1}(u_1)^2 + d_{\Gamma_1}(u_2)^2] + [d_{\Gamma_1}(u_1)^2 + d_{\Gamma_1}(y)^2] \\
&+ [d_{\Gamma_1}(u_{t-1})^2 + d_{\Gamma_1}(u_t)^2] - [d_{\Upsilon}(u_1)^2 + d_{\Upsilon}(u_2)^2] \\
&- [d_{\Upsilon}(u_{t-1})^2 + d_{\Upsilon}(u_t)^2] - [d_{\Upsilon}(u_t)^2 + d_{\Upsilon}(y)^2] \\
&= [d_{\Gamma_1}(u_1)^2 + 4] + [d_{\Gamma_1}(u_1)^2 + d_{\Gamma_1}(y)^2] + 5 - 16 \\
&- [d_{\Gamma_1}(u_1) - 1]^2 - d_{\Gamma_1}(y)^2 \\
&= 2d_{\Gamma_1}(u_1)^2 - d_{\Gamma_1}(u_1)^2 - 8 + 2d_{\Gamma_1}(u_1) \\
&= d_{\Gamma_1}(u_1)^2 + 2d_{\Gamma_1}(u_1) - 8 > 0; \;\; d_{\Gamma_1}(u_1) \geq 2
\end{aligned}$$

As a result, the proof is complete. □

Let Γ be a connected graph. Two vertices x and y are said to be equivalent, If $\Gamma - x \cong \Gamma - y$. Evidently, $\mid \aleph(x) \mid = \mid \aleph(y) \mid$ and their neighbors contain identical lists of degrees for all of the graph's vertices.

Transformation 4: Let Γ_0 be a graph and x, y are two nodes in Γ_0 with $d_{\Gamma_0}(x) = u$ and $d_{\Gamma_0}(y) = v$ and $\aleph_{\Gamma_0}(y) \subseteq \aleph_{\Gamma_0}(x)$. Let Γ be the graph derived by affixing S_{s+1} and S_{t+1} on the nodes x and y of Γ_0, respectively. If Υ is the graph gained by removing t vertices having degree one at y in Γ and joining them to x of Γ. As a result Υ is obtained from Γ by transformation 4 as presented in Figure 5.

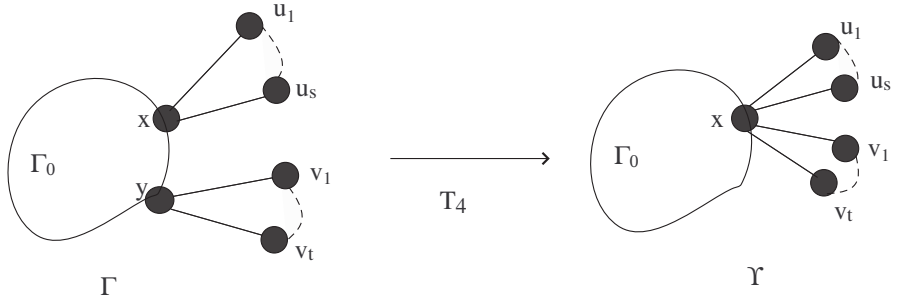

FIGURE 5. Transformation 4

Lemma 2.4. *If Υ is derived from Γ using transformation 4, then*

$$\mathcal{F}(\Gamma) < \mathcal{F}(\Upsilon)$$

Proof. Since $d_{\Gamma_0}(x) = u$ and $d_{\Gamma_0}(y) = v$ and $\aleph_{\Gamma_0}(y) \subseteq \aleph_{\Gamma_0}(x)$, $u > v$. Thus, by the definition of forgotten topological invariant,

