IEEE Access
Multidisciplinary ⋮ Rapid Review ⋮ Open Access Journal

Received October 9, 2019, accepted November 9, 2019, date of publication November 13, 2019, date of current version December 2, 2019.

Digital Object Identifier 10.1109/ACCESS.2019.2953338

Exact Formula and Improved Bounds for General Sum-Connectivity Index of Graph-Operations

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ABSTRACT For a molecular graph Γ, the general sum-connectivity index is defined as $\chi_\beta(\Gamma) = \sum_{vw\in E(\Gamma)}[d_\Gamma(v) + d_\Gamma(w)]^\beta$, where $\beta \in \mathbb{R}$ and $d_\Gamma(v)$ denotes the degree of the vertex v in the molecular graph Γ. The problem of finding best possible upper and lower bound for certain topological index is of fundamental nature in extremal graph theory. Akhtar and Imran [J. Inequal. Appl. (2016) 241] obtained the sharp bounds of general sum-connectivity index for four graph operations (F-sum graphs) introduced by Eliasi and Taeri [Discrete Appl. Math. 157: 794-803, 2009)]. In this paper, for $\beta \in \mathbb{N}$, we figured out and improved the sharp bounds of the general sum-connectivity index for F-sum graphs, where $F \in \{R, Q, T\}$. Several examples are presented to elaborate and compare the results of improved bounds with existing sharp bounds. In addition, we obtained exact formula of general sum-connectivity index for F-sum graphs, when $F = S$.

INDEX TERMS Molecular graphs, topological indices, Cartesian product, total graph, F-sum graphs.

I. INTRODUCTION

Assume $\Gamma = (V(\Gamma), E(\Gamma))$ be a simple, connected and finite molecular graph. We denote vertex set and edge set by $V(\Gamma)$ and $E(\Gamma) \subseteq V(\Gamma) \times V(\Gamma)$, respectively. The order and size of graph are denoted by $|V(\Gamma)| = n$ and $|E(\Gamma)| = m$, respectively. Each vertex of a molecular graph represents atom and each edge depicts bonding of two atoms. The degree of a vertex $v \in V(\Gamma)$, symbolize by $d_G(v)$, is the number of incident edges with v. A path graph or linear graph P_n of length $n-1$ be a graph consisting of vertex set $\{v_i : i = 1, 2, \ldots, n\}$ and edge set $\{v_iv_{i+1} : i = 1, 2, \ldots, n-1\}$. A cycle C_n having length n be a graph consisting of vertex set $\{v_i : i = 1, 2, \ldots, n\}$ and edge set $\{v_iv_{i+1} : i = 1, 2, \ldots, n-1\} \cup \{v_nv_1\}$.

Molecular graphs Γ illustrate the constitution of molecular structures, where vertices correspond to atoms and edges to covalent bonds between atoms. A Topological index (TI) is a numeric quantity computed mathematically from parameters of a molecular graph and correlates the meaningful information with the organic compound under study. TI's remain invariant with respect to symmetry properties (isomorphism) of Γ. Various types of valency, distance, spectral, and counting polynomials related TI's of molecular graphs are proposed in literature, however, degree related TI's are extensively investigated due to their significance. To conduct QSAR/QSPR analysis, topological invariants (being input) play essential role to better understand the complexity of molecules, physico-chemical and biological properties of corresponding chemical compound [1]–[8].

First Zagreb and second Zagreb indices are among the pioneer TI's which were introduced by Gutman and Trinajstić (1972) and are defined as [9]:

$$M_1(\Gamma) = \sum_{v\in V} d_v^2 = \sum_{vw\in E} (d_v + d_w).$$

$$M_2(\Gamma) = \sum_{vw\in E} (d_v d_w).$$

Li and Zheng (2005) extended the concept of first Zagreb index and provided the idea of first general Zagreb index (FGZI), which is given by [10]:

$$M^\alpha(\Gamma) = \sum_{v\in V(\Gamma)} d_\Gamma^\alpha(v) = \sum_{vw\in E(\Gamma)} [d_\Gamma^{\alpha-1}(v) + d_\Gamma^{\alpha-1}(w)].$$

where $\alpha \in \mathbb{R}$, $\alpha \neq 0$ and $\alpha \neq 1$. It is obvious that we get the first Zagreb index $M_1(\Gamma)$ and forgotten topological

The associate editor coordinating the review of this manuscript and approving it for publication was Yilun Shang.

index $F(\Gamma)$ by setting $\alpha = 2$ and $\alpha = 3$ in FGZI, respectively [9], [11].

Milan Randić (1975) introduced a TI with the name branching connectivity index [12]. It earned high rank in chemical graph theory due to its applied nature and its formula is given by $R_{\frac{-1}{2}}(\Gamma) = \sum_{vw\in E(\Gamma)} \frac{1}{\sqrt{d_v d_w}}$. Böllöbás and Erdös (1998) extended the idea and proposed general Randić index (GRI) which is defined as [13]:

$$R_\alpha(\Gamma) = \sum_{vw\in E(\Gamma)} [d_\Gamma(v)d_\Gamma(w)]^\alpha, \quad \alpha \in \mathbb{R},\ \alpha \neq 0.$$

Clearly, $\alpha = \frac{-1}{2}$ gives the classical Randić index $R_{-\frac{1}{2}}(\Gamma)$ and $\alpha = 1$ provides second Zagreb index $M_2(\Gamma)$.

The additive version of Randić index is known as sum-connectivity index which was initiated by Zhou and Trinajstić (2009) and its formula is given as [14]:

$$\chi_{-\frac{1}{2}}(\Gamma) = \sum_{vw\in E(\Gamma)} \frac{1}{\sqrt{d_v + d_w}}.$$

In [15], Zhou and Trinajstić (2010) presented the concept of general sum-connectivity index (GSCI) and established Nordhaus-Gaddum-type results for GSCI. It is defined as follows:

$$\chi_\beta(\Gamma) = \sum_{vw\in E(\Gamma)} [d_\Gamma(v) + d_\Gamma(w)]^\beta, \quad \beta \in \mathbb{R}.$$

The significance and effectiveness of GSCI can be witnessed by its relation with diverse TI's, e.g., χ_1 is the first Zagreb index, χ_2 is the hyper-Zagreb index, $2\chi_{-1}$ is the harmonic index, and $\chi_{-\frac{1}{2}}$ is the classical sum-connectivity index. Moreover, both $R_{-\frac{1}{2}}(\Gamma)$ and $\chi_{-\frac{1}{2}}(\Gamma)$ correlate well with each other as well as with the π-electron energy of benzenoid hydrocarbons [16]. Chemical applications and mathematical properties of these indices are investigated and presented in [17]–[22]. Now, we state two important results from basic mathematics which will be used in the main results.

Binomial and Trinomial Theorem

Binomial and trinomial theorems are quick way to expand (multiplying out) binomial and trinomial expression involving higher powers. Their formal expressions are presented below, respectively.

$$(x_1 + x_2)^n = \sum_{i=0}^{n} \binom{n}{i} x_1^{n-i} x_2^{i}. \tag{1}$$

$$(x_1 + x_2 + x_3)^n = \sum_{\substack{a,b,c\\ a+b+c=n}} P_{a,b,c}\, x_1^a x_2^b x_3^c. \tag{2}$$

where $P_{a,b,c} = \frac{(a+b+c)!}{a!\,b!\,c!}$.

