Hacettepe Journal of
Mathematics & Statistics

Hacet. J. Math. Stat.
Volume XX (x) (XXXX), 1 – 12
DOI : 10.15672/hujms.xx

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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Received: 21.01.2023; Accepted: 02.01.2024

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.

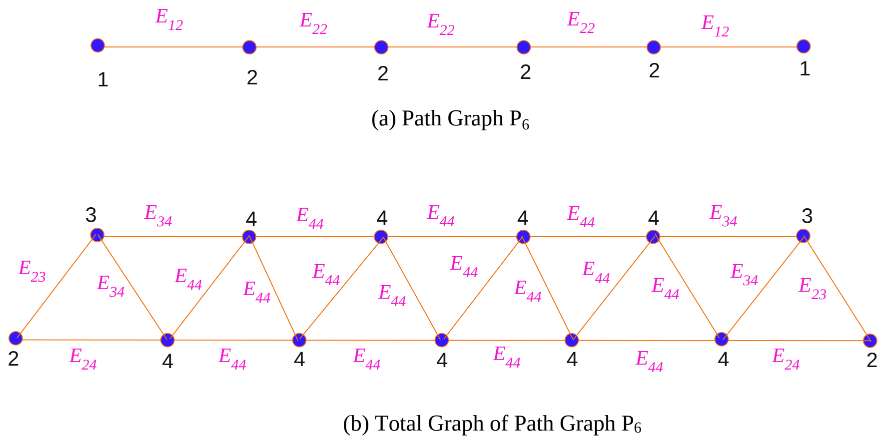


Figure 1. Graphical illustration of (a)path graph P_6 and (b)its total graph $\Gamma(P_6)$

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

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

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

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

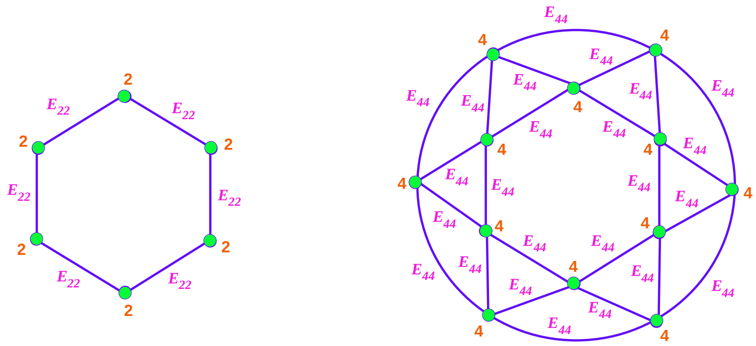
Define $g(\mu) = \frac{2}{2^{\alpha}}(\mu - 3) - (-13 + 4\mu) \times (\frac{2}{5^{\alpha}})$.
For $\mu \geq 4$, $g(\mu)$ is strictly decreasing function when $(\frac{2}{5})^{\alpha} > \frac{1}{4}$, also $g(4) < 0$ also holds for $(\frac{2}{5})^{\alpha} > \frac{1}{4}$ Consequently, $H^{\alpha}(P_n) - H^{\alpha}(\Gamma(P_n)) \leq g(\mu) \leq g(4) < 0$ 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 C6

(b) Total Graph of Cycle Graph C6

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

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

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

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

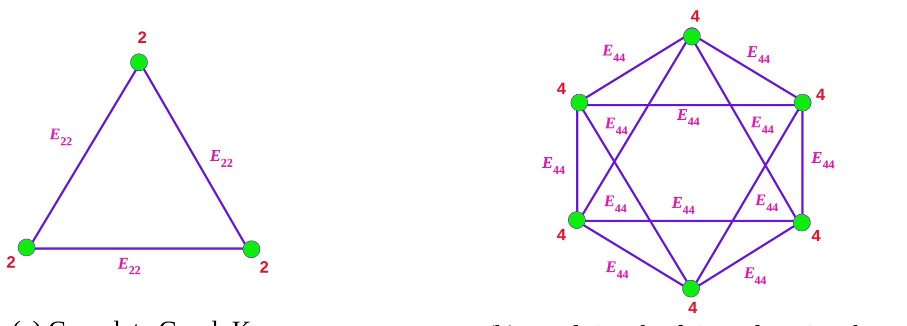
Define $f(\nu) = 2\nu\times(\frac{1}{2})^{\alpha}-8\nu\times(\frac{1}{5})^{\alpha}$. Also,

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

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.

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

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

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

$$\phi(\beta) < (3\beta-5)^{\alpha-1}g(\beta) < 0$$

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*

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

Proof.

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

where $f(\vartheta) = \frac{1}{(3\vartheta-5)^\alpha}\big[(6+3\alpha)\vartheta^2+(-13-3\alpha)\vartheta-5\big]$ 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 $(\frac{2}{5})^{\alpha}<4$ 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 $\Omega(\vartheta)=2^{\alpha}\vartheta(\vartheta-1)[\frac{1}{(3\vartheta-5)^{\alpha}}-\frac{(\vartheta+1)}{(6\vartheta-8)^{\alpha}}]$ is increasing and decreasing for $\alpha>\frac{-1}{2}$ and $\alpha<\frac{-1}{2}$ respectively. Also $\Omega(3)=6\cdot 2^{\alpha}[\frac{1}{4^{\alpha}}-\frac{4}{10^{\alpha}}]<0$ if and only if $(\frac{2}{5})^{\alpha}<\frac{1}{4}$ 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.

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

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

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

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

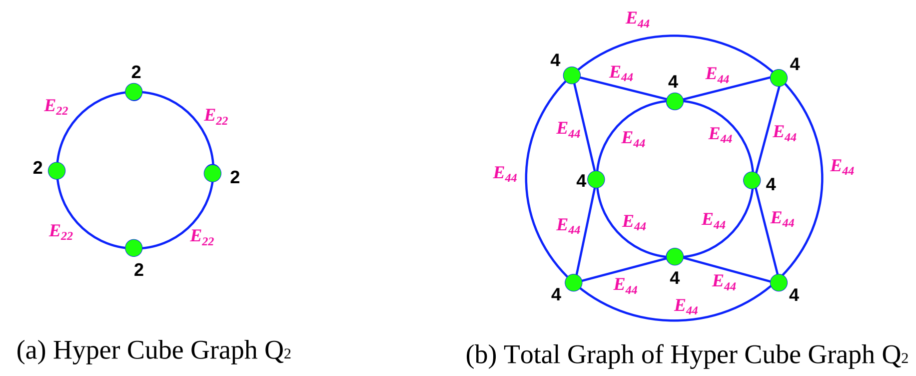


Figure 4. Graphical illustration of (a)hypercube Q_2 and (b) its total graph $\Gamma(Q_2)$

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.

Acknowledgment. This work is supported by Ansebo (Chongqing) Biotechnology Co., Ltd. under the Research Project of Optimization of Plant Cell Automation Production Model (H2139).

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