$$\begin{aligned}
\mathcal{F}(\Upsilon) - \mathcal{F}(\Gamma) &= \sum_{i=1}^{s}[d_\Upsilon(x)^2 + d_\Upsilon(u_i)^2 - d_\Gamma(x)^2 - d_\Gamma(u_i)^2] \\
&+ \sum_{i=1}^{t}[d_\Upsilon(x)^2 + d_\Upsilon(v_i)^2 - d_\Gamma(y)^2 - d_\Gamma(v_i)^2] \\
&+ \sum_{w\in\aleph_{\Gamma_0}(y)}[d_\Upsilon(x)^2 + d_\Upsilon(w)^2 + d_\Upsilon(y)^2 + d_\Upsilon(w)^2] \\
&- \sum_{w\in\aleph_{\Gamma_0}(y)}[d_\Gamma(x)^2 + d_\Gamma(w)^2 + d_\Gamma(y)^2 + d_\Gamma(w)^2] \\
&= s[(u+s+t)^2 + 1 - (u+s)^2 - 1] + t[(t+s+u)^2 \\
&+ 1 - (t+v)^2 - 1] + \sum_{w\in\aleph_{\Gamma_0}(y)}[(s+t+u)^2 + d_{\Gamma_0}(w)^2 + v^2 \\
&+ d_{\Gamma_0}(w)^2 - (u+s)^2 - (v+t)^2 - 2d_{\Gamma_0}(w)^2] \\
&= s[t^2 + 2t(u+s)] + t[(s+u)^2 + 2t(s+u) - v^2 - 2tv] \\
&+ \sum_{w\in\aleph_{\Gamma_0}(y)}[2st + 2tu - 2tv] \\
&= 3st^2 + 3ts^2 + 4stu + t(u^2 - v^2) + 2t^2(u-v) \\
&+ \sum_{w\in\aleph_{\Gamma_0}(y)}[2t(s+u-v)] > 0; \;\; (s,t) \geq 1
\end{aligned}$$

As a result, the proof is complete. □

3. AI AND MACHINE LEARNING APPLICATIONS FOR F-INDEX ANALYSIS

On the one hand, the derivation of extremal F-index bounds for tricyclic graphs provides foundational knowledge. On the other hand, integrating AI/ML Approaches bridges theoretical graph theory with real-world applications. Relevant to our study, these applications may be in the fields of drug discovery, materials science, and chemical informatics. In the following, we discuss three novel AI-driven frameworks that leverage the extremal bounds established in this work.

3.1. **Predictive Modeling with Graph Neural Networks (GNNs).** In this proposed framework, scalable models are developed to predict F-indices for large or synthesized tricyclic graphs. In this way, reliance on exhaustive enumeration is reduced, shown in figure 6.

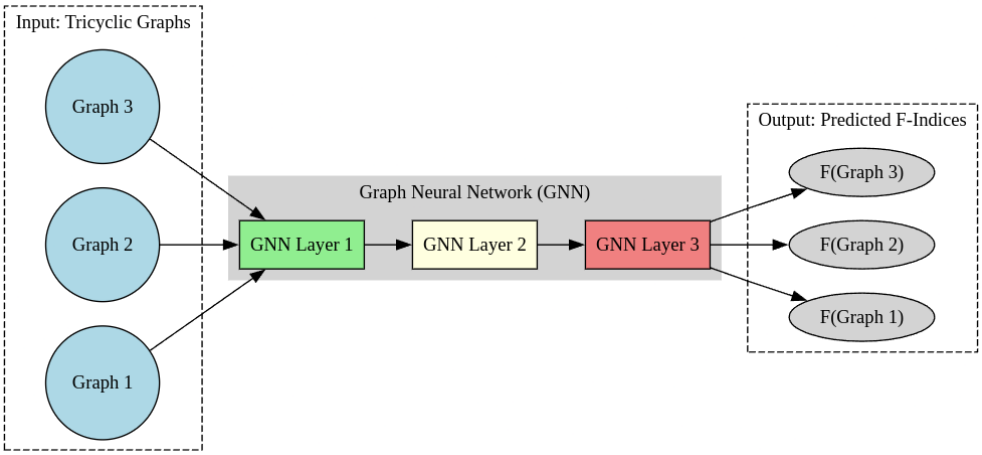

FIGURE 6. Predictive modeling via graph neural networks (GNNs)