Cartesian product is a convenient and elegant tool to develop a larger network from smaller graphs and is crucial for design as well as analysis of networks [23]. The cartesian product of two simple graphs Γ_1 and Γ_2 is a new graph denoted by $\Gamma_1 \square\, \Gamma_2$ whose vertex set is $V(\Gamma_1) \square\, V(\Gamma_2) = V(\Gamma_1) \times V(\Gamma_2)$ and whose edge set is the set of all pairs $(v_1, w_1)(v_2, w_2)$ such that either $v_1v_2 \in E(\Gamma_1)$ and $w_1 = w_2$, or $w_1w_2 \in E(\Gamma_2)$ and $v_1 = v_2$. Thus, every edge of Γ_1 and every edge of Γ_2 contributes 4 edges in $\Gamma_1 \square\, \Gamma_2$. Moreover, $|V(\Gamma_1 \square\, \Gamma_2)| = n_1 n_2$ and $|E(\Gamma_1 \square\, \Gamma_2)| = e_1 n_2 + e_2 n_1$.

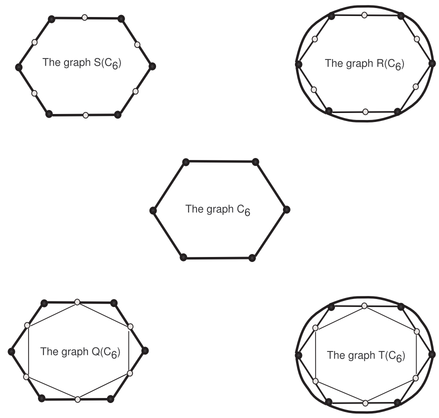

FIGURE 1. **Base graph C_6 along with its derived graphs.**

For a connected-simple graph Γ, the subdivided graph $S(\Gamma)$, the triangle parallel $R(\Gamma)$, line superposition $Q(\Gamma)$ [24], and the total graph $T(\Gamma)$ [25] can be constructed as follows:

1) $S(\Gamma)$ is derived from base graph Γ by placing an additional node (hollow) on every edge of Γ.
2) $R(\Gamma)$ is achieved from $S(\Gamma)$ by connecting the end (solid) vertices of the original edges of Γ that are incident with thin vertices.
3) $Q(\Gamma)$ is attained from $S(\Gamma)$ by linking those pairs of new vertices (hollow) by edges which have common adjacent (solid) vertex.
4) $T(\Gamma)$ is constructed from $S(\Gamma)$ by applying $R(\Gamma)$ and $Q(\Gamma)$, simultaneously.

Above mentioned operations are applied on the base graph C_6 and derived graphs $S(C_6)$, $R(C_6)$, $Q(C_6)$, and $T(C_6)$ are depicted in Figure 1. For two simple-connected graphs Γ_1 & Γ_2 and $F \in \{S, R, Q, T\}$, Eliasi and Taeri [26] developed four new graphs by applying the notion of cartesian product on $F(\Gamma_1)$ and Γ_2 and resultant graphs, denoted by $(\Gamma_1 +_F \Gamma_2)$, are called F-sum graphs. The vertex set of F-sum graph $\Gamma_1 +_F \Gamma_2$ is $V(\Gamma_1 +_F \Gamma_2) = V(F(\Gamma_1)) \times (V(\Gamma_2)) = (V(\Gamma_1) \cup E(\Gamma_1)) \times (V(\Gamma_2))$ such that two vertices (v_1, v_2) and (w_1, w_2) of $V(\Gamma_1 +_F \Gamma_2)$ are adjacent if and only if $[v_1 = w_1 \in V(\Gamma_1)$ and $(v_2, w_2) \in E(\Gamma_2)]$ or $[v_2 = w_2 \in V(\Gamma_2)$ and $(v_1, w_1) \in E(F(\Gamma_1))]$. In $\Gamma_1 +_F \Gamma_2$, we recognize $|V(\Gamma_2)|$ copies of the graph $F(\Gamma_1)$ provided that vertices of these copies are labeled with vertices of Γ_2. The vertices of Γ_1 and vertices in $E(\Gamma_1)$ are referred as solid and hollow vertices in $\Gamma_1 +_F \Gamma_2$, respectively and connecting only solid vertices having same symbol in $F(\Gamma_1)$ in such a way that their adjacency in Γ_2 is preserved. For further clarity, see Figure 2.

Numerous extremal results regarding GSCI for various classes of graphs were investigated by active researchers. Du *et al.* [27], [28] discussed minimum GSCI of unicyclic graphs, maximum GSCI of n-vertex tree and characterize

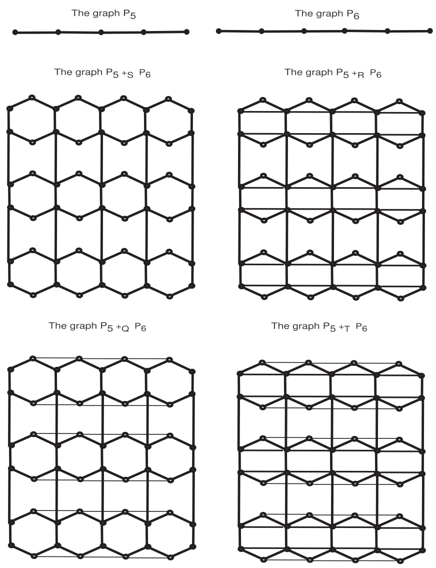

FIGURE 2. Graphs P_5 and P_6 along with their F-sum graphs.

extremal trees for certain value of α. Ramane *et al.* [29] studied and provided exact formulae for GSCI, GRI, FGZI, and co-indices of certain families of graphs. Furthermore, exact formulae, as well as bounds on several indices of unicyclic, bicyclic, and F-sum graphs were provided in [30]–[35]. Akhter and Imran [36] obtained sharp bounds for GSCI of F-sum graphs.

In this paper, we improved the sharp bounds for F-sum graphs offered in [36] for $\beta \in \mathbb{N}$ and $F \in \{R, Q, T\}$ by employing different technique. We observe that advantage of improved bounds over sharp bounds are due to the involvement of certain eminent TI's of the base graphs in it, whereas sharp bounds involve order, size, smallest degree, and largest degree of Γ, only. As a consequence, we observed and analyzed that our results perform equally well for any kind of parameters, while the sharp bounds deviate from exact value for big values of β, $\Delta(\Gamma)$ or small value of $\delta(\Gamma)$. In addition, we derived exact formula for GSCI of graph $\Gamma_1 +_S \Gamma_2$ in terms of certain topological indices of base graphs.

