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Characterization of extremal graphs for geometric-arithmetic index with given cut vertices and correlation with eigenvalues

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Abstract. This paper links spectral and chemical graph theories by examining the geometric-arithmetic and normalized Laplacian indices via Rayleigh's quotient principle. Spectral graph theory elucidates structural properties through the examination of eigenvalues and eigenvectors, whereas chemical graph theory represents molecular structures, presenting applications in chemistry. We concentrate on the collection $\mathbb{G}_n^k$, which includes all n-vertex graphs exhibiting connectivity 1 and containing precisely k cut vertices, such that the elimination of a cut vertex results in the disconnection of the graph. Precise limits for the geometric-arithmetic index in $\mathbb{G}_n^k$ are established through auxiliary graph operations. Additionally, we enhance these bounds by analyzing the relationship between the normalized Laplacian index and the geometric-arithmetic index via the Rayleigh quotient, thereby offering a more profound understanding of the structural interaction of indices within these graphs.

1. Introduction

Chemical graph theory is an interdisciplinary area that seeks to connect chemistry with graph theory. The study of the relationship between the eigenvalues of a matrix representation and the primary form of a graph is the goal of spectral graph theory.

The topological index [5] is a numerical measure provided by graph theory to chemists for modelling molecules and chemical compounds. Topological indices are widely utilized in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies to predict the physio-chemical characteristics of molecules. In many scientific fields, topological indices are essential, especially in chemistry and bioinformatics, where they offer important insights into the structural features and attributes of molecules. These indices capture crucial details regarding connectivity, branching, and symmetry and measure the topological characteristics of molecular networks. Topological indices help forecast the biological activities and characteristics of molecules in medicinal chemistry and drug design, directing the creation of novel pharmaceutical substances. These indices aid in the comprehension of the

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chemical and electrical characteristics of materials in the field of materials science. Furthermore, network theory, the analysis of complex systems, and quantitative structure-activity relationship (QSAR) research employ topological indices. Their applicability includes the analysis of DNA and protein structures in bioinformatics and environmental chemistry, where they help evaluate the behavior of pollutants. Overall, the variety of uses highlights how important topological indices are as effective instruments for describing molecular structures and their characteristics across a number of scientific fields. For further study, we refer to [2, 7, 10].

In 2009, Vukičević [18] introduced the geometric-arithmetic index (GA index for short) as an attempt to outperform the predictive ability. The definition of GA index the index of any graph Ω is defined as follows [18],

$$GA = GA(\Omega) = \sum_{pq \in E(\Omega)} \frac{2\sqrt{\deg_\Omega(p) \cdot \deg_\Omega(q)}}{(\deg_\Omega(p) + \deg_\Omega(q))},$$

where pq is an edge of the graph Ω and $\deg_\Omega(p)$ (resp. $\deg_\Omega(q)$) is the degree of vertex p (resp. vertex q). The GA index is acknowledged to have significantly superior forecasting accuracy for multiple physicochemical characteristics such as boiling point, entropy, enthalpy and standard enthalpy of vaporization, enthalpy of formation, and acentric component [1].

Investigating the mathematical behavior of topological indices is a contemporary research topic these days. Extremal graphs are of great importance in chemical graph theory [3, 17]. For example, Li [11] characterized the extremal results for all graphs, and their line graphs for GA index and Bermudo [3] characterized the graphs achieving upper bounds of trees with domination number for GA index. There are numerous results on GA, which can be read herein [8, 9, 12, 13, 16, 19].

Let M be a real symmetric matrix of order n; we order and denote the eigenvalues by $\lambda_1(M) \leq ... \leq \lambda_n(M)$ and the singular values by $\sigma_1(M) \leq ... \leq \sigma_n(M)$. If G is a graph and M is a real symmetric matrix associated with G, then the M-energy of G is

$$E_M(G) = \sum_{i=1}^{n} |\lambda_i(M) - \frac{tr(M)}{n}|, \tag{1}$$

where $tr(M)$(sum of diagonal entries) is equal to $trace(M)$(sum of its eigenvalues). Formally, using Equation (1) with M taken to be L, the normalized Laplacian energy (or L-energy) [15] of a graph G is

$$E_L(G) = \sum_{i=1}^{n} |\lambda_i(L) - 1|, \tag{2}$$

which is equivalent to

$$E_L(G) = \sum_{i=1}^{n} |\lambda_i(I - L)|, \tag{3}$$

To advance from the previous framework in extremal graph theory, specifically inspired by [1, 3, 8, 9, 12, 13, 16, 17, 19] and various applications of geometric-arithmetic index GA, our research takes a ground-breaking step forward. Initially, we extend the existing literatures to attain sharp bounds on GA index with given cut vertices and characterize the extremal graphs achieving bounds. Further research delves into the domain of spectral graph theory to introduce a novel direction to the extremal characterization by employing the Rayleigh quotient principle to establish a correlation between GA index and the normalized Laplacian index.

2. Preliminaries

We exclusively concentrate on discrete, connected, and simple graphs. Let $\Omega = (V, E)$ be a simple connected graph, where $V = V(\Omega)$ is a vertex set and $E = E(\Omega)$ is an edge set. If $p \in V(\Omega)$, then neighborhood of vertex p is defined as $N_\Omega(p) = \{q \in V(\Omega) | \, pq \in E(\Omega)\}$. The degree of a vertex v is the number of edges incident to it, denoted by $\deg_\Omega(v)$. For an edge $pq \in E(\Omega)$, the graph $\Omega - pq$ is obtained by deleting $pq \in E(\Omega)$ from Ω.

Let $\mathbb{P}_n$ (resp. $\mathbb{S}_n$) be the path (resp. star) graph of order n. A block of any graph Ω is a maximally connected subgraph without a cut-vertex. The block graph is a graph in which every block of it is a complete subgraph. A clique of a graph Ω is an induced subgraph of Ω that is complete.

Regarding the geometric arithmetic index of a graph, we start with the following auxiliary lemmas and transformations.

Theorem 2.1. *[14] Let Ω be a connected graph with zero cut vertex such that $|V(\Omega)| \geq 3$, then there exists a cycle containing all its vertices.*

Remark 2.2. *Every non-trivial connected graph contains at least two vertices that are not cut vertices.*

Proposition 2.3. *[14] Suppose $\Omega = (V, E)$ is a graph with at least one cycle then $|E| > |N|$.*

Theorem 2.4. *[14] Every non-pendant vertex of the tree is a cut vertex.*

Let $\mathbb{G}_n^k$ be a set of all graphs with n vertices and k cut vertices.

Lemma 2.5. *[6] Let $\Omega \in \mathbb{G}_n^k$ be a connected graph, then $GA(\Omega) > GA(\Omega - pq)$ for any edge $pq \in \Omega$.*

Theorem 2.6. *Assume that T is a tree graph of order n. Then $GA(\mathrm{T}) \geq 2(n-1)\frac{\sqrt{n-1}}{n}$, with equality holds if and only if $\mathrm{T} \cong \mathbb{S}_n$.*

In general, the Theorem 2.6 holds for all connected graphs Ω.