3.1.1. *Methodology:* Firstly, in Dataset Generation, it is proposed to synthesize a diverse dataset of tricyclic graphs (with $m \leq 50$) using combinatorial generators. In this approach, each graph is labeled with its F-index. Secondly, for Graph Representation, to encode graphs using adjacency matrices or degree sequences. These are augmented with vertex-level features (e.g., degree, connectivity). Thirdly, for Model Architecture, to Train a Graph Convolutional Network (GCN) or Graph Attention Network (GAT) [20]. This is performed to regress F-indices, using the extremal bounds as validation checkpoints. For example, predictions which exceed theoretical maxima or minima signal model errors. Lastly, regarding Interpretability, it is proposed to apply gradient-based attribution (e.g., Saliency Maps). This is useful in identifying substructures (e.g., branching patterns) most influential to F-index values [16]. The significance of this framework is, that it enables rapid screening of virtual chemical libraries for molecules with desired F-index ranges. In addition, the proposed framework validates theoretical bounds by detecting anomalies in model predictions.

3.2. **Generative Design via Variational Autoencoders (VAEs).** In the VAE proposed framework, novel tricyclic graphs with F-indices is generated near the derived extremal values. This helps in the design of materials with customized electronic properties, shown in figure 7.

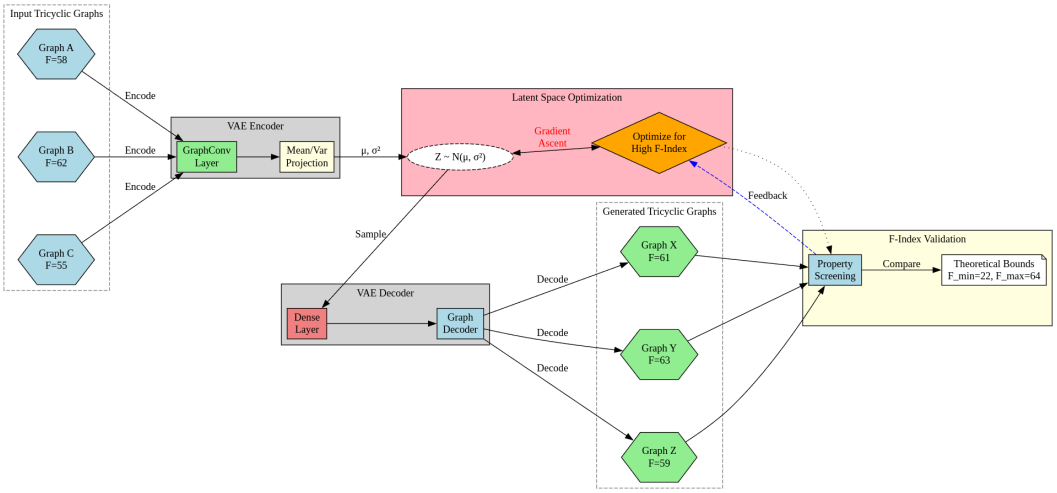

FIGURE 7. Generative design using variational autoencoders (VAEs)

3.2.1. *Methodology:* Firstly, in Latent Space Construction, a VAE on the tricyclic graph dataset is trained, which maps graphs to a continuous latent space Z. Secondly, for the Controlled Generation part, gradient-based optimization is used in Z to steer generation toward regions corresponding to high or low F-indices, according to the extremal bounds. Lastly, for the Validity Constraints stage, graph-theoretic rules (e.g., tricyclicity, connectivity) are integrated into the loss function. This integration ensures chemically plausible outputs [23]. For this framework, a case study is proposed as follows. Generate tricyclic graphs with F-indices close to the upper bound (maximally branched structures) for applications in conductive polymers. In these, high π-electron density correlates with conductivity. The proposed framework is highly significant in, Accelerating the discovery of functional materials. This is possible by prioritizing synthetically accessible candidates. The framework is also appropriate for demonstrating the utility of topological indices as optimization targets in generative AI.