II. RESULTS AND DISCUSSION

In this section, the main results regarding general sum-connectivity index for the F-sum graphs $\Gamma_1 +_S \Gamma_2$, $\Gamma_1 +_R \Gamma_2$, $\Gamma_1 +_Q \Gamma_2$ and $\Gamma_1 +_T \Gamma_2$, where Γ_1 and Γ_2 are considered to be connected simple graphs. Throughout $n_1 = V(\Gamma_1)$, $n_2 = V(\Gamma_2)$, $e_1 = |E(\Gamma_1)|$, $e_2 = |E(\Gamma_2)|$, $V(S(\Gamma_1)) = n_1 + e_1$, $|E(S(\Gamma_1))| = 2e_1$, $M^0(\Gamma_1) = n_1$, $M^1(\Gamma_1) = 2e_1$, $M^1(\Gamma_2) = 2e_2$, $M^2(\Gamma_1) = M_1(\Gamma_1)$, $M^2(\Gamma_2) = M_1(\Gamma_2)$, $R_1(\Gamma_2) = M_2(\Gamma_2)$, $\chi_0(\Gamma_2) = e_2$, $\chi_1(\Gamma_1) = M_1(\Gamma_1)$

Theorem 1: Let Γ_1 and Γ_2 be two connected, simple and finite graphs and $\beta \in \mathbb{N}$, then the GSCI of S-sum graph (subdivision) is

$$\chi_\beta(\Gamma_1 +_S \Gamma_2) = \sum_{i=0}^{\beta} \binom{\beta}{i} \Big[2^{\beta-i} M^{\beta-i}(\Gamma_1)\chi_i(\Gamma_2) + \chi_{\beta-i}(S(\Gamma_1)) M^i(\Gamma_2) \Big].$$

Proof: Let $d(w, v) = d_{(\Gamma_1 +_S \Gamma_2)}(w, v)$ be the degree of a vertex (w, v) in the graph $(\Gamma_1 +_S \Gamma_2)$. Then using the definition of GSCI for graph operation S, we have

$$\begin{aligned}
\chi_\beta(\Gamma_1 +_S \Gamma_2) &= \sum_{\substack{(w_1,v_1)(w_2,v_2)\\ \in E(\Gamma_1 +_S \Gamma_2)}} \big[d(w_1, v_1) + d(w_2, v_2)\big]^\beta \\
&= \sum_{w \in V(\Gamma_1)} \sum_{v_1 v_2 \in E(\Gamma_2)} \big[d(w, v_1) + d(w, v_2)\big]^\beta \\
&\quad + \sum_{v \in V(\Gamma_2)} \sum_{w_1 w_2 \in E(S(\Gamma_1))} \big[d(w_1, v) + d(w_2, v)\big]^\beta \\
&= S1 + S2. \qquad (3)
\end{aligned}$$

Consider

$$\begin{aligned}
S1 &= \sum_{w \in V(\Gamma_1)} \sum_{v_1 v_2 \in E(\Gamma_2)} \big[d(w, v_1) + d(w, v_2)\big]^\beta \\
&= \sum_{w \in V(\Gamma_1)} \sum_{v_1 v_2 \in E(\Gamma_2)} \big[d_{\Gamma_1}(w) + d_{\Gamma_2}(v_1) + d_{\Gamma_1}(w) + d_{\Gamma_2}(v_2)\big]^\beta \\
&= \sum_{w \in V(\Gamma_1)} \sum_{v_1 v_2 \in E(\Gamma_2)} \big[2d_{\Gamma_1}(w) + (d_{\Gamma_2}(v_1) + d_{\Gamma_2}(v_2))\big]^\beta.
\end{aligned}$$

Using binomial theorem, we get

$$\begin{aligned}
S1 &= \sum_{w \in V(\Gamma_1)} \sum_{v_1 v_2 \in E(\Gamma_2)} \Bigg[\sum_{i=0}^{\beta} \binom{\beta}{i} 2^{\beta-i} d_{\Gamma_1}^{\beta-i}(w) \\
&\quad \times (d_{\Gamma_2}(v_1) d_{\Gamma_2}(v_2))^i \Bigg] \\
&= \sum_{i=0}^{\beta} \binom{\beta}{i} \Bigg[2^{\beta-i} \sum_{w \in V(\times\Gamma_1)} d_{\Gamma_1}^{\beta-i}(w) \\
&\quad \sum_{v_1 v_2 \in E(\Gamma_2)} (d_{\Gamma_2}(v_1) + d_{\Gamma_2}(v_2))^i \Bigg] \\
&= \sum_{i=0}^{\beta} \binom{\beta}{i} \Big[2^{\beta-i} M^{\beta-i}(\Gamma_1) \chi_i(\Gamma_2) \Big]. \\
S2 &= \sum_{v \in V(\Gamma_2)} \sum_{w_1 w_2 \in E(S(\Gamma_1))} \big[d(w_1, v) + d(w_2, v)\big]^\beta \\
&= \sum_{v \in V(\Gamma_2)} \sum_{w_1 w_2 \in E(S(\Gamma_1))} \big[d_{S(\Gamma_1)}(w_1) + d_{\Gamma_2}(v) + d_{S(\Gamma_1)}(w_2)\big]^\beta \\
&= \sum_{v \in V(\Gamma_2)} \sum_{w_1 w_2 \in E(S(\Gamma_1))} \big[(d_{S(\Gamma_1)}(w_1) + d_{S(\Gamma_1)}(w_2)) + d_{\Gamma_2}(v)\big]^\beta. \qquad (4)
\end{aligned}$$

Again, using binomial theorem, we have

$$\begin{aligned}
S2 &= \sum_{v \in V(\Gamma_2)} \sum_{w_1 w_2 \in E(S(\Gamma_1))} \Bigg[\sum_{i=0}^{\beta} \binom{\beta}{i} \\
&\quad \times (d_{S(\Gamma_1)}(w_1) + d_{S(\Gamma_1)}(w_2))^{\beta-i} (d_{\Gamma_2})^i(v) \Bigg]
\end{aligned}$$

$$= \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[\sum_{w_1w_2\in E(S(\Gamma_1))}(d_{S(\Gamma_1)}(w_1)+d_{S(\Gamma_1)}(w_2))^{\beta-i} \times \sum_{v\in V(\Gamma_2)}(d_{\Gamma_2})^i(v)\Big]$$

$$= \sum_{i=0}^{\beta}\binom{\beta}{i}\big[\chi_{\beta-i}(S(\Gamma_1))M^i(\Gamma_2)\big]. \quad (5)$$

Plugging equations (4) and (5) in equation (3), we get

$$\chi_\beta(\Gamma_1 +_S \Gamma_2) = \sum_{i=0}^{\beta}\binom{\beta}{i}\big[2^{\beta-i}M^{\beta-i}(\Gamma_1)\chi_i(\Gamma_2) + \chi_{\beta-i}(S(\Gamma_1))M^i(\Gamma_2)\big].$$

This concludes the proof.

