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Research Article

On some bounds of degree based topological indices for total graphs

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Abstract

In this paper, we discuss the concept of total graph and computed some topological indices. If Θ is a simple graph, then the elements of Θ are the vertices Θ_V and edges Θ_E. For $e = u\acute{u} \in \Theta_E$, the vertex u and edge e, as well as $\acute{u}$ and e, are incident. We define the general harmonic (GH) index and general sum connectivity (GS) index for graph Θ regarding incident vertex-edge degrees as: $H^\alpha(\Theta) = \sum_{e\acute{u}} \left(\frac{2}{\aleph_{\acute{u}}+\aleph_e}\right)^\alpha$ and $\hat{\chi}^\alpha(\Theta) = \sum_{e\acute{u}} (\aleph_{\acute{u}} + \aleph_e)^\alpha$, where α is any real number. In this article, we derive the closed formulas for a few standard graphs for (GH) and (GS) indices and then go on to calculate the lowest and the greatest general harmonic index, as well as the general sum-connectivity index, for various graphs that correspond to their total graphs.

Mathematics Subject Classification (2020). 05C07,05C09,05C10.

Keywords. general harmonic index; general sum connectivity index; incident; total graphs

1. Introduction

Chemical Graph Theory is a branch of Mathematical Chemistry that uses graph theory tools numerically to analyze chemical phenomena [3,23]. It has a significant impact on the realm of chemical sciences [10]. The vertices of a molecule are the atoms, and the links between the atoms are the valency bonds. A topological descriptor is an extracted numerical value from the molecular graph [24,25]. It is used to understand the physicochemical properties of chemical compounds [11,12]. The interesting characteristic of topological indices is to apprehend a couple of the features of an atomic structure in a single number. Starting with Wiener's foundational work [29], plenty of topological descriptor have been anticipated and investigated [28].
Let $\Theta = (\Theta_V, \Theta_E)$ be a simple graph having l vertices and m edges, with vertex and edge sets Θ_V and Θ_E, individually. And $\aleph_u$ is used to symbolize the degree of vertex u [17,18]. In a simple graph Θ, $u\acute{u}$ is the symbol for the edge e that connects the vertices u and $\acute{u}$.

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For the edge$e = u\acute{u}$ of the graph Θ, then the vertices u and $\acute{u}$ are associated with edge e. The degree of an edge $\aleph_e$ is calculated by the formula $\aleph_e = \aleph_u + \aleph_{\acute{u}} - 2$, where $u\acute{u} = e$. The total $\Gamma(\Theta)$ graph is a derived graph with $(\Gamma(\Theta))_V = \Theta_V + \Theta_E$ and $u\acute{u} \in (\Gamma(\Theta))_E \Leftrightarrow$ u and $\acute{u}$ are associated or incident in Θ. For more details see [26, 27].
During the past few decades, edge end-vertex degrees were employed to calculate topological indices. Several indices have been recognized as helpful tools in theoretical-chemistry. The most familiar of these descriptors is discussed in [22] . This molecular descriptor (Randić sum connectivity) has been the subject of over a thousand studies and a number of books [14, 21]. Scientists have been working on improving the Randić index's predictive power for many years. As a result, a significant amount of additional topological indices, analogous to the novel Randić index, are introduced. The Zagreb type indices are the most important Randić successors [13]. The harmonic index, described in [8], is another noteworthy topological descriptor and is defined as:

$$H(\Theta) = \sum_{u\acute{u}\in\Theta_E} \frac{2}{(\aleph_u + \aleph_{\acute{u}})}.$$

Favaron et al. in [9] explored the connection between the harmonic index and graph eigenvalues. Zhong [31, 32] calculates the extreme values of harmonic indices for trees, general graphs, and unicyclic graphs. The general harmonic index is introduces by Yan et al. in [30] and is defined as:

$$H^{\alpha}(\Theta) = \sum_{u\acute{u}\in\Theta_E} \left(\frac{2}{\aleph_u + \aleph_{\acute{u}}}\right)^{\alpha}.$$

Getting inspiration from the Randić [1], Zagreb [12], and harmonic indices, two new indices namely, the sum connectivity and the general sum connectivity indices were defined by Zhou and Trinajstic in [33, 34] as:

$$\hat{\chi}(\Theta) = \sum_{u\acute{u}\in\Theta_E} \frac{1}{\sqrt{\aleph_u + \aleph_{\acute{u}}}}.$$

$$\hat{\chi}^{\alpha}(\Theta) = \sum_{u\acute{u}\in\Theta_E} (\aleph_u + \aleph_{\acute{u}})^{\alpha}.$$

Some extremal characteristics of $\hat{\chi}(\Theta)$ and $\hat{\chi}^{\alpha}(\Theta)$ are discussed in [5, 6, 35]. To account for contributions from pairs of nearby vertices, the Zagreb type indices were suggested. Following them, a slew of other indices are calculated [2, 7]. After being inspired by Kulli's work [15, 16, 19, 20], we define the generalized harmonic index and generalized sum connectivity index regarding incident vertex-edge degrees.

Definition 1.1. We establish the general harmonic (GH) index for graphs with regard to incident vertex-edge degrees as:

$$H^{\alpha}(\Theta) = \sum_{e\acute{u}} \left(\frac{2}{\aleph_{\acute{u}} + \aleph_e}\right)^{\alpha}. \tag{1.1}$$

Definition 1.2. We establish the general sum-connectivity (GS) index for graphs with regard to incident vertex-edge degrees as:

$$\hat{\chi}^{\alpha}(\Theta) = \sum_{e\acute{u}} (\aleph_{\acute{u}} + \aleph_e)^{\alpha}. \tag{1.2}$$

Firstly, we'll derive the closed formulas for a few standard graphs for equation (1.1) and equation (1.2). Secondly, we'll calculate the lowest and the greatest general harmonic (GH) index, as well as the general sum-connectivity (GS) index, across various graphs that correspond to their total graphs.