3.3. **Reinforcement Learning (RL) for Extremal Graph Exploration.** This proposed framework is to deploy RL agents to navigate the tricyclic graph space. It also encompasses rediscovering/extending extremal graphs and validating theoretical results, shown in figure 8.

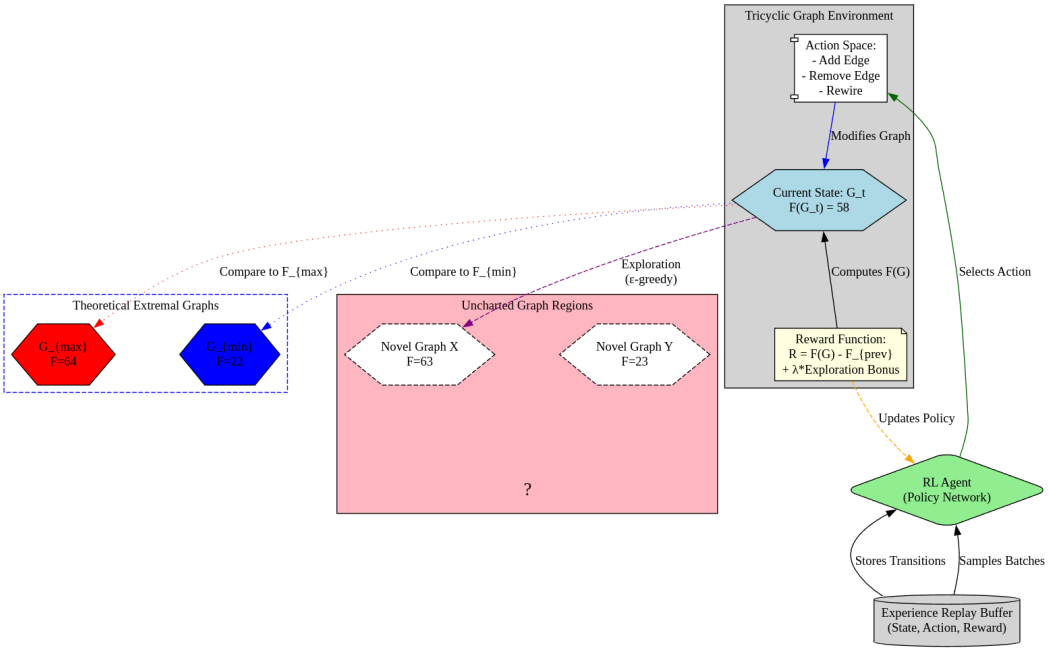

FIGURE 8. AI-driven optimization employing reinforcement learning (RL)

3.3.1. *Methodology:* Firstly, in the State-Action Formulation, specify State and Actions.

(1) State: It is the current graph configuration (encoded as a vector).
(2) Actions: These are edge additions/removals preserving tricyclicity.

Secondly, in the Reward Function, Penalize deviations from target F-index bounds. For example:

$$Reward = \begin{cases} +1, \text{if } F(\Gamma) \text{ approaches upper bound} \\ -1, \text{if } F(\Gamma) \text{ diverges.} \end{cases}$$

Lastly, in the Agent Training phase, use Proximal Policy Optimization (PPO) to learn edge-modification policies that maximize cumulative reward. Expected results are, the RL agent successfully reconstructs the extremal graphs identified analytically, confirming their optimality. Additionally, it discovers alternative near-optimal configurations in larger graphs ($m > 20$), and suggests potential extensions to the bounds. The framework is significant in that it provides an automated framework for exploring complex graph spaces that are beyond human analytical capacity. In addition, it bridges combinatorial optimization with deep learning, enabling adaptive hypothesis testing.