Example 1: Let $\Gamma_1 = P_4$, $\Gamma_2 = C_3$, $\beta = 3$, and $F = S$. Then $n_1 = M^0(\Gamma_1) = 4$, $n_2 = M^0(\Gamma_2) = 3$, $e_1 = \chi_0(\Gamma_1) = 3$, $e_2 = \chi_0(\Gamma_2) = 3$, $\delta_{\Gamma_1} = 1$, $\Delta_{\Gamma_1} = 2$, $\delta_{\Gamma_2} = 2$, $\Delta_{\Gamma_2} = 2$, $\chi(\Gamma_1) = 10$, $\chi_2(\Gamma_1) = 34$, $\chi_3(\Gamma_1) = 118$,

First, we compute sharp lower bound γ_2 and sharp upper bound γ_1 using formulae derived in [36] $\gamma_2 = 2^\beta n_1e_2(\delta_{\Gamma_1} + \delta_{\Gamma_2})^\beta + 2n_2e_1(2\delta_{\Gamma_1} + \delta_{\Gamma_2})^\beta = 7200$ $\gamma_1 = 2^\beta n_1e_2(\Delta_{\Gamma_1} + \Delta_{\Gamma_2})^\beta + 2n_2e_1(2\Delta_{\Gamma_1} + \Delta_{\Gamma_2})^\beta = 10752$

Here, we compute GSCI using formula derived in theorem 1

$$\begin{aligned}\chi_3(P_4 +_S C_3) &= \sum_{i=0}^{3}\binom{3}{i}\Big[2^{3-i}M^{3-i}(\Gamma_1)\chi_i(\Gamma_2) + \chi_{3-i}(S(\Gamma_1))M^i(\Gamma_2)\Big]\\
&= 8\,M^3(\Gamma_1)\chi_0(\Gamma_2) + \chi_3(S(\Gamma_1))M^0(\Gamma_2)\\
&\quad + 3(4\,M^2(\Gamma_1)\chi(\Gamma_2) + \chi_2(S(\Gamma_1))M(\Gamma_2))\\
&\quad + 3(2\,M(\Gamma_1)\chi_2(\Gamma_2) + \chi(S(\Gamma_1))M^2(\Gamma_2))\\
&\quad + M^0(\Gamma_1)\chi_3(\Gamma_2) + \chi_0(S(\Gamma_1))M^3(\Gamma_2)\\
&= 8(18)(3) + 3(310) + 12(10)(12) + 18(82)\\
&\quad + 6(6)(48) + 36(22) + 4(192) + 24(6) = 7710.\end{aligned}$$

In graph $P_4 +_S C_3$, we observe 6 edges each with end vertex degrees $(2, 3)$, $(3, 3)$, and $(4, 4)$ and 12 edges having end vertex degrees $(2, 4)$. Now, we calculate exact value of GSCI of $P_4 +_S C_3$ for $\beta = 3$.

$$\chi_3(P_4 +_S C_3) = \sum_{vw\in E(P_4+_SC_3)}(d_{P_4}(v) + d_{C_3}(w))^3 = 7710.$$

In addition, we computed actual value of $\chi_3(P_4 +_S P_4)$ to be 6812 and the sharp bounds on GSCI is given by $\gamma_2 = 1416 < 6812 < 11328 = \gamma_1$, whereas result obtained using formula presented in theorem 1 is exactly 6812.

Theorem 2: Let Γ_1 and Γ_2 be two connected, simple and finite graphs and $\beta \in \mathbb{N}$, then the improved lower and upper bounds for GSCI of R-sum graph (triangle parallel) are $L_R \leq \chi_\beta(\Gamma_1 +_R \Gamma_2) \leq U_R$, where

$$L_R = \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[4^{(\beta-i)}M^{(\beta-i)}(\Gamma_1)\chi_i(\Gamma_2) + 2^\beta M^{(\beta-i)}(\Gamma_2)\chi_i(\Gamma_1)\Big] + \sum_{\substack{a,b,c\\a+b+c=\beta}} P_{a,b,c}\, 2^{a+c+1}e_1(\delta_{\Gamma_1})^a M^b(\Gamma_2),$$

$$U_R = \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[4^{(\beta-i)}M^{(\beta-i)}(\Gamma_1)\chi_i(\Gamma_2) + 2^\beta M^{(\beta-i)}(\Gamma_2)\chi_i(\Gamma_1)\Big] + \sum_{\substack{a,b,c\\a+b+c=\beta}} P_{a,b,c}\, 2^{a+c+1}e_1(\Delta_{\Gamma_1})^a M^b(\Gamma_2).$$

where $P_{a,b,c} = \frac{(a+b+c)!}{a!\,b!\,c!}$. Equality holds iff Γ_1 is regular graph.

Proof: Let $d(w, v) = d_{(\Gamma_1+_R\Gamma_2)}(w, v)$ be the degree of a vertex (w, v) in the graph $(\Gamma_1 +_R \Gamma_2)$. Then GSCI for graph operation R is computed as

$$\begin{aligned}\chi_\beta(\Gamma_1 +_R \Gamma_2) &= \sum_{(w_1,v_1)(w_2,v_2)\in E(\Gamma_1+_R\Gamma_2)}\big[d(w_1, v_1)+d(w_2, v_2)\big]^\beta\\
&= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\big[d(w, v_1) + d(w, v_2)\big]^\beta + \sum_{v\in V(\Gamma_2)}\sum_{w_1w_2\in E(R(\Gamma_1))}\big[d(w_1, v) + d(w_2, v)\big]^\beta.\end{aligned}$$

For every edge $w_1w_2 \in E(R(\Gamma_1))$ and vertex $v \in V(\Gamma_2)$, we have two choices and are presented below

$$\begin{aligned}\chi_\beta(\Gamma_1 +_R \Gamma_2) &= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\big[d(w, v_1) + d(w, v_2)\big]^\beta\\
&\quad + \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(R(\Gamma_1))\\ w_1,\ w_2\in V(\Gamma_1)}}\big[d(w_1, v) + d(w_2, v)\big]^\beta\\
&\quad + \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(R(\Gamma_1))\\ w_1\in V(\Gamma_1)\\ w_2\in V(R(\Gamma_1))-V(\Gamma_1)}}\big[d(w_1, v) + d(w_2, v)\big]^\beta\\
&= S3 + S4 + S5. \qquad (6)\end{aligned}$$

$$\begin{aligned}S3 &= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\big[d(w, v_1) + d(w, v_2)\big]^\beta\\
&= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\big[2d_{R(\Gamma_1)}(w) + d_{\Gamma_2}(v_1) + d_{\Gamma_2}(v_2)\big]^\beta\\
&= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\big[4d_{\Gamma_1}(w) + (d_{\Gamma_2}(v_1) + d_{\Gamma_2}(v_2))\big]^\beta.\end{aligned}$$

$$S3 = \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\Big[\sum_{i=0}^{\beta}\binom{\beta}{i}4^{\beta-i}d_{\Gamma_1}^{\beta-i}(w) \times (d_{\Gamma_2}(v_1) + d_{\Gamma_2}(v_2))^i\Big]$$

$$= \sum_{i=0}^{\beta}\binom{\beta}{i}\Bigg[4^{\beta-i}\sum_{w\in V(\Gamma_1)} d_{\Gamma_1}^{\beta-i}(w) \times \sum_{v_1v_2\in E(\Gamma_2)}(d_{\Gamma_2}(v_1)+d_{\Gamma_2}(v_2))^i\Bigg]$$

$$= \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[4^{\beta-i}M^{\beta-i}(\Gamma_1)\chi_i(\Gamma_2)\Big]. \qquad (7)$$

Subsequent summation consists of edges of triangle parallel graph $R(\Gamma_1)$ such that both end points are in $V(\Gamma_1)$. In this scenario $d_{R(\Gamma_1)}(w) = 2d_{\Gamma_1}(w)$.