For $n \geq 4$, the path graph P_n has two types of edges $\mid \Theta_{E_{12}} \mid= 2$ and $\mid \Theta_{E_{22}} \mid= n-3$ while total graph graph of P_n has four types of edges. i-e. $\mid \Gamma_{E_{23}} \mid= 2$, $\mid \Gamma_{E_{24}} \mid= 2$, $\mid \Gamma_{E_{34}} \mid= 4$, and $\mid \Gamma_{E_{44}} \mid= 4n-13$, see details in Figure 1.

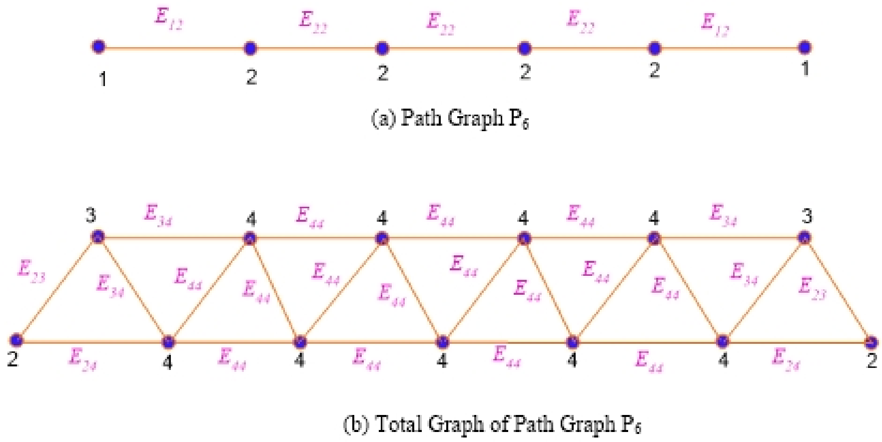


Figure 1. Graphical illustration of (a)path graph P_6 and (b)its total graph $\Gamma(P_6)$

Theorem 1.3. *For $n \geq 4$, if $\Gamma(P_n)$ is the total graph of P_n (path graph), then for $\alpha > -2$ and $\alpha < -2$, P_n has the largest and smallest GS index, respectively.*

Proof. By using equation (1.2), we can see that

$$\begin{aligned}
\hat{\chi}^{\alpha}(P_n) &= \sum_{\acute{u}e}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}] \\
&= \sum_{i=1}^{2}\sum_{\acute{u}u\in E_i(P_n)}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}+(\aleph_u+\aleph_e)^{\alpha}] \\
&= (2^{\alpha}+3^{\alpha})\times 2+2\times 4^{\alpha}(-3+n) \\
&= 2^{\alpha+1}+2\times 3^{\alpha}+2^{2\alpha+1}(n-3)
\end{aligned}$$

$$\begin{aligned}
\hat{\chi}^{\alpha}(\Gamma(P_n)) &= \sum_{\acute{u}e}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}] \\
&= \sum_{i=1}^{4}\sum_{\acute{u}u\in E_i(\Gamma(P_n))}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}+(\aleph_u+\aleph_e)^{\alpha}] \\
&= 2(6^{\alpha}+8^{\alpha})+2(5^{\alpha}+6^{\alpha})+4(8^{\alpha}+9^{\alpha})+2\times 10^{\alpha}(-13+4n) \\
&= 2\times 10^{\alpha}(-13+4n)+2\times(5^{\alpha}+9^{\alpha})+4\times(6^{\alpha}+8^{\alpha})
\end{aligned}$$

$$\begin{aligned}
\hat{\chi}^{\alpha}(P_n)-\hat{\chi}^{\alpha}(\Gamma(P_n)) &= 2\times 4^{\alpha}(-3+n)-2\times 10^{\alpha}(-13+4n)+2^{\alpha+1} \\
&+ 2\times 3^{\alpha}-2\times 5^{\alpha}-4\times 6^{\alpha}-6\times 8^{\alpha}-4\times 9^{\alpha} \qquad (1.3)
\end{aligned}$$

Define $h(\nu)=2\times 4^{\alpha}(-3+\nu)-2\times 10^{\alpha}(-13+4\nu)$.
For $\nu \geq 4$, $h(\nu)$ is strictly decreasing function when $\alpha > -2$, also

$$\begin{aligned}
h(4) &= 2\times 4^{\alpha}-6\times 10^{\alpha}+2\times 2^{\alpha}+2\times 3^{\alpha}-2\times 5^{\alpha}-4\times 6^{\alpha}-6\times 8^{\alpha}-4\times 9^{\alpha} \\
&= 2\times(2^{\alpha}+3^{\alpha}-5^{\alpha}-6^{\alpha})-2\times(3\times 8^{\alpha}+2\times 9^{\alpha}+3\times 10^{\alpha}) \\
&< 0, \quad for \;\; \alpha > -2.
\end{aligned}$$

Consequently, $\hat{\chi}^\alpha(P_n) - \hat{\chi}^\alpha(\Gamma(P_n)) \leq h(\nu) \leq h(4) < 0$ for $\alpha > -2$. Which implies that $\hat{\chi}^\alpha(P_n) < \hat{\chi}^\alpha(\Gamma(P_n))$ for $\alpha > -2$. By similar calculations, $\hat{\chi}^\alpha(P_n) > \hat{\chi}^\alpha(\Gamma(P_n))$ for $\alpha < -2$ and hence the the proof. □

Theorem 1.4. *For $n \geq 4$, if $\Gamma(P_n)$ is the total graph of P_n (path graph), then for $(\frac{2}{5})^\alpha > \frac{1}{4}$ and $(\frac{2}{5})^\alpha < \frac{1}{4}$, P_n has the smallest and largest GH index, respectively.*