(1) Saliency Maps: Heatmaps highlighting graph substructures (e.g., branched chains) most influential to the GNN's F-index prediction. Example: A high-saliency edge indicates its removal would drastically change F.

(2) PPO (Proximal Policy Optimization): An RL algorithm training agents to modify graphs via edge swaps. Analogous to teaching a robot to rebuild molecules while maximizing reward (e.g., +1 for nearing $F_{\max}$).
(3) Latent Space Optimization: In the VAE, a 'hidden blueprint' of graphs. Steer this space (e.g., via gradients) to generate graphs with $F \approx 8m + 76$ (lower bound) or $F \approx F_{\max}$ (upper bound).

We propose generating 500 tricyclic graphs (connected graphs with n vertices and $n + 2$ edges) using combinatorial generation algorithms (combgen) [7]. The generation process follows these steps:

Vertex Range

Graphs will be generated across orders $m = 6$ to $m = 20$. This covers:
Small graphs $m = 6$: Minimal tricyclic structures (e.g., three fused cycles)
Medium graphs $m = 10 - 15$: Intermediate complexity
Larger graphs $m = 20$: Approaching practical molecular sizes

Generation Method

Algorithm: Systematic combinatorial enumeration ensuring:
Connectivity
Exactly $m + 2$ edges
No duplicate graphs (isomorphism checking)
Output: Edge-list representations (e.g., $[(v_1, v_2), (v_2, v_3), ...]$)

Labeling

Each graph is labeled with its Forgotten index F calculated as:

$$F(G) = \sum_{v \in V} [d(v)]^3$$

where $d(v)$ = degree of vertex v.
Example: A 6-vertex tricyclic graph might have $F = 124$.

Distribution

Balanced sampling across vertex sizes
Diverse topologies: Linear chains, branched structures, fused cycles
Includes extremal graphs from Theorem 1 (e.g., Ω_m^1)

Implementation Tools

python
Pseudocode for graph generation from combgen import tricyclic-generator
dataset = []
for m in range $(6, 21)$: $m = 6$ to 20
for m in range (25): 25 graphs per order
Γ = tricyclic-generator m-vertices= m
F-index = $\sum(d(v)^3$ for d in Γ.degree sequence())
dataset.append $(\Gamma, F - index)$.

Practical Significance

This dataset bridges theoretical graph theory with ML applications by:
Providing computable labels F for supervised learning
Enabling benchmarking of GNN performance
Including chemically relevant structures (e.g., $m = 20$ mimics real organic molecules)

4. Results and Discussion

In this section, we derived the extremal tricyclic graphs for Forgotten topological invariant. We have employed the transformations that were just explained in order to achieve the intended result.

