The Gourava Co-Indices of Graph

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Abstract:- This Paper explores the concept of Gourava co-indices, inspired by the analogous discussions on Zagreb indices in prior literature. Gourava co-indices are a novel extension of graph theoretical concepts, focusing on the relationships and patterns within molecular structures. Moreover, we present several key relations and properties associated with Gourava co-indices, providing a comprehensive framework for further research and practical applications in areas such as drug discovery, material science, and computational chemistry.

Keywords:- *Zagreb Indices, Co-Indices, Gourava Indices, Gourava Co-Indices, Complete Graph, Tree Graph, Uniform Edge, Uniform Graph.*

I. INTRODUCTION

➢ *Background:*

Consider a simple, connected graph, G, having vertex group V(G) = {v_{a1}, v_{a2}, . . ., v_{ap}} and edge group E(G) with |E(G)| = q. Whenever any two vertices say x and y are part of V(G) and share an edge, they are represented by xy ∈ E(G). The degree of the vertex x in the vertex group V(G) is defined as the count of edges that are connected to x, represented or denoted as $\deg_G(x)$. Throughout this study, we adopt standard references for terms and symbols.

In the realm of molecular graph theory, molecular arrangement is commonly represented by molecular graphs to analyse various properties of chemical compounds theoretically. A crucial concept in this field is the molecular structure index, a graph invariant that correlates physio-chemical properties with numerical values. Utilizing adjacency, degree, and distance matrices from graph theory, one can elucidate the structural features of molecules, leading to the development of vertex degree-based topological indices and distance-based topological indices [5,6,8,9,10]. The application of molecular structure indices is integral to elucidating structure-property relationships and other relevant properties [1,7,11].

The initial Zagreb indices, Namely the Ist Zagreb Index and IInd Zagreb index were first introduced as components of a topological formula to calculate the total π-energy of conjugated molecules by Gutman et al [1]. These indices play a crucial role as fundamental branching indices. Their utility extends across various fields, notably in QSPR (Quantitative Structure-Property Relationships) and QSAR (Quantitative Structure-Activity Relationship) studies, where they have been extensively applied and analyzed.

The Ist and IInd Zagreb Indices of Graphs are defined as follows:

$$M_1(G) = \sum_{xy\in E(G)}[d_G(x) + d_G(y)] \;\; or \sum_{x\in V(G)} d_G^2(x),$$

$$M_2(G) = \sum_{xy\in G}[d_G(x).d_G(y)]$$

Drawing inspiration from the definitions of the Zagreb indices and their broad applications, V.R. Kulli introduced the first and second Gourava indices of a molecular graph in [2] as outlined below:

$$GO_1(G) = \sum_{xy\in G}[\{(d_G(x) + d_G(y)\} + d_G(x).d_G(y)],$$

$$GO_2(G) = \sum_{xy\in G}[\{(d_G(x) + d_G(y)\}.d_G(x).d_G(y)]$$

Exploring a finite simple graph, denoted as G, comprising p vertices and q edges. The sets of vertices are symbolized by V(G) and sets of edges in G are symbolised E(G). The complement of G, designated as $\overline{G}$ is a simple graph sharing the same vertex group V(G). In $\overline{G}$, two vertices x and y are termed adjacent, linked by an edge xy, solely if they are not adjacent in G. Hence, xy ∈ E (($\overline{G}$)) if and only if xy ∉ E(G). (This definition excludes loops in $\overline{G}$). It's evident that E(G) ∪ E ($\overline{G}$) = E(K_p), and the count of edges in the complement graph is denoted by |E ($\overline{G}$)| = $\frac{p(p-1)}{2} - q$.. The degree of a vertex x in G is represented by d(x); accordingly, the degree of the same vertex in ($\overline{G}$) is expressed as $d_{\overline{G}}(x) = p-1-(d_G(x))$. The subscript G can be removed when the referred graph is evident from the context.