Proof. Consider $\mathrm{T}(\Omega)$ represents the spanning tree of any connected graph Ω with n vertices. Then, by Lemma 2.5 and Theorem 2.6, we have

$$GA(\Omega) \geq GA(\mathrm{T}(\Omega)) \geq 2(n-1)\frac{\sqrt{n-1}}{n},$$

with equality if and only if $\Omega \cong \mathbb{S}_n$. □

Theorem 2.7. *[4] Consider connected graph Ω with pendant vertices with $B_{ij} = \{\frac{1}{\deg_\Omega(i)} + \frac{1}{\deg_\Omega(j)}\}$. Then*

$$GA(\Omega) \geq \frac{2}{D_1(\Omega)} \sum_{ij \in E_r(\Omega)} \frac{1}{B_{ij}} + \frac{2}{\sqrt{D_2(\Omega)}} \sum_{ij \in E_p(\Omega)} \frac{1}{B_{ij}},$$

Where E_p are pendant edges, $E_r(\Omega) = E(\Omega) - E_p(\Omega)$ and $D_1(\Omega)$ is the maximum degree among all vertices in $E_p(\Omega)$ whereas $D_2(\Omega)$ is the maximum degree in non-pendant edges.

Suppose the set of cut vertices in Ω represented by $C(\Omega)$ and the shortest distance between p and q in Ω labeled by $d_\Omega(p, q)$.

Definition 2.8. *The two distinct cut vertices are known as closed cut vertices in a connected graph Ω if it satisfies $d_\Omega(p, r) < d_\Omega(p, q)$ and $d_\Omega(q, r) < d_\Omega(p, q)$ for some p, q, and r cut vertices.*

Definition 2.9. *Suppose two distinct cut vertices p and q in any graph Ω. The $CVIS(\Omega)$ represents the induced subgraph by two close-cut vertices p and q is defined as the subgraph with vertex set and edge set comprising cut vertices (p, q) and vertex $s \in V(\Omega) \setminus C(\Omega)$ such that $d_{\Omega-p}(s, q) < d_{\Omega-p}(s, r)$ and $d_{\Omega-q}(s, p) < d_{\Omega-q}(s, r)$, where $r \in C(\Omega) \setminus \{p, q\}$ and $y_1 y_2 \in E(\Omega)$ edges respectively, where $y_1, y_2 \in V(CVIS(\Omega))$.*

Definition 2.10. *Suppose two distinct cut vertices p and q in a connected graph Ω. The vertex set of close-cut vertex graph is symbolized by $V(CCV(\Omega))$ a collection of cut vertices of Ω and each pair of cut vertices is associated with an edge if it is close cut vertices.*

Definition 2.11. *Let p be at least one cut vertex in any graph Ω. Let $\Omega - p = \cup_{i=1}^{t}\Omega_i \ \forall\ t \geq 2$ be a graph without cut vertex. Then, $[V(\Omega_i)\bigcup\{p\}]$ is an end block of Ω with respect to cut vertex p.*

Now, we establish a transformation namely α-transformation 2.1 on $\Omega \in \mathbb{G}_n^k$. Figure 1 explains the structure of transformation 2.1.

Transformation 2.1. *Let Ω_o and Ω_o' be two subgraphs adjoining by cut vertex p where Ω_o' comprises the vertices $p_1, p_2, ..., p_r$ such that $p_1, p_2, ..., p_r$ form a cycle, which is denoted by Ω.*

Next, suppose that Ω_α is a generated graph from Ω by deletion of edges and addition of pendant edges by applying transformation 2.1 *such that $\Omega_\alpha = \Omega - \{p_1p_2, .., p_{r-1}p_r\} + \{pp_1, pp_2, .., pp_{r-1}\}$.*

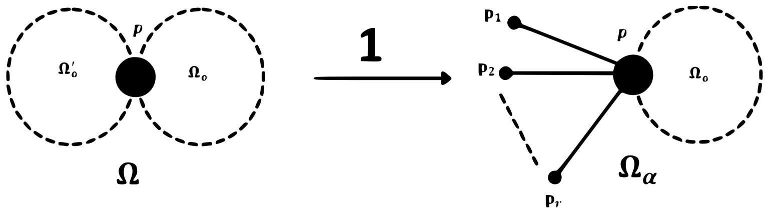


Figure 1: Employed transformation 2.1 in lemma 2.12.

Lemma 2.12. *Let Ω_α be an $\alpha-$ transformed graph from $\Omega \in \mathbb{G}_n^k$. Then*

$$GA(\Omega_\alpha) < GA(\Omega)$$

Proof. Let p be a cut vertex of two subgraphs Ω_o and Ω_o' such that Ω_o' comprises the vertices $p_1, p_2, ..., p_i \ \forall$ $1 \leq i \leq r$, which form a cycle. Let $\Omega_\alpha = \Omega - \{p_1p_2, .., p_{r-1}p_r\} + \{pp_1, pp_2, .., pp_{r-1}\}$. The resulting graph Ω_α is a generated graph from Ω by deletion of edges and associating pendant edges at cut vertex p. This shifting of edges between $GA(\Omega)$ and $GA(\Omega_\alpha)$ requires the following relationship.

$$\begin{aligned}
GA(\Omega) - GA(\Omega_\alpha) &= \frac{2\sqrt{\deg_\Omega(p)\cdot\deg_\Omega(p_1)}}{\deg_\Omega(p)+\deg_\Omega(p_1)} + \frac{2\sqrt{\deg_\Omega(p_1)\cdot\deg_\Omega(p_2)}}{\deg_\Omega(p_1)+\deg_\Omega(p_2)} \\
&+ \frac{2\sqrt{\deg_\Omega(p_2)\cdot\deg_\Omega(p_3)}}{\deg_\Omega(p_2)+\deg_\Omega(p_3)} + \frac{2\sqrt{\deg_\Omega(p_{r-1})\cdot\deg_\Omega(p_r)}}{\deg_\Omega(p_{r-1})+\deg_\Omega(p_r)} \\
&+ \frac{2\sqrt{\deg_\Omega(p_r)\cdot\deg_\Omega(p_1)}}{\deg_\Omega(p_r)+\deg_\Omega(p_1)} - \sum_{i=1}^{r}\frac{2\sqrt{\deg_\Omega(p_1)\cdot\deg_\Omega(p_i)}}{\deg_\Omega(p_1)+\deg_\Omega(p_i)} \\
&= 2\frac{2\sqrt{x\cdot 2}}{x+2} + (r-2)\frac{2\sqrt{2\cdot 2}}{2+2} - (r-1)\frac{2\sqrt{x+(r-1)\cdot 1}}{x+r} \\
&> 0
\end{aligned}$$

The proof is complete. □

Next, we derive another transformation namely β-transformation 2.2 on $\Omega \in \mathbb{G}_n^k$.