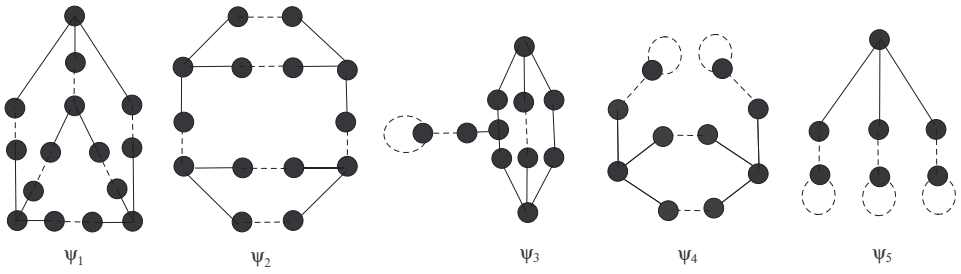

FIGURE 9. ψ_i in Ω_m^1

Theorem 4.1. *Let* Γ *be any tricyclic graph with order* m*, then*

$$\mathcal{F}(\Gamma) \geq 8m + 76; \;\; m \geq 4$$

equality holds if and only if $\Gamma \in \Omega_m^1$

Proof. Suppose Γ be a tricyclic graph. Using Lemma 2.2, Γ can be transformed into any one of the fifteen braces indicated in Figure 10. In the meanwhile, for each graph Γ there is a graph $\omega_i \in \Omega_m^0$, where $i \leq 15$, such that $\mathcal{F}(\omega_i) \leq \mathcal{F}(\Gamma)$ using Lemma 2.3. Clearly, $\mathcal{F}(\psi_i) = 8m + 76$, for $i = 1, 2, 3, 4, 5$.
As a result, the proof is complete. □

Theorem 4.2. *Let* Γ *be any tricyclic graph of size* $m + 2$ *and order* m*, then*

$$\mathcal{F}(\Gamma) \leq m^3 - 3m^2 + 4m + 82; \;\; m \geq 4$$

equality holds if and only if $\Gamma \cong S_m^{m+2}$

Proof. Suppose Γ be a tricyclic graph, as indicated in Figure 9, Γ can be converted into any one of η_i by repeatedly applying transformation 2 and 4. Alternatively, for any graph Γ having $m+2$ edges and of order m there is a $\eta_i \in \Omega_m^2$,where $i \leq 6$ such that $\mathcal{F}(\Gamma) \leq \mathcal{F}(\omega_i)$ by Lemma 2.2 and 2.4. Observe that,

$$\begin{aligned}
\mathcal{F}(\eta_1) &= m^3 - 3m^2 + 4m + 64 \\
\mathcal{F}(\eta_2) &= m^3 - 3m^2 + 4m + 52 \\
\mathcal{F}(\eta_3) &= m^3 - 3m^2 + 4m + 40 \\
\mathcal{F}(\eta_4) &= m^3 - 3m^2 + 4m + 28 \\
\mathcal{F}(S_m^{k_4}) &= m^3 - 3m^2 + 4m + 76 \\
\mathcal{F}(S_m^{m+2}) &= m^3 - 3m^2 + 4m + 82
\end{aligned}$$