Proof. By using equation (1.1), we can see that

$$\begin{aligned} H^\alpha(P_n) &= \sum_{\acute{u}e} (\frac{2}{\aleph_{\acute{u}} + \aleph_e})^\alpha \\ &= \sum_{i=1}^{2} \sum_{\acute{u}u \in E_i(P_n)} [(\frac{2}{\aleph_{\acute{u}} + \aleph_e}) + (\frac{2}{\aleph_u + \aleph_e})] \\ &= 2 \times (1 + (\frac{2}{3})^\alpha) + 2 \times (\frac{1}{2^\alpha})(-3 + n) \end{aligned}$$

$$\begin{aligned} H^\alpha(\Gamma(P_n)) &= \sum_{\acute{u}e} (\frac{2}{\aleph_{\acute{u}} + \aleph_e})^\alpha \\ &= \sum_{i=1}^{4} \sum_{\acute{u}u \in E_i(\Gamma(P_n))} [(\frac{2}{\aleph_{\acute{u}} + \aleph_e}) + (\frac{2}{\aleph_u + \aleph_e})] \\ &= (\frac{2}{5^\alpha})(-13 + 4n) + 4 \times [(\frac{1}{4})^\alpha + (\frac{2}{9})^\alpha] + 2 \times [(\frac{1}{3})^\alpha + (\frac{1}{4})^\alpha] \\ &+ 2 \times [(\frac{2}{5})^\alpha + (\frac{1}{3})^\alpha] \end{aligned}$$

$$\begin{aligned} H^\alpha(P_n) - H^\alpha(\Gamma(P_n)) &= \frac{2}{2^\alpha} \times (-3 + n) - (\frac{2}{5^\alpha}) \times (-13 + 4n) + 2 \\ &+ 2 \times (\frac{2}{3})^\alpha - 2 \times (\frac{2}{5})^\alpha - (\frac{4}{3^\alpha}) - (\frac{2}{4^\alpha}) - (\frac{4}{2^\alpha}) - 4 \times (\frac{2}{9})^\alpha \end{aligned} \quad (1.4)$$

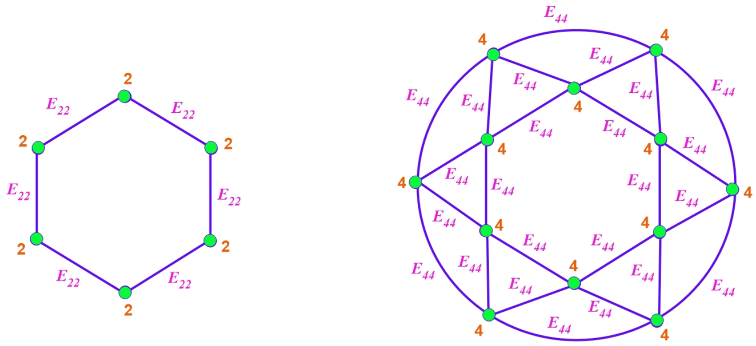
Define $g(\mu) = \frac{2}{2^\alpha}(\mu - 3) - (-13 + 4\mu) \times (\frac{2}{5^\alpha})$.
For $\mu \geq 4$, $g(\mu)$ is strictly decreasing function when $(\frac{2}{5})^\alpha > \frac{1}{4}$, also $g(4) < 0$ also holds for $(\frac{2}{5})^\alpha > \frac{1}{4}$ Consequently, $H^\alpha(P_n) - H^\alpha(\Gamma(P_n)) \leq g(\mu) \leq g(4) < 0$ for $(\frac{2}{5})^\alpha > \frac{1}{4}$. Which implies that $H^\alpha(P_n) < H^\alpha(\Gamma(P_n))$ for $(\frac{2}{5})^\alpha > \frac{1}{4}$. By similar calculations, $H^\alpha(P_n) > H^\alpha(\Gamma(P_n))$ for $(\frac{2}{5})^\alpha < \frac{1}{4}$ and hence the the proof. □

For $n \geq 3$, the cyclic graph C_n is 2 regular graph, so there is only one type of edges $\Theta_{E_{22}}$ with frequency n. If $\Gamma(C_n)$ is the total graph of cycle C_n, then it is a 4 regular graph. There is only one type of edges $\Gamma_{E_{44}}$ with frequency $4n$ The total graph derived from the cyclic graph C_n has $2n$ vertices and edges $4n$, see details in Figure 2.

Theorem 1.5. *For $n \geq 3$, $\Gamma(C_n)$ has the greatest and the smallest GS index for $\alpha < -2$ and $\alpha > -2$, respectively.*

Proof. By using equation (1.2), we can see that

$$\begin{aligned} \hat{\chi}^\alpha(C_n) &= \sum_{\acute{u}e} [(\aleph_{\acute{u}} + \aleph_e)^\alpha] \\ &= \sum_{\acute{u}u \in E(C_n)} [(\aleph_{\acute{u}} + \aleph_e)^\alpha + (\aleph_u + \aleph_e)^\alpha] \\ &= 2n \times 4^\alpha \end{aligned}$$



(a) Cycle Graph C_6 (b) Total Graph of Cycle Graph C_6

Figure 2. Graphical illustration of (a)cycle graph C_6 and (b)its total graph $\Gamma(C_6)$

$$\begin{aligned}\hat{\chi}^{\alpha}(\Gamma(C_n)) &= \sum_{\acute{u}e}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}] \\ &= \sum_{\acute{u}u\in E(\Gamma(C_n))}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}+(\aleph_u+\aleph_e)^{\alpha}] \\ &= 8n\times 10^{\alpha}\end{aligned}$$

$$\hat{\chi}^{\alpha}(C_n)-\hat{\chi}^{\alpha}(\Gamma(C_n)) = 2n\times 4^{\alpha}-8n\times 10^{\alpha} \tag{1.5}$$