Transformation 2.2. *Assume that p and q are two close-cut vertices in a connected graph Ω. Let Ω_A be an induced close-cut vertex subgraph $CVIS(\Omega)$. The union of $[p]$-component of Ω is represented by $\Omega_o - p$ which does not contain* *q and the union of* $[q]$*-component of* Ω *is represented by* $\Omega_o - q$ *which is not containing p. The cardinality of* Ω_o *and* $\Omega_o^{'}$ *greater than 2 such that* $p \in \Omega_o$ *and* $q \in \Omega_o^{'}$.

Suppose there exist some cut vertices on the cycle other than close cut vertices p, q *if they neither comprise in* $\Omega_o - p$ *nor in* $\Omega_o - q$. *Otherwise, there exists a path containing cut vertex, say* $r \in C(\Omega)$ *to p (or q) and r passing through* Ω *if we select cut vertex* $r \in C(\Omega) \setminus (\Omega_o - p) \cup (\Omega_o - q)$ *such that* $r \in C(\Omega)$ *is close cut vertex to p (or q). Consequently, It shows* $r \in C(\Omega)$ *comprising in* $[p]$*-component of* Ω *(or* $[q]$*-component of* Ω*) which means* $r \in (\Omega_o - p)$ *(or* $r \in (\Omega_o - q)$*), is a contradiction. Next, we suppose that edge-disjoint subgraph, say* Ω_B *such that* $\Omega_B = \Omega[V(\Omega) \setminus V(\Omega_o) \cup V(\Omega_o^{'}) \cup V(\Omega_A) \cup \{p, q\}] - pq$ *where* $pq \in E(\Omega_A)$*, which is symbolized by* Ω.

Next, we deduce the Ω_β *from* Ω *by deletion of all edges of* $E(\Omega_A)$ *between* p, q *except pq is connected to cut vertex p (or q) as a pendent vertex. This shifting of edges between* Ω *and* Ω_β *named Transformation* 2.2.

Similarly, we deduced Ω_γ *from* Ω *by deletion of all edges of* $E(\Omega_A)$ *between* p, q *except pq connected to cut vertex p (or q) as a pendent vertex (*$|E(\Omega_A)| - 2$*), if all the others cut vertices lie in* $(\Omega_o - p)$ *or* $(\Omega_o - q)$*. The Figure* 3*, clearly illustrated the transformation between* Ω_γ *and* Ω.

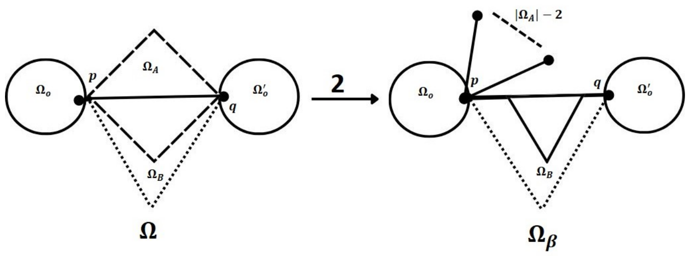


Figure 2: Transformation 2.2 used in Lemma 2.13.

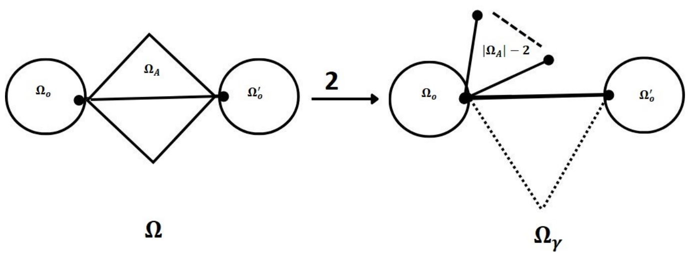


Figure 3: Employed transformation 2.2 in lemma 2.13.

The following lemma differentiates the geometric arithmetic indices of $\Omega \in \mathbb{G}_n^k$ in Ω_β and Ω_γ.

Lemma 2.13. *Let* Ω_β *and* Ω_γ *be a* $\beta, \gamma-$ *transformed graphs from* $\Omega \in \mathbb{G}_n^k$ *represent in the Figures* 2 *and* 3*. Then*

$$GA(\Omega_\beta) < GA(\Omega),$$

and

$$GA(\Omega_\gamma) < GA(\Omega).$$

Proof. Let p and q be two close-cut vertices in a connected graph Ω. Suppose that $\deg_\Omega(\Omega_o) = x > 0$ and $\deg_\Omega(\Omega_o) = y > 0$. Let Ω_A comprises $p, p_1, p_2, ..., p_t, q, p_{t+1}, ..$ vertices such that $p, p_1, p_2, ..., p_t, q, p_{t+1}, ..., p$ form a cycle. Similarly, Ω_B comprises the vertices $p, q_1, q_2, ..., q_s, q$. Furthermore, $|\Omega_o| \geq 2$ and $|\Omega_o^{'}| \geq 2$.

Next, we deduce $\Omega_\beta = \Omega - \{pp_1, p_1p_2, ..., p_tq\} + \{pp_1, pp_2, ..., pp - t\}$. This shifting of edges between $GA(\Omega)$ and Ω_β requires the following relationship.

$$\begin{aligned} GA(\Omega) - GA(\Omega_\beta) = {} & \frac{2\sqrt{(x+4)\cdot 2}}{x+6} + t\frac{2\sqrt{2\cdot 2}}{4} + \frac{2\sqrt{(x+4)(y+4)}}{x+y+8} \\ & + \frac{2\sqrt{(x+4)\cdot 2}}{x+6} + \frac{2\sqrt{(y+4)\cdot 2}}{y+6} + \frac{2\sqrt{(y+4)\cdot 2}}{y+6} \\ & - (t)\frac{2\sqrt{(x+3+t)\cdot 1}}{x+t+4} - \frac{2\sqrt{(x+t+3)(y+3)}}{x+y+t+6} \\ & - \frac{2\sqrt{(x+t+3)\cdot 2}}{x+t+5} - \frac{2\sqrt{(y+3)\cdot 2}}{y+5} \\ & > 0 \end{aligned}$$

The proof is complete. Similarly, $GA(\Omega) - GA(\Omega_\gamma) > 0$ satisfies. □

Next, we discuss ξ-transformation 2.3 on $\Omega \in \mathbb{G}_n^k$. The structure of Ω is explain in Figure 4.