$$S4 = \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(R(\Gamma_1))\\ w_1,\, w_2\in V(\Gamma_1)}}[d(w_1,v)+d(w_2,v)]^{\beta}$$

$$= \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(R(\Gamma_1))\\ w_1,\, w_2\in V(\Gamma_1)}}[2d_{\Gamma_2}(v)+d_{R(\Gamma_1)}(w_1) + d_{R(\Gamma_1)}(w_2)]^{\beta}$$

$$= \sum_{v\in V(\Gamma_2)}\sum_{w_1w_2\in E(\Gamma_1)}[2d_{\Gamma_2}(v)+2d_{\Gamma_1}(w_1)+2d_{\Gamma_1}(w_2)]^{\beta}$$

$$= \sum_{v\in V(\Gamma_2)}\sum_{w_1w_2\in E(\Gamma_1)}2^{\beta}[d_{\Gamma_2}(v)+(d_{\Gamma_1}(w_1)+d_{\Gamma_1}(w_2))]^{\beta}$$

$$= \sum_{v\in V(\Gamma_2)}\sum_{w_1w_2\in E(\Gamma_1)}2^{\beta}\Bigg[\sum_{i=0}^{\beta}\binom{\beta}{i}d_{\Gamma_2}^{\beta-i}(v) \times (d_{\Gamma_1}(w_1)+d_{\Gamma_1}(w_2))^i\Bigg] \quad \text{(using 1)}$$

$$= \sum_{i=0}^{\beta}\binom{\beta}{i}2^{\beta}\Bigg[\sum_{v\in V(\Gamma_2)}d_{\Gamma_2}^{\beta-i}(v) \times \sum_{w_1w_2\in E(\Gamma_1)}(d_{\Gamma_1}(w_1)+d_{\Gamma_1}(w_2))^i\Bigg]$$

$$= \sum_{i=0}^{\beta}\binom{\beta}{i}2^{\beta}M^{\beta-i}(\Gamma_2)\chi_i(\Gamma_1). \qquad (8)$$

Our next summation comprise of edges of graph $R(\Gamma_1)$ having end vertices in $V(\Gamma_1)$. It is evident from graph $R(\Gamma_1)$ that $d_{R(\Gamma_1)}(w) = 2$.

$$S5 = \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(R(\Gamma_1))\\ w_1\in V(\Gamma_1)\\ w_2\in V(R(\Gamma_1))-V(\Gamma_1)}}[d(w_1,v)+d(w_2,v)]^{\beta}.$$

$$S5 = \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(R(\Gamma_1))\\ w_1\in V(\Gamma_1),\ w_2\in V(R(\Gamma_1))-V(\Gamma_1)}}[d_{R(\Gamma_1)}(w_1) + d_{\Gamma_2}(v)+d_{R(\Gamma_1)}(w_2)]^{\beta}$$

$$= \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(R(\Gamma_1))\\ w_1\in V(\Gamma_1),\ w_2\in V(R(\Gamma_1))-V(\Gamma_1)}}[2d_{\Gamma_1}(w_1) + d_{\Gamma_2}(v)+2]^{\beta}$$

$$= \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(R(\Gamma_1))\\ w_1\in V(\Gamma_1),\ w_2\in V(R(\Gamma_1))-V(\Gamma_1)}}\Bigg[\sum_{\substack{a,b,c\\ a+b+c=\beta}}P_{a,b,c} \times 2^a d_{\Gamma_1}^a(w_1)d_{\Gamma_2}^b(v)2^c\Bigg]. \quad \text{(using 2)}$$

where $P_{a,b,c} = \frac{(a+b+c)!}{a!\, b!\, c!}$.

$$S5 = \sum_{\substack{a,b,c\\ a+b+c=\beta}}P_{a,b,c}\,2^{a+c}\Bigg[\sum_{\substack{w_1w_2\in E(R(\Gamma_1))\\ w_1\in V(\Gamma_1)\\ w_2\in V(R(\Gamma_1))-V(\Gamma_1)}}d_{\Gamma_1}^a(w_1) \times \sum_{v\in V(\Gamma_2)}d_{\Gamma_2}^b(v)\Bigg].$$

since $E(R(\Gamma_1)) = 2E(\Gamma_1) = 2e_1$, and $\delta_{\Gamma_1}(w) \le d_{\Gamma_1}(w)$ $\forall\, w \in V(\Gamma_1)$, therefore

$$S5 \ge \sum_{\substack{a,b,c\\ a+b+c=\beta}}P_{a,b,c}\,2^{a+c}\Big[2e_1(\delta_{\Gamma_1})^a M^b(\Gamma_2)\Big]$$

$$= \sum_{\substack{a,b,c\\ a+b+c=\beta}}P_{a,b,c}\,2^{a+c+1}e_1(\delta_{\Gamma_1})^a M^b(\Gamma_2). \qquad (9)$$

Consequently, by using equations (7)-(9) in equation (6), we get

$$\chi_{\beta}(\Gamma_1 +_R \Gamma_2) \ge \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[4^{(\beta-i)}M^{(\beta-i)}(\Gamma_1)\chi_i(\Gamma_2)+2^{\beta}\chi_i(\Gamma_1)M^{(\beta-i)}(\Gamma_2)\Big] + \sum_{\substack{a,b,c\\ a+b+c=\beta}}P_{a,b,c}\,2^{a+c+1}e_1(\delta_{\Gamma_1})^a M^b(\Gamma_2) = L_R.$$

Similarly, by using $\Delta_{\Gamma_1}(w) \ge d_{\Gamma_1}(w)$ $\forall\, w \in V(\Gamma_1)$, we get

$$\chi_{\beta}(\Gamma_1 +_R \Gamma_2) \le \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[4^{(\beta-i)}M^{(\beta-i)}(\Gamma_1)\chi_i(\Gamma_2)+2^{\beta}\chi_i(\Gamma_1)M^{(\beta-i)}(\Gamma_2)\Big] + \sum_{\substack{a,b,c\\ a+b+c=\beta}}P_{a,b,c}\,2^{a+c+1}e_1(\Delta_{\Gamma_1})^a M^b(\Gamma_2) = U_R.$$

Equality holds iff Γ_1 is regular graph. This concludes the proof.