The Zagreb indices can be understood as the additive and multiplicative contributions of pairs of adjacent vertices to weighted variations of Wiener numbers and polynomial [12]. Intriguingly, it has been found that analogous contributions from non-neighbouring pairs of vertices become notable while calculating the weighted Wiener polynomials of specific composite graphs [13]. These contributions, spanning across the edges of the complement of G, are referred to as Zagreb co-indices. To formally define the first Zagreb coindex of a graph G.

$$\bar{M}_1(G) = \sum_{xy \notin E(G)} [d_G(x) + d_G(y)]$$

$$\bar{M}_2(G) = \sum_{xy \notin E(G)} [d_G(x).d_G(y)]$$

The formal presentation of these new invariants was introduced in [13], anticipating that they would enhance our capability to measure the impacts of pairs of non-adjacent vertices on different characteristics of molecules. In this article, we delve into the computation of Gourava Co-indices, defined as follows:

$$\overline{GO}_1(G) = \sum_{xy \notin E(G)} [\{(d_G(x) + d_G(y)\} + d_G(x).d_G(y)]$$

$$\overline{GO}_2(G) = \sum_{xy \notin E(G)} [\{(d_G(x) + d_G(y)\}.d(x).d_G(y)]$$

II. BASIC PROPERTIES OF ZAGREB CO-INDICES FROM [14]

- *Result 1. Assuming a Simple Graph G Having p Vertices, q Edges, then*

$$M_1(\overline{G}) = M_1(G) + 2(p-1)(\overline{q} - q)$$

- *Proof:*

$$M_1\overline{(G)} = \sum_{x \in V(\overline{G})} d^2_{\overline{G}}(u) = \sum_{u \in V(G)} (p - 1 - (d_G(x))^2$$

$$= \sum_{x \in V(G)} (p-1)^2 - 2(p-1) \sum_{x \in V(G)} d_G(x) + \sum_{x \in V(G)} (d_G(x)^2)$$

$$= p(p-1)^2 - 4q(p-1) + M_1(G)$$

- *Result 2: Assuming a Simple Graph G having p Vertices, q Edges, then*

$$\bar{M}_1(G) = 2q(p-1) - M_1(G)$$

- *Proof:*

$$\bar{M}_1(G) = \sum_{xy \notin E(G)} [d_G(x) + d_G(y)]$$

$$= \sum_{xy \in E(\overline{G})} [(p - 1 - d_{\overline{G}}(x)) + (p - 1 - d_{\overline{G}}(y)]$$

$$= \sum_{xy \in E(\overline{G})} [(2p - 2 - (d_{\overline{G}}(x) + d_{\overline{G}}(y))]$$

$$= \sum_{xy \in E(\overline{G})} (2(p-1) + \sum_{xy \in E(\overline{G})} (d_{\overline{G}}(x) + d_{\overline{G}}(y))$$

$$= 2(p-1)\overline{q} - M_1(G) = 2(q-1)p - M_1(G)$$

- *(Substituting the Value of* $M_1(\overline{G})$ *from Result 1)*

- *Result 3: Assuming a Simple Graph G having p Vertices, q Edges,* then

$$\bar{M}_2(G) = (2q)^2 - M_2(G) - \frac{1}{2} M_1(G)$$

- *Proof: follows from [14]*

- *Result 4: Assuming a Simple Graph G having p Vertices, q Edges,* then

$$M_2(\overline{G}) = \bar{M}_2(G) + (p-1)\ M_1(\overline{G}) + \overline{q}(p-1)^2$$

- *Proof:*

$$\bar{M}_2(G) = \sum_{xy \notin E(G)} [d_G\,(x).\, d_G\,(y)]$$

$$= \ \sum_{xy \in E(\overline{G})} \left[(p-1-d_{\overline{G}}\,(x)\right).\,(p-1-d_{\overline{G}}\,(y)]$$

$$= \ \sum_{xy \in E(\overline{G})} (p-1)^2 - (p-1)\sum_{xy \in E(\overline{G})} d_{\overline{G}}\,(x) + d_{\overline{G}}\,(y) + \sum_{xy \in E(\overline{G})} d_{\overline{G}}\,(x) d_{\overline{G}}\,(y)$$

$$= (p-1)^2\,\overline{q} + (p-1)\ \ M_1\left(\overline{G}\right) + \bar{M}_2(G)$$

- *Corollary 1:*

$$M_2\left(\overline{G}\right) = (2q)^2 - \ M_2(G) - \frac{1}{2}\, M_1(G) + (p-1)\ \ M_1(G) + 2(p-1)^2(\overline{q} - q) - \overline{q}(\,p-1)^2$$

- *Proof:*

- By substituting the value of $\bar{M}_2(G)$ from result 3 in result 4, we get the above stated result.
- After getting all these things we now tend to establish relation between Gourava and Zagreb Co-indices.