Transformation 2.3. *Let Ω be a graph containing vertices $p_1, p_2, ..., p_l, q_{r+1}, q_{r+2} ..., q_s$ such that vertices form a nested cycle. Any subgraph can be attached to any vertex of nested cycles.*

Next, we deduce $\Omega_\xi = \Omega - \{p_{r-1}p_r + p_1p_l\} + \{p_{r-1}p_l\}$, we declare that Ω_ξ transformed graph from Ω by ξ-transformation 2.3.

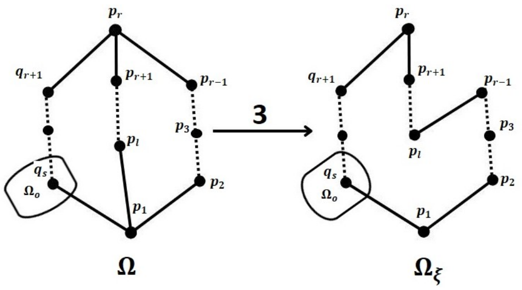


Figure 4: Employed transformation 2.3 in lemma 2.14.

Lemma 2.14. *Assume that Ω_ξ is a transformed graph by applying ξ−transformation on $\Omega \in \mathbb{S}_n^k$. We obtain $GA(\Omega) > GA(\Omega_\xi)$.*

Proof. Suppose that Ω comprises two nested cycles, that is, a bicycle graph. The bicycle graph transformed into a unicycle by applying ξ−transformation 2.3. This transformation of edges between $GA(\Omega)$ and $GA\Omega_\xi$

is expressed as the following relation,

$$
\begin{aligned}
GA(\Omega) - GA(\Omega_\xi) &= \frac{2\sqrt{\deg_\Omega(p_1)\cdot\deg_\Omega(p_2)}}{\deg_\Omega(p_1)+\deg_\Omega(p_2)} + \frac{2\sqrt{\deg_\Omega(p_1)\cdot\deg_\Omega(p_l)}}{\deg_\Omega(p_1)+\deg_\Omega(p_l)} \\
&+ \frac{2\sqrt{\deg_\Omega(p_1)\cdot\deg_\Omega(q_m)}}{\deg_\Omega(p_1)+\deg_\Omega(q_s)} + \frac{2\sqrt{\deg_\Omega(p_r)\cdot\deg_\Omega(p_{r-1})}}{\deg_\Omega(p_r)+\deg_\Omega(p_{r-2})} \\
&+ \frac{2\sqrt{\deg_\Omega(p_r)\cdot\deg_\Omega(p_{r+1})}}{\deg_\Omega(p_r)+\deg_\Omega(p_{r+1})} + \frac{2\sqrt{\deg_\Omega(p_r)\cdot\deg_\Omega(q_{r+1})}}{\deg_\Omega(p_r)+\deg_\Omega(p_{r+1})} \\
&- \frac{2\sqrt{deg_{\Omega_\xi}(p_1)\cdot\deg_\Omega(p_2)}}{deg_{\Omega_\xi}(p_1)+deg_{\Omega_\xi}(p_2)} - \frac{2\sqrt{\deg_{\Omega_\xi}(p_1)\cdot\deg_\Omega(q_m)}}{\deg_{\Omega_\xi}(p_1)+\deg_{\Omega_\xi}(q_s)} \\
&- \frac{2\sqrt{\deg_{\Omega_\xi}(p_r)\cdot\deg_\Omega(p_{r+1})}}{\deg_{\Omega_\xi}(p_r)+\deg_{\Omega_\xi}(p_{r+1})} - \frac{2\sqrt{\deg_{\Omega_\xi}(p_l)\cdot\deg_\Omega(p_{r-1})}}{\deg_{\Omega_\xi}(p_l)+\deg_{\Omega_\xi}(pr-1)} \\
&= 6\frac{2\sqrt{3\cdot 2}}{5} - 5\frac{2\sqrt{4}}{4} \\
&> 0
\end{aligned}
$$

Which is the required result. □

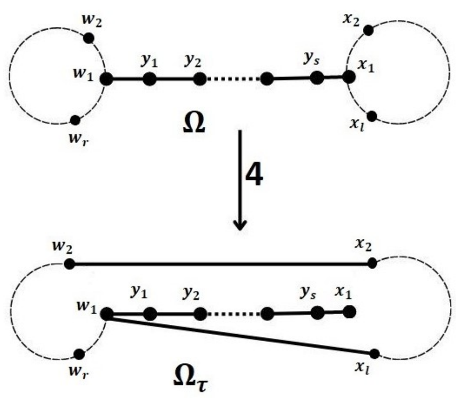


Figure 5: Employed transformation 2.4 in lemma 2.15.

Transformation 2.4. *Now, we established the $\tau-$transformation by employing it to $\Omega \in \mathbb{G}_n^k$. Let Ω be a graph containing vertices $w_1, w_2, ..., w_r, x_1, x_2..., x_l$ and $y_1, y_2, ..., y_s$ such that $w_1, w_2, ..., w_r$ (resp. $x_1, x_2..., x_l$) form a cycles C_r (resp. C_l) and induces path $y_1, y_2, ..., y_s$.*

Next, we extract $\Omega_\tau = \Omega - \{w_1w_2, x_1x_2, x_1x_l\} + \{w_2x_2, w_1y_s\}$, we declare that Ω_τ transformed graph from Ω by τ-transformation 2.4.

Lemma 2.15. *Assume that Ω_τ is a transformed graph by applying $\tau-$transformation on $\Omega \in \mathbb{G}_n^k$ depicted in Figure* 5. *We obtain $GA(\Omega) > GA(\Omega_\tau)$.*

Proof. Notice that Ω contains a path $y_1, y_2, ..., y_s$ such that one end vertex of path y_1 identifying by cycle $w_1, w_2, ..., w_r$ and another end vertex of path y_s associates the cycle $x_1, x_2..., x_l$. Suppose that Ω_τ be transformed from Ω by deletion of w_1w_2, x_1x_2, x_1x_l edges and addition of w_2x_2, w_1y_s edges. This shifting of edges between $GA(\Omega)$ and $GA(\Omega_\tau)$ suggests the following relation:

$$\begin{aligned} GA(\Omega) - GA(\Omega_\tau) &= \frac{2\sqrt{3\cdot 2}}{5} + \frac{2\sqrt{3\cdot 2}}{5} + \frac{2\sqrt{3\cdot 2}}{5} + \frac{2\sqrt{3\cdot 2}}{5} + \frac{2\sqrt{3\cdot 2}}{5} + \frac{2\sqrt{3\cdot 2}}{5} \\ &- \frac{2\sqrt{2\cdot 2}}{4} - \frac{2\sqrt{3\cdot 2}}{5} - \frac{2\sqrt{3\cdot 2}}{5} - \frac{2\sqrt{3\cdot 2}}{5} - \frac{2\sqrt{2\cdot 1}}{3} \\ &= 6\frac{2\sqrt{3\cdot 2}}{5} - 3\frac{2\sqrt{3\cdot 2}}{5} - \frac{2\sqrt{2\cdot 2}}{4} - \frac{2\sqrt{1\cdot 2}}{3} \\ &> 0 \end{aligned}$$

The proof is complete. □

Lemma 2.16. *Let $\Omega \in \mathbb{G}_n^k$ be a graph such that $k < n-2$. We have $GA(\Omega) < GA(\Omega')$ for $\Omega' \in \mathbb{G}_n^k$. Then Ω has a unique cycle of order $n-k$.*

Proof. Suppose Ω contains at least one cycle because Ω is not a tree. Suppose on the contrary Ω contains more than one cycle.