Define $h(\nu)=2\nu\times 4^{\alpha}-8\nu\times 10^{\alpha}$. Also,

$$\begin{aligned} h(3) &= 6\times 4^{\alpha}-12\times 10^{\alpha} \\ &= 6\times 4^{\alpha}(1-2(\frac{5}{2})^{\alpha}) \\ &< 0, \quad\Leftrightarrow\quad (\frac{5}{2})^{\alpha}>\frac{1}{2}.\end{aligned}$$

which holds for $\alpha>-2$, so $h(3)<0$ for $\alpha>-2$. And $h'(\nu)=2(4^{\alpha}-4\times 10^{\alpha})<0$ for $\alpha>-2$. Consequently, $\hat{\chi}^{\alpha}(C_n)-\hat{\chi}^{\alpha}(\Gamma(C_n))\leq h(\nu)\leq h(3)<0$ for $\alpha>-2$. Which implies that $\hat{\chi}^{\alpha}(C_n)<\hat{\chi}^{\alpha}(\Gamma(C_n))$ for $\alpha>-2$. By similar calculations, $\hat{\chi}^{\alpha}(C_n)>\hat{\chi}^{\alpha}(\Gamma(C_n))$ for $\alpha<-2$ and hence the the proof. □

Theorem 1.6. *For $n\geq 3$, $\Gamma(C_n)$ has the greatest and the smallest GH index for $(\frac{2}{5})^{\alpha}<\frac{1}{4}$ and $(\frac{2}{5})^{\alpha}>\frac{1}{4}$, respectively.*

Proof. By using equation (1.1), we can see that

$$\begin{aligned} H^{\alpha}(C_n) &= \sum_{\acute{u}e}(\frac{2}{\aleph_{\acute{u}}+\aleph_e})^{\alpha} \\ &= \sum_{\acute{u}u\in E(C_n)}[(\frac{2}{\aleph_{\acute{u}}+\aleph_e})^{\alpha}+(\frac{2}{\aleph_u+\aleph_e})^{\alpha}] \\ &= 2\times(\frac{2}{2+2})^{\alpha}\times n=2n\times(\frac{1}{2})^{\alpha}\end{aligned}$$

$$\begin{aligned} H^{\alpha}(\Gamma(C_n)) &= \sum_{\acute{u}e} (\frac{2}{\aleph_{\acute{u}} + \aleph_e})^{\alpha} \\ &= \sum_{\acute{u}u \in E(\Gamma(C_n))} [(\frac{2}{\aleph_{\acute{u}} + \aleph_e})^{\alpha} + (\frac{2}{\aleph_u + \aleph_e})^{\alpha}] \\ &= 2 \times (\frac{2}{4+6})^{\alpha} \times 4n = 8n \times (\frac{1}{5})^{\alpha} \end{aligned}$$

$$H^{\alpha}(C_n) - H^{\alpha}(\Gamma(C_n)) = 2n \times (\frac{1}{2})^{\alpha} - 8n \times (\frac{1}{5})^{\alpha} \tag{1.6}$$

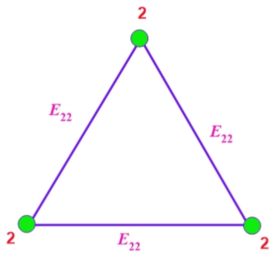
Define $f(\nu) = 2\nu \times (\frac{1}{2})^{\alpha} - 8\nu \times (\frac{1}{5})^{\alpha}$. Also,

$$\begin{aligned} f(3) &= \frac{6}{2^{\alpha}} - \frac{24}{5^{\alpha}} \\ &= 6 \times (\frac{1}{2^{\alpha}} - \frac{4}{5^{\alpha}}) \\ &< 0, \quad \Leftrightarrow \quad (\frac{2}{5})^{\alpha} > \frac{1}{4} \end{aligned}$$

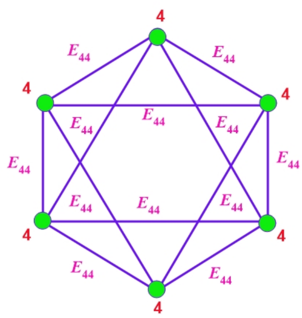
So $f(3) < 0$ for $(\frac{2}{5})^{\alpha} > \frac{1}{4}$. And $f'(\nu) = 2(\frac{1}{2^{\alpha}} - 4 \times \frac{1}{5^{\alpha}}) < 0$ for $(\frac{2}{5})^{\alpha} > \frac{1}{4}$. Consequently, $H^{\alpha}(C_n) - H^{\alpha}(\Gamma(C_n)) \leq f(\nu) \leq f(3) < 0$ for $(\frac{2}{5})^{\alpha} > \frac{1}{4}$. Which implies that $H^{\alpha}(C_n) < H^{\alpha}(\Gamma(C_n))$ for $(\frac{2}{5})^{\alpha} > \frac{1}{4}$. By similar calculations, $H^{\alpha}(C_n) > H^{\alpha}(\Gamma(C_n))$ for $(\frac{2}{5})^{\alpha} < \frac{1}{4}$ and hence the the proof. □

Lemma 1.7. *$\Gamma(K_n)$ is $(2n-2)$ regular graph and has order and size $\frac{n^2+n}{2}$ and $\frac{n}{2} \cdot (n-1)(n+1)$ respectively.*

Proof. Each vertex, say u', will be connected to $n-1$ vertices, see details in Figure 3. As a result, these vertices will be connected to u' by $n-1$ edges. Therefore, the degree of u' in $\Gamma(K_n)$ will be $2n-2$. i-e. $\Gamma(K_n)$ is $2n-2$ regular. As $\mid V(K_n) \mid = n$ and $\mid E(K_n) \mid = \frac{n}{2} \times (n-1)$, so by using definition of $\Gamma(K_n)$, $\mid V(\Gamma(K_n)) \mid = \frac{n}{2} \times (n-1) + n = \frac{n^2+n}{2}$. Using the regularity and order of $\Gamma(K_n)$, we have $\sum_{u' \in V(\Gamma(K_n))} (\aleph_{u'}) = \frac{n^2+n}{2} \cdot (2n-2)$. With the help of Hand shaking lemma, $\mid E(\Gamma(K_n)) \mid = \frac{n}{2} \cdot (n-1)(n+1)$. □