- *We know*

$$GO_1(G) = \sum_{xy \in G} [\{(d_G\,(x) + d_G\,(y)\} + d_G\,(x).\, d_G\,(y)]$$

$$= \sum_{xy \in G} \{(d_G\,(x) + d_G\,(y)\} + \sum_{xy \in G} d_G\,(x).\, d_G\,(y)$$

$$= M_1(G) + M_2(G)$$

- *Proposition 1:*

$$\overline{GO}_1(G) = \bar{M}_1(G) + \bar{M}_2(G)$$

- *Proof:*

$$\text{R.H.S} \quad \bar{M}_1(G) + \bar{M}_2(G)$$

$$= 2q(p-1) - \ \ M_1(G) + (2q)^2 - \ M_2(G) - \frac{1}{2}\, M_1(G)$$

$$= 2q(p-1) - \frac{3}{2}\, M_1(G) - \ M_2(G) + (2q)^2$$

$$\text{L.H.S} \quad \overline{GO}_1(G) = \sum_{xy \notin G} [\{(d_G\,(x) + d_G\,(y)\} + d_G\,(x).\, d_G\,(y)]$$

$$= \sum_{xy \in E(\overline{G})} [(p-1-d_{\overline{G}}\,(x)) + (p-1-d_{\overline{G}}\,(y)] + \left[(p-1-d_{\overline{G}}\,(x)\right).\,(p-1-d_{\overline{G}}\,(y)]$$

$$= \sum_{uv \in E(\overline{G})} \left[(2p-2) - p(d_{\overline{G}}\,(x) + d_{\overline{G}}\,(y)\right) + (p-1)^2 + \quad (d_{\overline{G}}\,(x).\, d_{\overline{G}}\,(y))]$$

$$= \sum_{xy \in E(\overline{G})} ((p)^2 - 1) - p \sum_{xy \in E(\overline{G})} (d_{\overline{G}}\,(x) + d_{\overline{G}}\,(y)) + \sum_{xy \in E(\overline{G})} d_{\overline{G}}\,(x) d_{\overline{G}}\,(y)$$

$$= ((p)^2 - 1)\,\overline{q}p\ \ M_1\left(\overline{G}\right) + \ \ M_1\left(\overline{G}\right)$$

- *Substituting the Values of*

$$M_1(\overline{G})\ and\ \ M_2(\overline{G})$$

$$=((p)^2-1)\overline{q}-p(M_1(G)+2(p-1)(\overline{q}-q))+(2q)^2-\ M_2(G)\ -\tfrac{1}{2}\,M_1(G)+(p-1)\ M_1(G)+2(p-1)^2(\overline{q}-q)-\overline{q}(p-1)^2$$

$$=((p)^2-1-(p-1)^2)\overline{q}+(2(p-1)^2-2p\,(p-1)(\overline{q}-q)-M_2(G)-\tfrac{3}{2}\,M_1(G)+(2q)^2$$

$$=-2p\overline{q}+(2-2p)(\,\overline{q}-q)-\ M_2(G)-\tfrac{3}{2}\,M_1(G)+(2q)^2$$

$$=2q(p-1)-\tfrac{3}{2}\,M_1(G)-\ M_2(G)+(2q)^2\ =R.H.\ S$$

III. SECOND GOURAVA INDEX

- *Unlike how First Gourava Index behaves, the Second Gourava Index does not Adhere to*

$$GO_2(G)=\ M_1(G)\,M_2(G)$$

- *As Summation is not Distributed over Multiplication*

- *So, Clearly*

$$GO_2(G)\neq\ M_1(G)\,M_2(G)$$

- *But for Certain* ***Special Cases*** *q*

$$GO_2(G)=\ M_1(G)\,M_2(G)$$

- *We will now Discuss those Special Cases.*

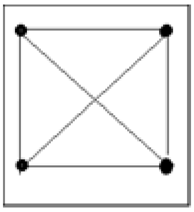
- *Uniform Graphs and Uniform Edges*

There exist graphs where the degrees of corresponding vertices in both the graph and its complement are equal. We refer to these edges as "Uniform edges," and such graphs are termed "Uniform Graphs."

Upon observation, Complete graphs, Cyclic Graphs, and Tree Graphs are examples of Uniform Graphs.