Claim 2.17. *Each cycle contains a unique path.*

Proof. [Proof of Claim 2.17] Let $C_1, C_2, C_3, ..., C_r$ be cycles for $r \geq 2$ with a common walk, by repeatedly applying lemma 2.14 Implies that $GA(\Omega) > GA(\Omega')$, which contradicts the choice of Ω, which leads to the claim 2.17. □

By Claim 2.17 and Lemma 2.15 repeatedly applying $GA(\Omega) > GA(\Omega'')$ which is again contradicts the choice of Ω. Hence, Ω contains a unique cycle. □

3. Sharp Lower bound of geometric arithmetic with given cut vertices.

Let $\mathbb{G}_n^k$ be a set of all graphs with n vertices and k cut vertices. In this section, we determine the lower bound on the geometric arithmetic invariant in $\mathbb{G}_n^k$ by implementing auxiliary results from section 2. Graphs attaining the lower bound have also been classified. For $n, k \geq 1$, suppose $\mathbb{S}_{n-k}$ is a star graph of order $n-k$ with central vertex $p \in \mathbb{S}_{n-k}$. The family $\mathbb{S}_n^k$ is acquired by adjoining a path $\mathbb{P}_k$ with the vertex $p \in \mathbb{S}_{n-k}$.

Theorem 3.1. *Assume that Ω is a graph in $\mathbb{G}_n^k$ such that $k = 0$. Then*

$$GA(\Omega) \geq n,$$

where equality is satisfied if and only if $\Omega = \mathbb{C}_n$.

Proof. As we know, Ω has no cut vertex. By employing Theorem 1, there exists a cycle containing all vertices of Ω. Since Ω is connected and contains a cycle so, by proposition 3 and definition of geometric arithmetic, we have

$$\begin{aligned} GA(\Omega) &= \sum_{pq\in E(G)} \frac{2\sqrt{2.2}}{2+2} \\ &= m \\ &\geq n, \end{aligned}$$

By Lemma 2.16, $\Omega \in \mathbb{G}_n^0$ achieves minimum unique cycle of length n then $\Omega \cong \mathbb{P}_n^0 \cong \mathbb{C}_n^0 \cong \mathbb{C}_n$. □

Lemma 3.2. *There exist exactly zero cycles in Ω_{min}.*

Proof. Let Ω_{min} be the graph from family $\mathbb{G}_n^k$ such that $GA(\Omega_{min}) < GA(\Omega)$ for any $\Omega \in \mathbb{G}_n^k \setminus \Omega_{min}$. Suppose that $\mathbb{C}$ is a cycle in a connected close-cut vertex graph of Ω_{min}, say $CCV(\Omega_{min})$, such that $\mathbb{C}$ comprises the vertices $C_{i_1}, C_{i_2}, ..., C_{i_t} C_{i_1}$ $(t \geq 3)$. If $| V(CCV(\Omega_{min})) | \geq 3$ for some edges on the cycle $\mathbb{C}$, say $C_{i_t}, C_{i_{t+1}}$, then clearly for applying $\beta-$Transformation 2.2, we can find $\Omega^{'}$ with precisely k cut vertices, then $GA(\Omega^{'} < GA(\Omega_{min}))$, which is a contradiction to our choice of Ω_{min}. Next, suppose that $| V(CCV(\Omega_{min})) | = 2$ for some edges $C_{i_t}, C_{i_{t+1}}$ then $\mathbb{C}$ is a cycle. The number of cut vertices remains the same in Ω_{min} if we remove any edge from cycle $\mathbb{C}$, but it generates the new graph, say $\Omega^{''}$. By applying Lemma 2.5, $GA(\Omega^{''} < GA(\Omega_{min}))$, which is again a contradiction to our choice of Ω_{min}.

As we know, close-cut vertex graph of Ω_{min}, $CCV(\Omega_{min})$ has no cycle. So, an induced subgraph of the close-cut vertex graph of Ω_{min} must have precisely two cut vertices p, q. Otherwise, we will find a contradiction on Ω_{min} by applying $\gamma-$Transformation 2.2. Suppose that r is a vertex on Ω_{min} but r is not a cut vertex. Since, the induced subgraph of close cut vertex graph of Ω_{min} must have precisely two cut vertices p, q. Therefore, $r \notin | V(CVIS(\Omega_{min})) |$ as $| V(CVIS(\Omega_{min})) | = 2$ for close-cut vertices p and q. Consequently, r must be in the end block of Ω_{min}. □

Next, we discuss a sharp lower bound for graphs in $\mathbb{G}_n^k$ where $n, k \geq 1$.

Theorem 3.3. *Suppose that $\Omega \in \mathbb{G}_n^k$ is a connected graph, then*

$$GA(\Omega) \geq (n-k) \cdot \frac{2\sqrt{n-k}}{n-k+1} + \frac{2\sqrt{2(n-k)}}{n-k+2} + k - 2 + \frac{2\sqrt{2}}{3},$$

with equality hold if and only if $\Omega = \mathbb{S}_n^k$.

Proof. Let Ω be a connected graph with $k = 0$. Therefore Ω comprises zero cut edge, and then by employing Theorem 3.1, $GA(\Omega) \geq n$ holds. If Ω comprises exactly one cut vertex, then by employing Theorem 2.6, we have $GA(\Omega) \geq GA(\mathrm{T}(\Omega)) \geq 2(n-1)\frac{\sqrt{n-1}}{n}$.

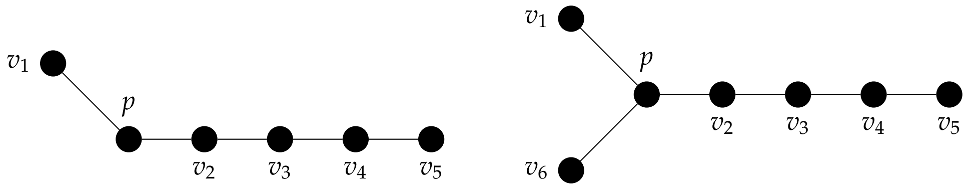
Next, let Ω be a graph with $k \geq 2$. Let Ω_{min} be the graph from family $\mathbb{G}_n^k$ such that $GA(\Omega_{min}) < GA(\Omega)$ for any $\Omega \in \mathbb{G}_n^k \setminus \Omega_{min}$. Moreover, we will prove $\Omega_{min} \cong \mathbb{S}_n^k$.