(a) Complete Graph K3



(b) Total Graph of Complete Graph K3

Figure 3. Graphical illustration of (a)complete graph K_3 and (b) its total graph $\Gamma(K_3)$

Lemma 1.8. *Let $\beta \geq 3$, the function $\phi(\beta)$ is a strictly decreasing and increasing function for $\alpha > \frac{-1}{3}$ and $\alpha < \frac{-1}{3}$ respectively, where*

$$\phi(\beta) = \beta(\beta-1)[(3\beta-5)^{\alpha} - (\beta+1)(6\beta-8)^{\alpha}]$$

Proof.

$$\begin{aligned}
\phi'(\beta) &= (3\beta-5)^{\alpha-1}[(2\beta-1)(3\beta-5)+3\alpha\beta(\beta-1)] \\
&- (6\beta-8)^{\alpha-1}[(2\beta-1)(\beta+1)+(\beta^2-\beta)(6\beta-8)+(\beta^2-\beta)(\beta+1)\times 6\alpha] \\
&= (3\beta-5)^{\alpha-1}[(6-3\alpha)\beta^2+(-13+3\alpha)\beta+5] \\
&- (6\beta-8)^{\alpha-1}[6(1+\alpha)\beta^3-12\beta^2+9\beta-1] \qquad (1.7)
\end{aligned}$$

The convexity of $x^{\alpha-1}$ together with the Jensen's inequality implies that

$$(6\beta-8)^{\alpha-1} < (3\beta-5)^{\alpha-1}+3(\beta-1)^{\alpha-1}$$

Therefore, by using above inequality in equation (1.7), we have

$$\phi'(\beta) < (3\beta-5)^{\alpha-1}[(-6-6\alpha)\beta^3+(18-3\alpha)\beta^2+(-22+3\alpha)\beta+6]$$
$$\phi(\beta) < (3\beta-5)^{\alpha-1}g(\beta) < 0$$

for $\beta \geq 4$ and $\alpha > \frac{-1}{3}$, where $g(\beta) = a_1\beta^3+a_2\beta^2+a_3\beta+6$, and $a_1 = -6-6\alpha$, $a_2 = 18-3\alpha$, $a_3 = -22+3\alpha$. Since $1 \leq \alpha-1 \leq 2$ implies that $2 \leq \alpha \leq 3$. Consequently, $\phi(\beta)$ is strictly decreasing for $\alpha > \frac{-1}{3}$. Similarly, we can show $\phi(\beta)$ strictly increasing for $\alpha < \frac{-1}{3}$. □

Lemma 1.9. *Let $\vartheta \geq 3$, the function $\Omega(\vartheta)$ is a strictly decreasing and increasing function for $\alpha < \frac{-1}{2}$ and $\alpha > \frac{-1}{2}$ respectively, where*

$$\Omega(\vartheta) = 2^\alpha\vartheta(\vartheta-1)[\frac{1}{(3\vartheta-5)^\alpha} - \frac{(\vartheta+1)}{(6\vartheta-8)^\alpha}]$$

Proof.

$$\begin{aligned}
\Omega'(\vartheta) &= 2^\alpha(2\vartheta-1)[\frac{1}{(3\vartheta-5)^\alpha} - \frac{\vartheta+1}{(6\vartheta-8)^\alpha}] \\
&+ 2^\alpha(\vartheta^2-\vartheta)[\frac{3\alpha}{(3\vartheta-5)^\alpha} - \frac{1}{(6\vartheta-8)^\alpha} + \frac{6\alpha(\vartheta+1)}{(6\vartheta-8)^2}] \\
&= \frac{1}{(3\vartheta-5)^{alpha}}[2\vartheta-1+\frac{3\alpha(\vartheta^2-\vartheta)}{3\vartheta-5}] \\
&- \frac{1}{(6\vartheta-8)^\alpha}[(2\vartheta-1)(\vartheta+1)-(\vartheta^2-\vartheta)] + \frac{6(\vartheta+1)\vartheta(\vartheta-1)}{(6\vartheta-8)^2} \times \alpha \\
&= \frac{1}{(3\vartheta-5)^\alpha}[(6+3\alpha)\vartheta^2+(-13-3\alpha)\vartheta-5] + \frac{6\alpha(\vartheta+1)\vartheta(\vartheta-1)}{(6\vartheta-8)^2} \\
&- \frac{1}{(6\vartheta-8)^\alpha}[\vartheta^2+2\vartheta-1] \\
&\leq \frac{1}{(3\vartheta-5)^\alpha}[(6+3\alpha)\vartheta^2+(-13-3\alpha)\vartheta-5] + \frac{6\alpha(\vartheta+1)\vartheta(\vartheta-1)}{(6\vartheta-8)^2} \\
&= f(\vartheta)+g(\vartheta) \qquad (1.8)
\end{aligned}$$

where $f(\vartheta) = \frac{1}{(3\vartheta-5)^\alpha}[(6+3\alpha)\vartheta^2+(-13-3\alpha)\vartheta-5]$ and $g(\vartheta) = \frac{6\alpha(\vartheta+1)\vartheta(\vartheta-1)}{(6\vartheta-8)^2}$ both are strictly decreasing for $\alpha < \frac{-1}{2}$ and are strictly increasing for $\alpha > \frac{-1}{2}$. Consequently, inequality 1.8 implies that $\Omega(\vartheta)$ is strictly decreasing for $\alpha < \frac{-1}{2}$. Similarly, we can show $\Omega(\vartheta)$ is strictly increasing for $\alpha > \frac{-1}{2}$ □

Theorem 1.10. *If $\Gamma(K_n)$ is the total graph of complete graph where $n \geq 3$, then K_n give the largest and the smallest GS index for $\alpha < \frac{-1}{3}$ and $\alpha > \frac{-1}{3}$ respectively. Furthermore, for $\alpha = \frac{1}{3}$ and $\beta = 3$*

$$\hat{\chi}^\alpha(K_n) = \hat{\chi}^\alpha(\Gamma(K_n))$$

.