Example 2: Again considering same graphs and using information discussed in Example 1 but for $\beta = 2$ and $F = R$, we compute sharp lower and upper bounds using formulae derived in [36].

$$\gamma_2 = 2^{\beta}(n_1e_2+n_2e_1)\big(2\delta_{\Gamma_1}+\delta_{\Gamma_2}\big)^{\beta} + 2n_2e_1\big(2\delta_{\Gamma_1}+\delta_{\Gamma_2}+2\big)^{\beta} = 1992.$$

$$\gamma_1 = 2^{\beta}(n_1e_2+n_2e_1)\big(2\Delta_{\Gamma_1}+\Delta_{\Gamma_2}\big)^{\beta} + 2n_2e_1\big(2\Delta_{\Gamma_1}+\Delta_{\Gamma_2}+2\big)^{\beta} = 4176.$$

Here, we compute GSCI using formula derived in theorem 2

$$\begin{aligned}L_R &= \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[4^{(\beta-i)}M^{(\beta-i)}(\Gamma_1)\chi_i(\Gamma_2)+2^{\beta}\chi_i(\Gamma_1)\Big]\\ &\quad\times M^{(\beta-i)}(\Gamma_2)+\sum_{\substack{a,b,c\\a+b+c=\beta}}P_{a,b,c}\,2^{a+c+1}e_1(\delta_{\Gamma_1})^aM^b(\Gamma_2)\\ &= 16M^2(\Gamma_1)\chi_0(\Gamma_2)+4M^2(\Gamma_2)\chi_0(\Gamma_1)\\ &\quad+2\big(4M(\Gamma_1)\chi(\Gamma_2)+4M(\Gamma_2)\chi(\Gamma_1)\big)\\ &\quad+M^0(\Gamma_1)\chi_2(\Gamma_2)+4M^0(\Gamma_2)\chi_2(\Gamma_1)\\ &\quad+24P_{1,0,1}M^0(\Gamma_2)+6P_{1,1,0}M(\Gamma_2)\\ &\quad+6P_{0,1,1}M(\Gamma_2)+12P_{2,0,0}M^0(\Gamma_2)\\ &\quad+12P_{0,2,0}M^2(\Gamma_2)+12P_{0,0,2}M^0(\Gamma_2)\\ &= 16(10)(3)+4(12)(3)+8(6)(12)+8(6)(10)+4(48)\\ &\quad+12(34)+48(3)+6(24)+6(24)+24(3)+6(12)\\ &\quad+24(3)=2928.\end{aligned}$$

Similarly, using specific values from Example 1 to compute U_R, we have $U_R = 3432$. In graph $P_4 +_R C_3$, we observe 6 edges each with end vertex degrees (2, 4), (4, 4), and (4, 6), 12 edges having end vertex degrees (2, 4), and 9 edges having end vertex degrees (6, 6). Now, we calculate exact value of GSCI of $P_4 +_R C_3$ for $\beta = 2$.

$$\chi_2(P_4 +_R C_3) = \sum_{vw\in E(P_4+_RC_3)}(d_{P_4}(v)+d_{C_3}(w))^2 = 3264.$$

It is evident that our bounds $L_R = 2928 \le 3264 \le 3432 = U_R$ sound promising as compared against sharp bounds $\gamma_2 = 1992 \le 3264 \le 4176 = \gamma_1$, offered in [36].

Theorem 3: Let Γ_1 and Γ_2 be two connected, simple and finite graphs and $\beta \in \mathbb{N}$, then the improved lower and upper bounds for GSCI of Q-sum graph (triangle parallel) are $L_Q \le \chi_\beta(\Gamma_1 +_Q \Gamma_2) \le U_Q$, where

$$\begin{aligned}L_Q &= \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[2^{\beta-i}M^{\beta-i}(\Gamma_1)\chi_i(\Gamma_2)+n_2(2\delta_{\Gamma_1})^i\chi_{\beta-i}(\Gamma_1)\Big]\\ &\quad+\sum_{\substack{a,b,c\\a+b+c=\beta}}2P_{a,b,c}\Big[(\delta_{\Gamma_1})^aM^b(\Gamma_2)\chi_c(\Gamma_1)\Big],\\ U_Q &= \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[2^{\beta-i}M^{\beta-i}(\Gamma_1)\chi_i(\Gamma_2)+n_2(2\Delta_{\Gamma_1})^i\chi_{\beta-i}(\Gamma_1)\Big]\\ &\quad+\sum_{\substack{a,b,c\\a+b+c=\beta}}2P_{a,b,c}\Big[(\Delta_{\Gamma_1})^aM^b(\Gamma_2)\chi_c(\Gamma_1)\Big].\end{aligned}$$

where $P_{a,b,c} = \frac{(a+b+c)!}{a!\,b!\,c!}$. Equality holds iff Γ_1 is regular graph.

Proof: Let $d(w, v) = d_{(\Gamma_1+_Q\Gamma_2)}(w, v)$ be the degree of a vertex (w, v) in the graph $(\Gamma_1 +_Q \Gamma_2)$. Then GSCI for graph operation Q is computed as

$$\begin{aligned}&\chi_\beta(\Gamma_1 +_Q \Gamma_2)\\ &\quad= \sum_{(w_1,v_1)(w_2,v_2)\in E(\Gamma_1+_Q\Gamma_2)}\big[d(w_1,v_1)+d(w_2,v_2)\big]^\beta\\ &\quad= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\big[d(w,v_1)+d(w,v_2)\big]^\beta\\ &\qquad+\sum_{v\in V(\Gamma_2)}\sum_{w_1w_2\in E(Q(\Gamma_1))}\big[d(w_1,v)+d(w_2,v)\big]^\beta.\end{aligned}$$

For computational ease, all edges $w_1w_2 \in E(Q(\Gamma_1))$ provided vertex $v \in V(\Gamma_2)$ can be split into two sets which are expressed in following expression.

$$\begin{aligned}&\chi_\beta(\Gamma_1 +_Q \Gamma_2)\\ &= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\big[d(w,v_1)+d(w,v_2)\big]^\beta\\ &\quad+\sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(Q(\Gamma_1))\\ w_1\in V(\Gamma_1)w_2\in V(Q(\Gamma_1))-V(\Gamma_1)}}\big[d(w_1,v)+d(w_2,v)\big]^\beta\\ &\quad+\sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(Q(\Gamma_1))\\ w_1,w_2\in V(Q(\Gamma_1))-V(\Gamma_1)}}\big[d(w_1,v)+d(w_2,v)\big]^\beta\\ &\chi_\beta(\Gamma_1 +_Q \Gamma_2) = S6+S7+S8.\end{aligned}\tag{10}$$

$$\begin{aligned}&S6\\ &= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\big[d(w,v_1)+d(w,v_2)\big]^\beta\\ &= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\big[2d_{Q(\Gamma_1)}(w)+d_{\Gamma_2}(v_1)+d_{\Gamma_2}(v_2)\big]^\beta\\ &= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\big[2d_{\Gamma_1}(w)+(d_{\Gamma_2}(v_1)+d_{\Gamma_2}(v_2))\big]^\beta\\ &= \sum_{w\in V(\Gamma_1)}\sum_{v_1v_2\in E(\Gamma_2)}\Bigg[\sum_{i=0}^{\beta}\binom{\beta}{i}2^{\beta-i}d_{\Gamma_1}^{\beta-i}(w)(d_{\Gamma_2}(v_1)\\ &\quad+d_{\Gamma_2}(v_2))^i\Bigg]\ \text{(using 1)}\\ &=\sum_{i=0}^{\beta}\binom{\beta}{i}\Big[2^{\beta-i}\sum_{w\in V(\Gamma_1)}d_{\Gamma_1}^{\beta-i}(w)\sum_{v_1v_2\in E(\Gamma_2)}(d_{\Gamma_2}(v_1)+d_{\Gamma_2}(v_2))^i\Big]\\ &S6\\ &= \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[2^{\beta-i}M^{\beta-i}(\Gamma_1)\chi_i(\Gamma_2)\Big].\end{aligned}\tag{11}$$