Suppose if Ω_{min} comprises a tree then Ω_{min} contains k pendent vertices which already have been discussed in Theorem 2.7.

By employing Lemma 3.2, Ω_{min} comprises no cycle. Therefore, the end block of Ω_{min} contains no cycle. Suppose, on the contrary, the end block of Ω_{min} comprises a cycle with respect to cut vertex p, then clearly applying $\alpha-$transformation 2.1, we can find a new graph $\Omega^{'''}$ that shows $GA(\Omega^{'''} < GA(\Omega_{min}))$, which is a contradiction to our choice of Ω_{min}. According to the definition of end block, if Ω_{min} is a cycle, then Ω_{min} does not contain end block vertices or cut vertices. Also, even though $CCV(\Omega_{min})$ has no cycles, the cycle in Ω_{min} cannot be comprised of cut vertices. As a result, Ω_{min} has no cycle. The proof is complete. □

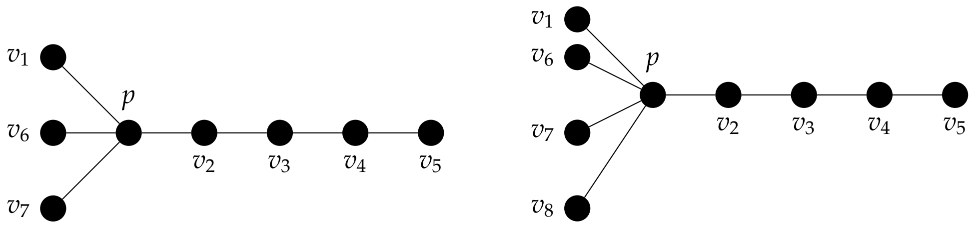
Example 3.4. *Consider a certain family $\mathbb{G}_n^4 \in \mathbb{G}_n^k$ to characterize the extremal graphs.*

Proof. Let $\mathbb{G}_n^k$ be a set of all graphs with n vertices and k cut-vertices. Let $\mathbb{G}_n^4$ be the set of all graphs with n vertices and 4 cut vertices. By employing the theorem 3.3, we deduce a certain family of graphs $\mathbb{S}_n^k$ with a minimum geometric arithmetic index. Figures 6, 7, and 8 illustrate the structural properties of the star graph $\mathbb{S}_n$ and the path graph $\mathbb{P}_n$ within the family $\mathbb{S}_n^k$ for $n = 6, 7, 8, 9, 10, 11$. The order of these graphs, determined by the number of vertices, directly affects the geometric-arithmetic (GA) index. Notably, among all graphs in the family $\mathbb{G}_n^k$, this structure attains the minimum geometric arithmetic index. □



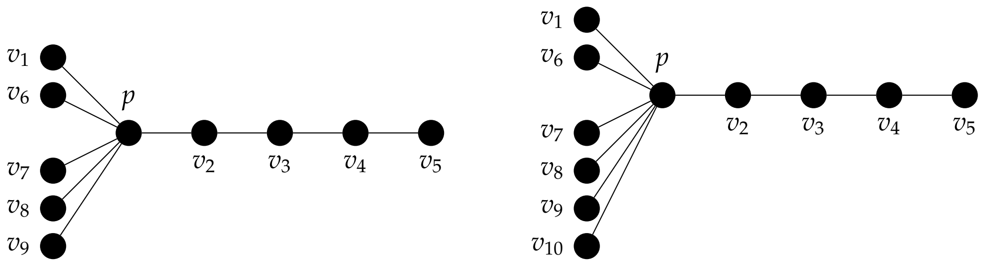
$GA(\mathbb{S}_6^4) \approx 5.828$ $GA(\mathbb{S}_7^4) \approx 6.520$

Figure 6: Extremal graphs among $\Omega \in \mathbb{G}_n^k$ graphs for n=6,7 and k=4



$GA(\mathbb{S}_8^4) \approx 7.085$ $GA(\mathbb{S}_9^4) \approx 7.573$

Figure 7: Extremal graphs among $\Omega \in \mathbb{G}_n^k$ graphs for n=8,9 and k=4



$GA(\mathbb{S}_{10}^4) \approx 8.007$ $GA(\mathbb{S}_{11}^4) \approx 8.405$

Figure 8: Extremal graphs among $\Omega \in \mathbb{G}_n^k$ graphs for n=10,11 and k=4

4. Sharp upper bound of geometric arithmetic with given cut vertices.

If a block of Ω is not an end block, then the block is considered to be an internal block. We refer to a block of Ω as being a nontrivial clique of Ω if it contains at least one clique with an order greater than 3. For any graph Ω, there exists a set of nontrivial cliques that are its terminal blocks. When a block within Ω is also a clique, we say that Ω has a nontrivial internal clique. We claim that graph Ω has an induced $\mathbb{K}_{1,n}(n \geq 3)$ if it has a vertex-induced subgraph that is isomorphic to $\mathbb{K}_{1,n}(n \geq 3)$.

Let $\mathbb{H}_n^k$ be a set of all graphs with n vertices and k cut vertices. Further, we characterize the extremal graphs attaining sharp upper bounds for the geometric arithmetic index in $\mathbb{H}_n^k$. Consider $\mathbb{K}_{n-k}$ is said to be a complete graph of order $n-k$ to central vertex $p \in \mathbb{K}_{n-k}$ such that $n, k \geq 1$. Obtaining the family $\mathbb{K}_n^k$ by attaching a path $\mathbb{P}_k$ to the vertex $p \in \mathbb{K}_{n-k}$.

Lemma 4.1. *There exists precisely one terminal clique in Ω_{max}.*

Proof. Let Ω_{max} be a graph which is generated by $\mathbb{H}_n^k$ such that $GA(\Omega) \leq GA(\Omega_{max})$ for any $\Omega \in \mathbb{H}_n^k \setminus \Omega_{max}$. Since Ω_{max} is not a tree for $1 \leq k \leq n-3$, then suppose on the contrary Ω_{max} is a tree. Assume that $N(u) = u_1, ..., u_t$, $(t \geq 3)$, where u is any arbitrary vertex of Ω_{max} such that $\deg_\Omega(u) \geq 3$. Let Ω' be a graph derived from Ω_{max} by adding an edge uu_1, where Ω' have exactly k cut vertices but $GA(\Omega') > GA(\Omega_{max})$ by employing Lemma 2.5, which is a contradiction to our choice of Ω_{max}. Consequently, at least one nontrivial clique exists in Ω_{max}.