Proof.

$$\begin{aligned}
\hat{\chi}^{\alpha}(K_n) &= \sum_{\acute{u}e}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}] \\
&= \sum_{\acute{u}u\in E(K_n)}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}+(\aleph_u+\aleph_e)^{\alpha}] \\
&= \frac{n(n-1)}{2}\times 2\times(3n-5)^{\alpha} \\
&= n(n-1)(3n-5)^{\alpha} \\
\hat{\chi}^{\alpha}(\Gamma(K_n)) &= \sum_{\acute{u}e}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}] \\
&= \sum_{\acute{u}u\in E(\Gamma(K_n))}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}+(\aleph_u+\aleph_e)^{\alpha}] \\
&= n(n-1)(n+1)(6n-8)^{\alpha}
\end{aligned}$$

$$\hat{\chi}^{\alpha}(K_n)-\hat{\chi}^{\alpha}(\Gamma(K_n)) = n(n-1)[(3n-5)^{\alpha}-(n+1)(6n-8)^{\alpha}].$$

By using Lemma 1.8, the function $\psi(n)=n(n-1)[(3n-5)^{\alpha}-(n+1)(6n-8)^{\alpha}$ is increasing and decreasing for $\alpha<\frac{-1}{3}$ and $\alpha>\frac{-1}{3}$ respectively. Also $\psi(3)=6(4^{\alpha}-4\cdot 10^{\alpha})<0$ if and only if $\left(\frac{2}{5}\right)^{\alpha}<4$ which holds for $\alpha>\frac{-1}{3}$. Therefore $\hat{\chi}^{\alpha}(K_n)<\hat{\chi}^{\alpha}(\Gamma(K_n))$. By the similar argument for $\alpha<\frac{-1}{3}$, we have the result $\hat{\chi}^{\alpha}(K_n)>\hat{\chi}^{\alpha}(\Gamma(K_n))$. Finally, for $\alpha=\frac{-1}{3}$ and $n=3$, we have $\hat{\chi}^{\alpha}(K_n)=\hat{\chi}^{\alpha}(\Gamma(K_n))$. □

Theorem 1.11. *If $\Gamma(K_n)$ is the total graph of complete graph where $n\geq 3$, then K_n give the largest and the smallest GH index for $\alpha>\frac{-1}{2}$ and $\alpha<\frac{-1}{2}$ respectively.*

Proof.

$$\begin{aligned}
H^{\alpha}(K_n) &= \sum_{\acute{u}e}[(\frac{2}{\aleph_{\acute{u}}+\aleph_e})^{\alpha}] \\
&= \sum_{\acute{u}u\in E(K_n)}[(\frac{2}{\aleph_{\acute{u}}+\aleph_e})^{\alpha}+(\frac{2}{\aleph_u+\aleph_e})^{\alpha}] \\
&= 2\times(\frac{2}{3n-5})^{\alpha}\times\frac{n}{2}\cdot(n-1) \\
&= \frac{n2^{\alpha}}{(3n-5)^{\alpha}}\times(n-1) \\
H^{\alpha}(\Gamma(K_n)) &= \sum_{\acute{u}e}[(\frac{2}{\aleph_{\acute{u}}+\aleph_e})^{\alpha}] \\
&= \sum_{\acute{u}u\in E(\Gamma(K_n))}[(\frac{2}{\aleph_{\acute{u}}+\aleph_e})^{\alpha}+(\frac{2}{\aleph_u+\aleph_e})^{\alpha}] \\
&= 2\times(\frac{2}{2n-2+4n-6})^{\alpha}\times\frac{n(n-1)(n+1)}{2} \\
&= \frac{2^{\alpha}}{(6n-8)^{\alpha}}\times n(n-1)(n+1) \\
H^{\alpha}(K_n)-H^{\alpha}(\Gamma(K_n)) &= 2^{\alpha}n(n-1)[\frac{1}{(3n-5)^{\alpha}}-\frac{(n+1)}{(6n-8)^{\alpha}}].
\end{aligned}$$

By using Lemma 1.9, the function $\Omega(\vartheta)=2^{\alpha}\vartheta(\vartheta-1)\left[\frac{1}{(3\vartheta-5)^{\alpha}}-\frac{(\vartheta+1)}{(6\vartheta-8)^{\alpha}}\right]$ is increasing and decreasing for $\alpha>\frac{-1}{2}$ and $\alpha<\frac{-1}{2}$ respectively. Also $\Omega(3)=6\cdot 2^{\alpha}\left[\frac{1}{4^{\alpha}}-\frac{4}{10^{\alpha}}\right]<0$ if and only if $\left(\frac{2}{5}\right)^{\alpha}<\frac{1}{4}$ which holds for $\alpha<\frac{-1}{2}$. Therefore $H^{\alpha}(K_n)<H^{\alpha}(\Gamma(K_n))$. By the similar argument for $\alpha>\frac{-1}{2}$, we have the result $H^{\alpha}(K_n)>H^{\alpha}(\Gamma(K_n))$. □

Lemma 1.12. *For $\beta \geq 2$, the function defined by $\tau(\beta) = 2^{\beta}[\beta \times (-2+3\beta)^{\alpha} - \beta \times (2+\beta)(-2+6\beta)^{\alpha}]$ is strictly increasing and decreasing for $\alpha < -3$ and $\alpha > -3$ respectively.*

Proof.