Next summation contains those edges of graph $\Gamma_1 +_Q \Gamma_2$ having one vertex in $V(\Gamma_1)$ and other in $V(Q(\Gamma_1)) - V(\Gamma_1)$

$$\begin{aligned}S7 &= \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(Q(\Gamma_1))\\ w_1\in V(\Gamma_1)\\ w_2\in V(Q(\Gamma_1))-V(\Gamma_1)}}\big[d(w_1,v)+d(w_2,v)\big]^\beta\\ S7 &= \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(Q(\Gamma_1))\\ w_1\in V(\Gamma_1)\\ w_2\in V(Q(\Gamma_1))-V(\Gamma_1)}}\big[d_{Q(\Gamma_1)}(w_1)\\ &\qquad+d_{\Gamma_2}(v)+d_{Q(\Gamma_1)}(w_2)\big]^\beta\\ &= \sum_{v\in V(\Gamma_2)}\sum_{\substack{w_1w_2\in E(Q(\Gamma_1))\\ w_1\in V(\Gamma_1)\\ w_2\in V(Q(\Gamma_1))-V(\Gamma_1)}}\big[d_{(\Gamma_1)}(w_1)+d_{\Gamma_2}(v)\\ &\qquad+d_{Q(\Gamma_1)}(w_2)\big]^\beta\end{aligned}$$

$$= \sum_{v \in V(\Gamma_2)} \sum_{\substack{w_1w_2 \in E(Q(\Gamma_1)) \\ w_1 \in V(\Gamma_1) \\ w_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} \Bigg[\sum_{\substack{a,b,c \\ a+b+c=\beta}} P_{a,b,c} d^a_{\Gamma_1}(w_1) d^b_{\Gamma_2}(v) d^c_{Q(\Gamma_1)}(w_2) \Bigg]. \quad \text{(using 2)}$$

We observe that $d_Q(\Gamma_1)(w_2) = d_{\Gamma_1}(u_i) + d_{\Gamma_1}(u_j) \; \forall \; w_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)$ such that w_2 is the vertex added into the edge $u_iu_j \in E(\Gamma_1)$. Moreover

$$\sum_{\substack{w_1w_2 \in E(Q(\Gamma_1)) \\ w_1 \in V(\Gamma_1) \\ w_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} d_{Q(\Gamma_1)}(w_2) = 2 \sum_{u_iu_j \in E(\Gamma_1)} \big(d_{\Gamma_1}(u_i) + d_{\Gamma_1}(u_j)\big).$$

Also using the fact $\delta_{\Gamma_1}(w) \le d_{\Gamma_1}(w) \; \forall \; w \in V(\Gamma_1)$, we have

$$\begin{aligned} S7 &\ge \sum_{\substack{a,b,c \\ a+b+c=\beta}} P_{a,b,c} \Bigg[(\delta_{\Gamma_1})^a \sum_{v \in V(\Gamma_2)} d^b_{\Gamma_2}(v) \times \sum_{\substack{w_1w_2 \in E(Q(\Gamma_1)) \\ w_1 \in V(\Gamma_1) \\ w_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} d^c_{Q(\Gamma_1)}(w_2) \Bigg] \\ &\ge \sum_{\substack{a,b,c \\ a+b+c=\beta}} P_{a,b,c} \Bigg[(\delta_{\Gamma_1})^a M^b(\Gamma_2) 2 \sum_{u_iu_j \in E(\Gamma_1)} (d_{\Gamma_1}(u_i) + d_{\Gamma_1}(u_j))^c \Bigg] \\ &= \sum_{\substack{a,b,c \\ a+b+c=\beta}} 2P_{a,b,c} \Big[(\delta_{\Gamma_1})^a M^b(\Gamma_2) \chi_c(\Gamma_1) \Big]. \end{aligned} \quad (12)$$

Following summation comprise of edges with both end vertices in $V(Q(\Gamma_1)) - V(\Gamma_1)$.

$$\begin{aligned} S8 &= \sum_{v \in V(\Gamma_2)} \sum_{\substack{w_1w_2 \in E(Q(\Gamma_1)) \\ w_1, w_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} [d(w_1, v) + d(w_2, v)]^\beta \\ &= \sum_{v \in V(\Gamma_2)} \sum_{\substack{w_1w_2 \in E(Q(\Gamma_1)) \\ w_1, w_2 \in V(Q(\Gamma_1)) - V(\Gamma_1)}} [d_{Q(\Gamma_1)}(w_1) + d_{Q(\Gamma_1)}(w_2)]^\beta \\ &= \sum_{v \in V(\Gamma_2)} \sum_{\substack{u_iu_j \in E(\Gamma_1) \\ u_ju_k \in E(\Gamma_1)}} [d_{\Gamma_1}(u_i) + d_{\Gamma_1}(u_j) + d_{\Gamma_1}(u_j) + d_{\Gamma_1}(u_k)]^\beta \\ &= \sum_{v \in V(\Gamma_2)} \sum_{\substack{u_iu_j \in E(\Gamma_1) \\ u_ju_k \in E(\Gamma_1)}} [(d_{\Gamma_1}(u_i) + d_{\Gamma_1}(u_k)) + 2d_{\Gamma_1}(u_j)]^\beta \\ &= \sum_{v \in V(\Gamma_2)} \sum_{\substack{u_iu_j \in E(\Gamma_1) \\ u_ju_k \in E(\Gamma_1)}} \Bigg[\sum_{i=0}^{\beta} \binom{\beta}{i} (d_{\Gamma_1}(u_j) + d_{\Gamma_1}(u_k))^{\beta - i} \times (2d_{\Gamma_1}(u_j))^i \Bigg] \quad \text{(using 1)} \\ &= \sum_{i=0}^{\beta} \binom{\beta}{i} \Bigg[\sum_{\substack{u_iu_j \in E(\Gamma_1) \\ u_ju_k \in E(\Gamma_1)}} (d_{\Gamma_1}(u_j) + d_{\Gamma_1}(u_k))^{\beta - i} \times \sum_{v \in V(\Gamma_2)} (2d_{\Gamma_1}(u_j))^i \Bigg] \\ &\ge \sum_{i=0}^{\beta} \binom{\beta}{i} \Bigg[n_2 (2\delta_{\Gamma_1})^i \sum_{u_ju_k \in E(\Gamma_1)} (d_{\Gamma_1}(u_j) + d_{\Gamma_1}(u_k))^{\beta - i} \Bigg] \end{aligned}$$

$$S8 = \sum_{i=0}^{\beta} \binom{\beta}{i} \Big[n_2 (2\delta_{\Gamma_1})^i \chi_{\beta - i}(\Gamma_1) \Big]. \quad (13)$$

Using equations (11)-(13) in equation (10), we have

$$\begin{aligned} &\chi_\beta(\Gamma_1 +_Q \Gamma_2) \\ &\ge \sum_{i=0}^{\beta} \binom{\beta}{i} \Big[2^{\beta - i} M^{\beta - i}(\Gamma_1) \chi_i(\Gamma_2) + n_2 (2\delta_{\Gamma_1})^i \chi_{\beta - i}(\Gamma_1) \Big] \\ &\quad + \sum_{\substack{a,b,c \\ a+b+c=\beta}} 2P_{a,b,c} \Big[(\delta_{\Gamma_1})^a M^b(\Gamma_2) \chi_c(\Gamma_1) \Big] = L_Q. \end{aligned}$$

Similarly,

$$\begin{aligned} &\chi_\beta(\Gamma_1 +_Q \Gamma_2) \\ &\ge \sum_{i=0}^{\beta} \binom{\beta}{i} \Big[2^{\beta - i} M^{\beta - i}(\Gamma_1) \chi_i(\Gamma_2) + n_2 (2\Delta_{\Gamma_1})^i \chi_{\beta - i}(\Gamma_1) \Big] \\ &\quad + \sum_{\substack{a,b,c \\ a+b+c=\beta}} 2P_{a,b,c} \Big[(\Delta_{\Gamma_1})^a M^b(\Gamma_2) \chi_c(\Gamma_1) \Big] = U_Q. \end{aligned}$$

Equality holds iff Γ_1 is regular graph. This concludes the proof.