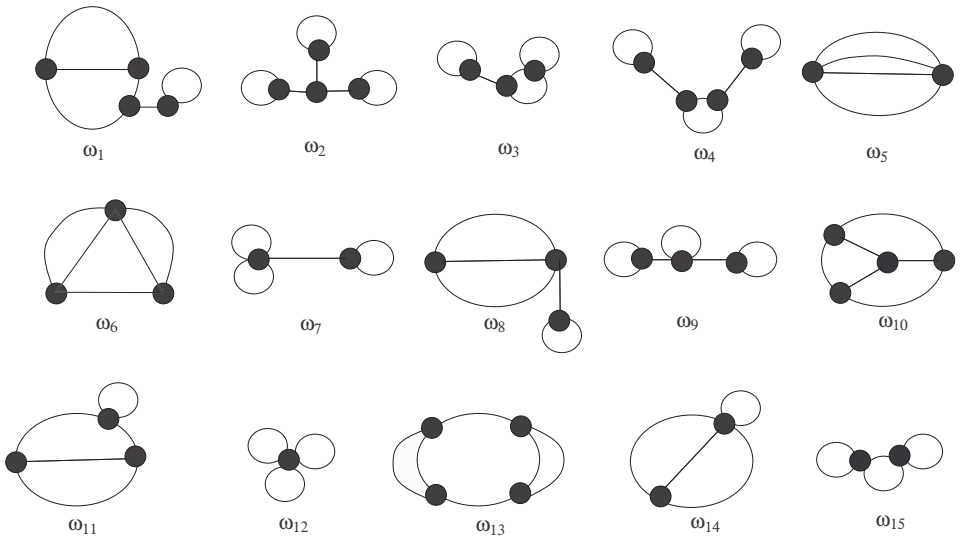

FIGURE 10. All possible braces ω_i of tricyclic graphs in Ω_m^0

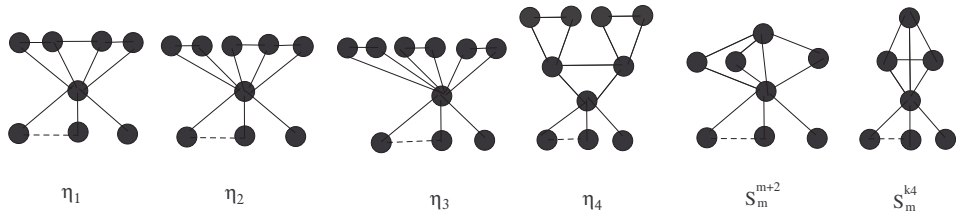

FIGURE 11. η_i in Ω_m^2

As a result, the proof is complete. □

5. CONCLUSION

In this work, we have observed the behavior of F-index under the graph transformations for tricyclic graphs of order m. We have observed that in transformation 1, when we converted vertex of internal path to pendent vertex then as a result, all the indices increased similarly, transformation 2 and 4, increased the indices under consideration which gave us upper bound, but in transformation 3, when we converted pendent path to internal path, as a result invariants decreased, which gave us lower bound. Further, extreme values of these chemical invariants are determined. In addition to theoretical contributions, this work pioneers in proposing the integration of artificial intelligence (AI) and machine

learning (ML) to enhance the utilization of topological indices in cheminformatics. We propose three transformative AI-driven frameworks: (i) Predictive modeling via graph neural networks (GNNs) to estimate F-indices for large-scale tricyclic graphs, circumventing combinatorial enumeration; (ii) Generative design using variational autoencoders (VAEs) to synthesize novel tricyclic architectures with near-optimal F-indices, enabling targeted materials discovery; and (3) Reinforcement learning (RL)-guided optimization to validate extremal structures and explore uncharted regions of the tricyclic graph space. This dual methodology-bridging rigorous mathematical analysis with data-driven AI-not only validates our derived bounds but also unlocks scalable strategies for molecular property prediction and design. By embedding F-index optimization within generative and exploratory AI pipelines, we advance cheminformatics into a paradigm where theoretical invariants directly inform actionable design principles, accelerating the discovery of functional materials with tailored π-electron properties. Future work will focus on experimental validation of AI-generated graphs and extending these synergies to higher cyclic systems. Moreover, the expected Outcome of the study is that the F-index improves model accuracy compared to baseline models, underscoring its physicochemical relevance.

6. Innovations and Strategic Directions

It is suggested to demonstrate the practical value of the F-index by incorporating it into a Quantitative Structure-Property Relationship (QSPR) model for predicting the boiling points of tricyclic hydrocarbons. To do this, in the Feature Engineering stage, combine F-index with other indices (e.g., Wiener, Zagreb) as input features. Next, in model Training, Train a Random Forest regressor on experimental boiling point data (e.g., NIST Chemistry WebBook). This work can be extended for more indices. Finally, for the validation, use SHAP (SHapley Additive exPlanations) to quantify F-index contributions, revealing its role in modeling non-covalent interactions [12, 9].

AUTHOR CONTRIBUTIONS

Conceptualization, Salma Kanwal; methodology, Maria Fazal and Muhammad Taskeen Raza; software, Maria Fazal and Muhammad Taskeen Raza; validation, Salma Kanwal, Maria Fazal and Muhammad Taskeen Raza; investigation, Salma Kanwal; writing-original draft, Maria Fazal and Muhammad Taskeen Raza; writing-review and editing, Salma Kanwal, Maria Fazal and Muhammad Taskeen Raza; visualization, Salma Kanwal, Maria Fazal and Muhammad Taskeen Raza; funding acquisition, Salma Kanwal and Maria Fazal. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest

Authors declared no conflicts of interest.

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