$$\begin{aligned}
\tau'(x) &= 2^{\beta}(1+\beta\ln 2)[(-2+3\beta)^{\alpha} - (\beta+2)(-2+6\beta)^{\alpha}] \\
&+ 2^{\beta} \times \beta[3\alpha(-2+3\beta)\alpha - 1 - (-2+6\beta)^{\alpha} - (2+\beta) \times 6\alpha(-2+6\beta)^{\alpha-1}] \\
&= 2^{\alpha}(-2+3\beta)^{\alpha-1}[(-2+3\beta)(1+x\ln 2) + 3\alpha\beta] \\
&- 2^{\alpha}(-2+2\beta)^{\alpha-1}[(-2+6\beta)(\ln 2(\beta)^2 + 2(1+\ln 2)\beta + 2) + 6\alpha\beta(\beta+2)] \quad (1.9)
\end{aligned}$$

The convexity of $u^{\alpha-1}$ together with the Jensens inequality implies that

$$(3\beta)^{\alpha-1} > (-2+6\beta)^{\alpha-1} - (-2+3\beta)^{\alpha-1}$$

Using above inequality in equation (1.9), we have

$$\begin{aligned}
\tau'(\beta) &< 2^{\beta}(-2+3\beta)^{\alpha-1}[3\beta - 2 + 3\ln 2\beta^2 - 2\ln 2\beta + 3\beta\alpha - (12\beta^2 + 8x - 4 \\
&+ 6\beta^3\ln 2 - 2\beta^2\ln 2 + 12\beta^2\ln 2 - 4\beta\ln 2 + 6\beta^2\alpha + 12\beta\alpha)] \\
&= 2^{\beta}(3\beta-2)^{\alpha-1}[(-6\times\ln 2)\beta^3 + (\ln 8 - 10\times\ln 2 - 12 - 6\alpha)\beta^2 \\
&+ (-5 - \ln 4 + 4\ln 2 - 9\alpha)\beta + 2] \\
\tau'(\beta) &< 2^{\beta}(-2+3\beta)^{\alpha-1} \times g(\beta) \quad (1.10)
\end{aligned}$$

where $g(\beta) = [(-6\times\ln 2)\beta^3 + (\ln 8 - 10\times\ln 2 - 12 - 6\alpha)\beta^2 + (-5 - \ln 4 + 4\ln 2 - 9\alpha)\beta + 2]$ $g'(\beta) < 0$ for $\alpha > -3$ and $g'(\beta) > 0$ for $\alpha < -3$, where $\beta \geq 2$. Consequently, $\tau(\beta)$ in increasing for $\alpha < -3$ and $\tau(\beta)$ is decreasing for $\alpha > -3$; $\beta \geq 2$. □

Lemma 1.13. *For $w \geq 3$, the function defined by $\phi(w) = w \times 2^{w+\alpha}[\frac{1}{(3w-2)^{\alpha}} - \frac{(w+2)}{(6w-2)^{\alpha}}]$ is strictly increasing and decreasing for $(\frac{7}{16})^{\alpha} < \frac{1}{5}$ and $(\frac{7}{16})^{\alpha} > \frac{1}{5}$ respectively.*

Lemma 1.13 can be proved analogously. The hypercube Q_n is n regular graph with order and size as 2^n and $n \times 2^{n-1}$ respectively , see details in Figure 4. By definition of total graph, $\Gamma(Q_n)$ has order and size as $n \cdot 2^{n-1} + 2 \cdot 2^{n-1} + = (n+2) \cdot 2^{n-1}$ and $2^{n-1} \cdot n(2n+n^2)$, respectively. Now for the hypercube Q_n, we calculate the smallest and

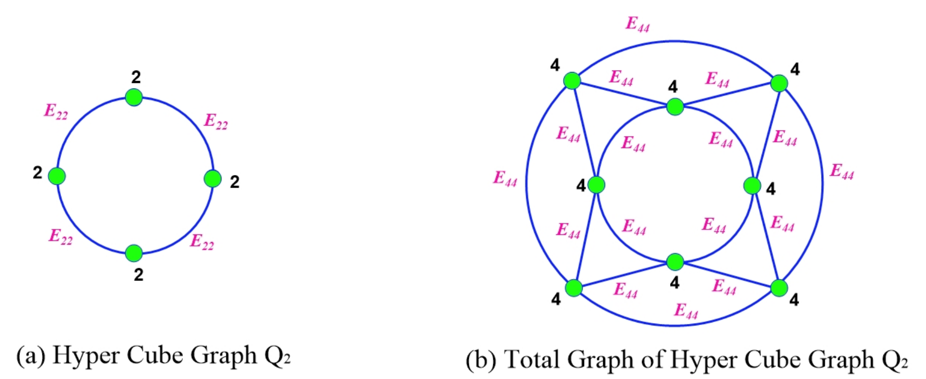


Figure 4. Graphical illustration of (a)hypercube Q_2 and (b) its total graph $\Gamma(Q_2)$

the largest GS index.

Theorem 1.14. *Let $\Gamma(Q_n)$ be the total graph of Q_n, then for $n \geq 2$, Q_n has the smallest and and the greatest GS index for $\alpha < -3$ and $\alpha > -3$ respectively.*

Proof.

$$\begin{aligned}\hat{\chi}^{\alpha}(Q_n) &= \sum_{\acute{u}e}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}]\\ &= \sum_{\acute{u}u\in E(Q_n)}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}+(\aleph_u+\aleph_e)^{\alpha}]\\ &= [(n+2(-1+n)^{\alpha}+(n+2(-1+n)^{\alpha}]\cdot 2^{n-1}\cdot n\\ &= 2^n\times n(3n-2)^{\alpha}\end{aligned}$$

$$\begin{aligned}\hat{\chi}^{\alpha}(\Gamma(Q_n)) &= \sum_{\acute{u}e}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}]\\ &= \sum_{\acute{u}u\in E(\Gamma(Q_n))}[(\aleph_{\acute{u}}+\aleph_e)^{\alpha}+(\aleph_u+\aleph_e)^{\alpha}]\\ &= [(2n+2(-1+2n))^{\alpha}+(2n+2(-1+2n))^{\alpha}]\cdot 2^{n-1}\cdot(2+n)\cdot n\\ &= 2^n\times(6n-2)^{\alpha}(2+n)n\end{aligned}$$

$$\hat{\chi}^{\alpha}(Q_n)-\hat{\chi}^{\alpha}(\Gamma(Q_n)) = n\times 2^n\big[(3n-2)^{\alpha}-(n+2)(6n-2)^{\alpha}\big] \tag{1.11}$$