Further, consider that Ω_{max} has at most one nontrivial terminal clique. Let $\mathbb{K}_i$ and $\mathbb{K}_j$ be two cliques such that $i, j \geq 3$ identify with any vertices u and v (u and v may be the same vertex) of connected graph H, respectively which is represented by Ω_1. Next, we replace $\mathbb{K}_i$ (resp. $\mathbb{K}_j$) with $\mathbb{K}_{i+j-2}$ (resp. $\mathbb{K}_2$), which is associated with Ω_2. By using the definition of the geometric arithmetic index, it is easy to calculate $GA(\Omega_1) \leq GA(\Omega_2)$, which is an obvious contradiction to our choice of Ω_{max}. Consequently, Ω_{max} contains at most one nontrivial terminal clique. □

Lemma 4.2. *There exists no induced $\mathbb{K}_{1,s}(s \geq 3)$ in Ω_{max}.*

Proof. Let Ω_{max} be a graph which is generated by $\mathbb{H}_n^k$ such that $GA(\Omega) \leq GA(\Omega_{max})$ for any $\Omega \in \mathbb{H}_n^k \setminus \Omega_{max}$. By employing Lemma 2.5, GA index increases by adding an edge between any two pendant vertices of $\mathbb{K}_{1,s}(s \geq 3)$, which is another graph with k cut vertices other than Ω_{max}, which is again a contradiction to our choice of Ω_{max}. Hence, Ω_{max} can not comprise induced $\mathbb{K}_{1,s}(s \geq 3)$. □

Note 4.1. *With zero cut vertex for $n = 2$, $\mathbb{H}_n^k$ comprises only the path of order two, and for $n = 3$, $\mathbb{H}_n^k$ comprises a complete graph of order 3. When $k \geq 1$, it ensures the existence of $n \geq 3$. Moreover, for $n = 3$ with $k \geq 1$, $\mathbb{H}_n^k$ comprises only the path of order three (P_3). So, we derived the following Theorem* 4.3 *with $n \geq 4$.*

Theorem 4.3. *Assume that Ω is a graph in $\mathbb{H}_n^k$ with $n \geq 4$, then*

$$GA(\Omega) \leq (n^2 - 3n + 2)\frac{\sqrt{(n-1)^2}}{2(n-1)} + (n-1)\frac{2\sqrt{n^2-n}}{2n-1} + \frac{2\sqrt{2n}}{n+2} + (n-3) + \frac{2\sqrt{2}}{3}$$

with equality holds if and only if $\Omega = \mathbb{K}_n^k$.

Proof. Let Ω_{max} be a graph which is generated by $\mathbb{H}_n^k$ such that $GA(\Omega) \leq GA(\Omega_{max})$ for any $\Omega \in \mathbb{H}_n^k \setminus \Omega_{max}$. Then, we will prove that $\Omega_{max} \cong \mathbb{K}_n^k$. The following first two cases for k are considered to be special.

$$\begin{cases} k = 0, & \text{By employing Lemma 2.5, the result is obvious.} \\ k = n-2, & P_k \text{ graph,} \\ 1 \leq k \leq n-3, & \text{Otherwise} \end{cases}$$

Consider that $1 \leq k \leq n-3$. Since any block is a clique in Ω_{max}. By employing the Lemma 2.5, GA index increases by adding new edges to any block of Ω_{max} then Ω_{max} with cut vertices. According to this argument, it is obvious that terminal cliques exist for cut vertex in Ω_{max} then Ω_{max} has a minimum of one terminal clique.

Claim 4.4. *If Ω_{max} contains no nontrivial terminal clique, then Ω_{max} contains at least one nontrivial internal clique.*

Proof. [Proof of claim 4.4] By employing Lemma 4.2, Ω_{max} cannot comprise an induced $\mathbb{K}_{1,s}(s \geq 3)$. it is abundantly clear that no two pendent paths can connect to the same vertex in a nontrivial internal clique of Ω_{max}. All vertices in Ω_{max} with a degree greater than and equal to 3 are connected in nontrivial cliques of Ω_{max}. Consequently, Ω_{max} must have a pendent path. There must be a nontrivial internal clique that is connected with either two pendent paths at different vertices or a pendent path at one vertex, say p, and to another subgraph of Ω_{max} at another vertex, say q. Assume that $N_{H_1}(p) = N_{H_1}(q)$, where H_1 is a connected graph with different vertices p, q where p (resp. q) is connected with a unique path of length $l \geq 1$ (resp. linked with H_2 connected graph). This resulting graph is denoted by Ω_3. Next, we transformed Ω_4 from Ω_3 by connecting unique path $l \geq 1$ with the vertex of H_1 and another end vertex with H_2 while possessing the same cut vertices in both resulting graphs. By employing the definition of the geometric arithmetic index, it is easy to obtain $GA(\Omega_3 < GA(\Omega_4)$, which is a contradiction to our choice of Ω_{max}. □

Claim 4.5. *There exists precisely one nontrivial terminal clique in Ω_{max}.*

Proof. [Proof of claim 4.5] According to Lemma 4.1, consider that Ω_{max} has nontrivial internal cliques; there must be at least one internal clique that is not trivial and connected to either two pendent paths at different vertices or a pendent path at one vertex, say p. Otherwise, Ω_{max} has at least two end cliques, which are not trivial, or Ω_{max} contains an induced $\mathbb{K}_{1,s}(s \geq 3)$, a contradiction. Similarly, as explained above, $GA(\Omega_3 < GA(\Omega_4)$ and obtain a contradiction once again. As a result, Ω_{max} has just one nontrivial terminal clique and no nontrivial interior cliques. □

All vertices in Ω_{max} are either of degree 1 or 2. Finally, $\Omega_{max} \cong \mathbb{K}_n^k$ and after some calculations, we have $GA(\Omega) \leq GA(\Omega_{max}) \leq (n^2 - 3n + 2)\frac{\sqrt{(n-1)^2}}{2(n-1)} + (n-1)\frac{2\sqrt{n^2-n}}{2n-1} + \frac{2\sqrt{2n}}{n+2} + (n-3) + \frac{2\sqrt{2}}{3}$. As a result, the proof is complete. □

Example 4.6. *Consider a certain family $\mathbb{H}_n^5 \in \mathbb{H}_n^k$ to characterize the extremal graphs.*

Proof. Let $\mathbb{H}_n^k$ be a set of all graphs with n vertices and k cut-vertices. Let $\mathbb{H}_n^5$ be the set of all graphs with n vertices and 5 cut vertices. By employing the theorem 4.3, we deduce a certain family of graphs $\mathbb{K}_n^k$ with a maximum geometric arithmetic index. Figures 9, 10, and 11 illustrate the structural properties of the star graph $\mathbb{K}_n$ and the path graph $\mathbb{P}_n$ within the family $\mathbb{K}_n^k$ for $n = 6, 7, 8, 9, 10, 11$. The order of these graphs, determined by the number of vertices, directly affects the geometric-arithmetic (GA) index. Notably, among all graphs in the family $\mathbb{H}_n^k$, this structure attains the maximum geometric arithmetic index. □