- *Illustration:*

- *Consider Complete Graph G= K_4*



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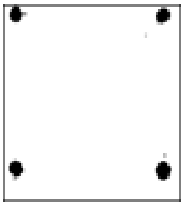
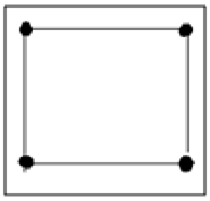


$\overline{G}$

Every edge in G possesses vertex degree 3 and 3

And $\overline{G}$ contains no edge

Consider Cyclic Graph G= C_4



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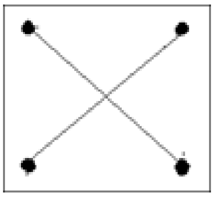
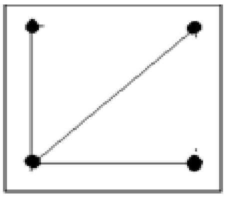


$\overline{G}$

Every edge in G possesses vertex degree 2 and 2

And every edge in $\overline{G}$ possesses vertex degree 1 and 1

- *Star Graph with 4 Vertices*



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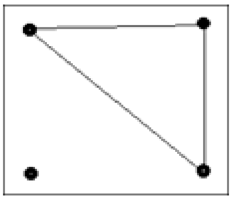

$\overline{G}$

Every edge in graph G has possesses degree 3 and 1

And every edge in $\overline{G}$ possesses vertex degree 2 and 2

- *Proposition 2: For Uniform Graphs:*

$$\overline{q}\ \overline{GO_2}(G)=\overline{M}_1(G).\overline{M}_2(G)$$

➢ *Proof:*

- *Case I: For Complete Graphs*

$$\text{LHS } \overline{q}\ \overline{GO}_2(G) = \overline{q} \sum_{xy\notin G} [\{(d_G(x) + d_G(y)\}.d(x).d_G(y)]$$

$$= \overline{q} \sum_{xy\notin G} [\{(p-1) + (p-1)\}.(p-1).(p-1)]$$

$$=2(p-1)^3\ \overline{q}^2$$

$$\text{RHS } \overline{M}_1(G).\overline{M}_2(G) = \sum_{xy\notin E(G)}[d_G(x) + d_G(y)] . \sum_{xy\notin E(G)}[d_G(x).d_G(y)]$$

$$= \sum_{xy\notin E(G)}[p-1+p-1] . \sum_{xy\notin E(G)}[(p-1).(p-1)]$$

$$=2(p-1)^3\ \overline{q}^2$$

- *Case 2: For Cyclic Graphs*

$$\text{LHS } \overline{q}\ \overline{GO}_2(G) = \overline{q} \sum_{xy\notin G} [\{(d_G(x) + d_G(y)\}.d(x).d_G(y)]$$

$$= \overline{q} \sum_{xy\notin G} [(2+2).(2).(2)]$$

$$=16\ \overline{q}^2$$

$$\text{RHS } \overline{M}_1(G).\overline{M}_2(G) = \sum_{xy\notin E(G)}[d_G(x) + d_G(y)] . \sum_{xy\notin E(G)}[d_G(x).d_G(y)]$$

$$= \sum_{xy\notin E(G)}[2+2] . \sum_{xy\notin E(G)}[(2.2)]$$

$$=4\ \overline{q}.\ 4\overline{q}$$

$$=16\ \overline{q}^2$$

- *Case 3: For Star Graphs*

$$\text{LHS } \overline{q}\ \overline{GO}_2(G) = \overline{q} \sum_{xy\notin G} [\{(d_G(x) + d_G(y)\}.d(x).d_G(y)]$$

$$= \overline{q} \sum_{xy\notin G} [(p-1+1).(p-1).(1)]$$

$$=p(p-1)\ \overline{q}^2$$

$$\text{RHS } \overline{M}_1(G).\overline{M}_2(G) = \sum_{xy\notin E(G)}[d_G(x) + d_G(y)] . \sum_{xy\notin E(G)}[d_G(x).d_G(y)]$$

$$= \sum_{xy\notin E(G)}[p-1+1] . \sum_{xy\notin E(G)}[(p-1).1]$$

$$=p\ \overline{q}\ .\ (p-1)\overline{q}$$

$$=p(p-1)\ \overline{q}^2$$

IV. CONCLUSION

In conclusion, this paper introduces the concept of Gourava co-indices, which extend the ideas of Zagreb indices to analyse relationships and patterns within molecular structures. We have also discussed some results that discuss relationship for Gourava and Zagreb Co-indices.

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