Let $\tau(u)=x\times 2^u\big[(3u-2)^{\alpha}-(u+2)(6u-2)^{\alpha}\big]$, then by using Lemma 1.12, $\tau(u)$ is strictly increasing and decreasing for $\alpha<-3$ and $\alpha>-3$ respectively. Also $\tau(3)=24(7^{\alpha}-5\times(16)^{\alpha})<0$ for $(\frac{7}{16})^{\alpha}<5$, which also satisfied by$\alpha>-3$. Consequently, $\hat{\chi}^{\alpha}(Q_n)-\hat{\chi}^{\alpha}(\Gamma(Q_n))\leq\tau(u)\leq\tau(3)<o$ for $\alpha>-3$, which implies that $\hat{\chi}^{\alpha}(Q_n)<\hat{\chi}^{\alpha}(\Gamma(Q_n))$ for $\alpha>-3$. By similar calculations, we can show that $\hat{\chi}^{\alpha}(Q_n)>\hat{\chi}^{\alpha}(\Gamma(Q_n))$ for $\alpha<-3$. □

Theorem 1.15. *Let $\Gamma(Q_n)$ be the total graph of Q_n, then for $n\geq 3$, Q_n has the smallest and and the greatest GH index for $(\frac{16}{7})^{\alpha}>\frac{1}{5}$ and $(\frac{16}{7})^{\alpha}>\frac{1}{5}$ respectively.*

Proof.

$$\begin{aligned}H^{\alpha}(Q_n) &= \sum_{\acute{u}e}[(\frac{2}{\aleph_{\acute{u}}+\aleph_e})^{\alpha}]\\ &= \sum_{\acute{u}u\in E(Q_n)}[(\frac{2}{\aleph_{\acute{u}}+\aleph_e})^{\alpha}+(\frac{2}{\aleph_u+\aleph_e})^{\alpha}]\\ &= n\times[(\frac{2}{n+2(-1+n)})^{\alpha}+(\frac{2}{n+2(-1+n)})^{\alpha}]\times 2^{n-1}\\ &= n\times\frac{2^{n+\alpha}}{(3n-2)^{\alpha}}\end{aligned}$$

$$\begin{aligned}H^{\alpha}(\Gamma(Q_n)) &= \sum_{\acute{u}e}[(\frac{2}{\aleph_{\acute{u}}+\aleph_e})^{\alpha}]\\ &= \sum_{\acute{u}u\in E(\Gamma(Q_n))}[(\frac{2}{\aleph_{\acute{u}}+\aleph_e})^{\alpha}+(\frac{2}{\aleph_u+\aleph_e})^{\alpha}]\\ &= [(\frac{2}{2(n-1+2n)})^{\alpha}+(\frac{2}{2(n-1+2n)})^{\alpha}]\cdot(2n+n^2)\cdot 2^{n-1}\\ &= (2n+n^2)\times\frac{2^{n+\alpha}}{(6n-2)^{\alpha}}\end{aligned}$$

$$H^{\alpha}(Q_n)-H^{\alpha}(\Gamma(Q_n)) = n\times 2^{n+\alpha}[\frac{1}{(3n-2)^{\alpha}}-\frac{(n+2)}{(6n-2)^{\alpha}}]. \tag{1.12}$$

Let $\phi(u) = u \times 2^{u+\alpha}[\frac{1}{(3u-2)^\alpha} - \frac{(u+2)}{(6u-2)^\alpha}]$, then by using Lemma 1.13, $\phi(u)$ is strictly increasing and decreasing for $(\frac{7}{16})^\alpha < \frac{1}{5}$ and $(\frac{7}{16})^\alpha > \frac{1}{5}$ respectively. Also $\phi(3) = 16(\frac{1}{7^\alpha} - \frac{5}{(16)^\alpha}) < 0$ for $(\frac{7}{16})^\alpha > \frac{1}{5}$. Consequently, $H^\alpha(Q_n) - H^\alpha(\Gamma(Q_n)) \leq \phi(u) \leq \phi(3) < 0$, for $(\frac{7}{16})^\alpha > \frac{1}{5}$, which implies that $H^\alpha(Q_n) < H^\alpha(\Gamma(Q_n))$ for $(\frac{7}{16})^\alpha > \frac{1}{5}$. By similar calculations, we can show that $H^\alpha(Q_n) > H^\alpha(\Gamma(Q_n))$ for $(\frac{7}{16})^\alpha < \frac{1}{5}$. □

2. Conclusion

The study of structural Graphs Theory is a large and growing field of study. First strategy for analysing structural qualities is to obtain quantitative measurements that scramble structural data of the entire system by a real number. The entire structure of networks has been examined using a vast compendium of quantitative descriptors and related graphs. The importance of degree-related topological indices in theoretical chemistry and nanotechnology is highlighted in these studies. As a result, one of the most successful study areas is the computation of degree-related indices.

This study deals with the derivation of closed expression of (GH) and (GS) indices in terms of incident vertex-edge degrees for the path graph P_n, cyclic graph C_n, complete graph K_n, and the hypercube graph Q_n for a definite pendent vertex for various estimations of α. Computing favourable results for the extremal (GS) and (GH) indices of various graphs with fixed parameters would be the most appealing.

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