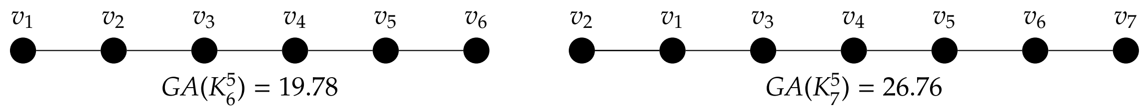


Figure 9: Extremal graphs among $\Omega \in \mathbb{H}_n^k$ graphs for n=6,7 and k=5

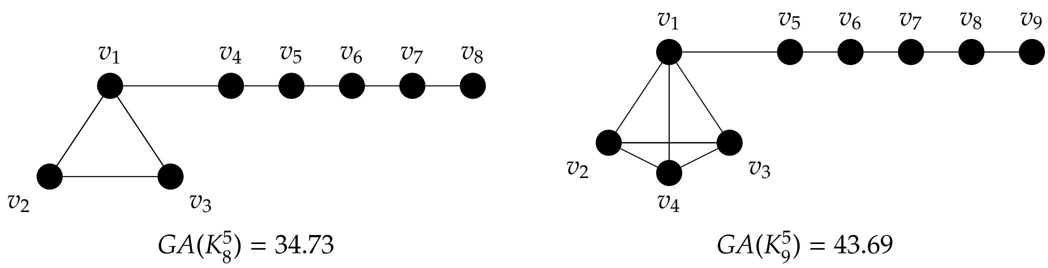


Figure 10: Extremal graphs among $\Omega \in \mathbb{H}_n^k$ graphs for n=8,9 and k=5

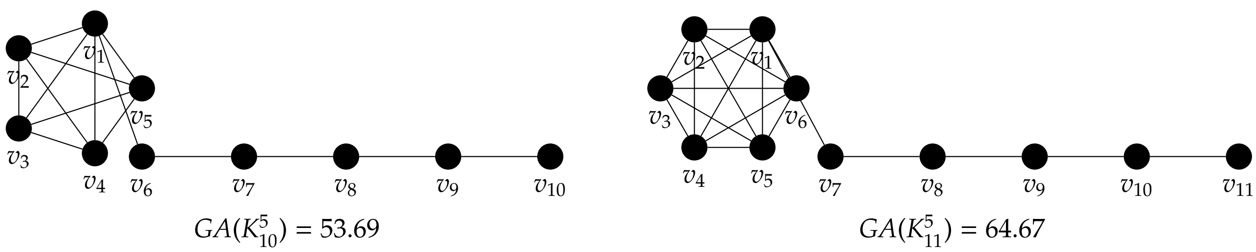


Figure 11: Extremal graphs among $\Omega \in \mathbb{H}_n^k$ graphs for n=10,11 and k=5

5. Correlation between geometric arithmetic and normalized Laplacian

Theorem 5.1. *Let Ω be a connected graph with n vertices and $\lambda_1, \lambda_2, ..., \lambda_n$ be eigenvalues. We have*

$$\frac{1}{\Delta}\sqrt{\frac{\lambda_n^2(n-1)-n}{2}} \leq GA(\Omega) \leq \Delta m(\lambda_n - 1)$$

where Δ represents the maximum degree of the graph and with left equalities satisfies if and only if G is the union of complete graphs.

Proof. It is easy to see

$$\frac{2\Delta}{deg_i + deg_j} \geq \frac{2\sqrt{deg_i deg_j}}{deg_i + deg_j} \geq \frac{2d}{deg_i + deg_j}$$

with the left equality holds if and only if $deg_i = deg_j = \Delta$ and the right equality holds if and only if $deg_i = deg_j = d$.

This implies that

$$GA(\Omega) \leq 2\Delta \sum_{\{i,j\}\in E} \frac{1}{deg_i + deg_j} \leq 2\Delta \frac{m(\lambda_n - 1)}{2} = \Delta m(\lambda_n - 1)$$

Conversely, Consider that

$$L = \begin{cases} (L)_{ii} = 1, & i = 1, \cdots, n \\ (L)_{ij} = -\frac{1}{\sqrt{deg_i deg_j}}, & i \neq j, i \sim j \\ (L)_{ij} = 0, & i \neq j, i \nsim j \end{cases}$$

be the normalized Laplacian matrix. Note that

$$\frac{2\Delta}{deg_i + deg_j} \geq \frac{2\sqrt{deg_i deg_j}}{deg_i + deg_j}$$
$$\frac{1}{\Delta}\sum_{\{i,j\in E\}} \sqrt{deg_i deg_j} = \frac{1}{\Delta}\sum_{\{i,j\in E\}} \frac{1}{(deg_i deg_j)^{-1/2}}$$

By employing Cauchy inequality, we have,

$$(\sum_{\{i,j\in E\}} \sqrt{deg_i deg_j})^2 \cdot \sum_{\{i,j\in E\}} \frac{1}{(deg_i deg_j)} \geq m^3$$
$$\geq \sqrt{\frac{m^3}{\sum_{\{i,j\in E\}} \frac{1}{(deg_i deg_j)}}}$$

So combining with $\lambda_1 = 0$, and by elementary properties of matrix theory and Rayleigh's quotient principle

$$\lambda_2^2 + \cdots + \lambda_n^2 = \sum_{i=1}^{n} \lambda_i^2 = \text{trace}(L^2) = \sum_{i=1}^{n}(L^2)_{ii} = n + 2\sum_{\{i,j\}\in E} \frac{1}{deg_i deg_j}$$

and thus,

$$\lambda_2 \leq \sqrt{\frac{n}{n-1} + \frac{2}{n-1}\sum_{\{i,j\}\in E}\frac{1}{deg_i deg_j}} \leq \lambda_n$$
$$\geq \sqrt{\frac{m^3}{(\lambda_n^2 - \frac{n}{n-1})\frac{n-1}{2}}}.$$

After simplification, we get the required result if and if Ω is a complete graph or a union of complete graphs. The proof is complete. $\square$

Conclusion

In this work, we have studied the geometric-arithmetic index with respect to eigenvalues in the framework of spectral and chemical graph theories. We obtained sharp lower and upper bounds on the geometric-arithmetic index for the family of graphs $\mathbb{G}_n^k$ and $\mathbb{H}_n^k$ with given cut vertices. Consequently, extremal families $\mathbb{S}_n^k$ and $\mathbb{K}_n^k$ have been characterized.
We also clearly found a strong relationship between the normalized Laplacian and geometric-arithmetic index by using the Rayleigh quotient concept. This relationship clarifies the interaction between topological indices and spectral graph parameters, therefore supporting the importance of spectral approaches in extremal graph theory.

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Conflict of interest
No conflict of interest to declare.

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