Example 3: For $F = Q$ and $\beta = 2$, we compute sharp lower and upper bounds for graphs presented in Example 1 by using formulae derived in

$$\begin{aligned} \gamma_2 &= 2^\beta n_1 e_2 \big(\delta_{\Gamma_1} + \delta_{\Gamma_2}\big)^\beta + 2n_2 e_1 \big(3\delta_{\Gamma_1} + \delta_{\Gamma_2}\big)^\beta \\ &\quad + 4^\beta n_2 (\delta_{\Gamma_1})^\beta \Big(\tfrac{M_1(\Gamma_1)}{2} - e_1 \Big) = 978 \\ \gamma_1 &= 2^\beta n_1 e_2 \big(\Delta_{\Gamma_1} + \Delta_{\Gamma_2}\big)^\beta + 2n_2 e_1 \big(3\Delta_{\Gamma_1} + \Delta_{\Gamma_2}\big)^\beta \\ &\quad + 4^\beta n_2 (\Delta_{\Gamma_1})^\beta \Big(\tfrac{M_1(\Gamma_1)}{2} - e_1 \Big) = 2304. \end{aligned}$$

Here, we compute GSCI using formula derived in theorem 3

$$\begin{aligned} &L_Q \\ &= 4M^2(\Gamma_1)\chi_0(\Gamma_2) + 3\chi_2(\Gamma_1) + 2\big(2M(\Gamma_1)\chi(\Gamma_2) + 6\chi(\Gamma_1)\big) \\ &\quad + M^0(\Gamma_1)\chi_2(\Gamma_2) + 12\chi_0(\Gamma_1) + 2P_{1,0,1}\big(M^0(\Gamma_2)\chi(\Gamma_1)\big) \\ &\quad + 2P_{1,1,0}\big(M(\Gamma_2)\chi_0(\Gamma_1)\big) + 2P_{0,1,1}\big(M(\Gamma_2)\chi(\Gamma_1)\big) \\ &\quad + 2P_{2,0,0}\big(M^0(\Gamma_2)\chi_0(\Gamma_1)\big) + 2P_{0,2,0}\big(M^2(\Gamma_2)\chi_0(\Gamma_1)\big) \\ &\quad + 2P_{0,0,2}\big(M^0(\Gamma_2)\chi_0(\Gamma_1)\big) = 4(10)(3) + 3(34) \\ &\quad + 2\big(2(6)(12) + 6(10)\big) + 4(48) + 12(3) + 12(10) + 18(3) \\ &\quad + 18(10) + 6(3) + 24(3) + 6(34) = 1584. \end{aligned}$$

Similarly, using required values from Example 1 to compute U_Q, we have $U_Q = 2058$. In graph $P_4 +_Q C_3$, we observe

12 edges each with end vertex degrees $(3,3)$, $(3,4)$, and $(4,4)$. Now, we compute exact value of GSCI of $P_4 +_Q C_3$ for $\beta = 2$.

$\chi_2(P_4 +_Q C_3) = \sum_{vw \in E(P_4 +_Q C_3)} (d_{P_4}(v) + d_{C_3}(w))^2 = 1788.$

It is obvious that our bounds $L_Q = 1584 \leq 1788 \leq 2058 = U_Q$ are better in contrast to the sharp bounds $\gamma_2 = 978 \leq 1788 \leq 2304 = \gamma_1$, offered in [36].

From Figure 2, it can readily be observed that T-sum graph (total graph) is closely related to R-sum graph and Q-sum graph graph. Consequently their degrees have following relation (i) $d_{\Gamma_1 +_T \Gamma_2}(w, v) = d_{\Gamma_1 +_R \Gamma_2}(w, v)$ for $w \in V(\Gamma_1)$ and $v \in V(\Gamma_2)$, (ii) $d_{\Gamma_1 +_T \Gamma_2}(w, v) = d_{\Gamma_1 +_Q \Gamma_2}(w, v)$ for $w \in V(T(\Gamma_1)) - V(\Gamma_1)$ and $v \in V(\Gamma_2)$. Following result is direct consequence of theorems 2 and 3

Theorem 4: Let Γ_1 and Γ_2 be two connected, simple and finite graphs and $\beta \in \mathbb{N}$, then the improved lower and upper bounds for GSCI of T-sum graph are $L_T \leq \chi_\beta(\Gamma_1 +_Q \Gamma_2) \leq U_T$, where

$$L_T = \sum_{\substack{a,b,c \\ a+b+c=\beta}} 2P_{a,b,c}\Big[(\delta_{\Gamma_1})^a M^b(\Gamma_2)\chi_c(\Gamma_1)\Big] + \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[2^{\beta-i}M^{\beta-i}(\Gamma_1)\chi_i(\Gamma_2) + 2^\beta M^{\beta-i}(\Gamma_2)\chi_i(\Gamma_1) + n_2(2\delta_{\Gamma_1})^i\chi_{\beta-i}(\Gamma_1)\Big]$$

$$U_T = \sum_{\substack{a,b,c \\ a+b+c=\beta}} 2P_{a,b,c}\Big[(\Delta_{\Gamma_1})^a M^b(\Gamma_2)\chi_c(\Gamma_1)\Big] + \sum_{i=0}^{\beta}\binom{\beta}{i}\Big[2^{\beta-i}M^{\beta-i}(\Gamma_1)\chi_i(\Gamma_2) + 2^\beta M^{\beta-i}(\Gamma_2)\chi_i(\Gamma_1) + n_2(2\Delta_{\Gamma_1})^i\chi_{\beta-i}(\Gamma_1)\Big]$$

where $P_{a,b,c} = \frac{(a+b+c)!}{a!\,b!\,c!}$. Equality holds iff Γ_1 is regular graph.

Example 4: For $F = T$ and $\beta = 2$, we compute sharp lower and upper bounds for graphs presented in Example 1 by using formulae derived in

$$\gamma_2 = 2^\beta(n_1e_2 + n_2e_1)\big(2\delta_{\Gamma_1} + \delta_{\Gamma_2}\big)^\beta + 2n_2e_1\big(4\delta_{\Gamma_1} + \delta_{\Gamma_2}\big)^\beta + 4^\beta n_2(\delta_{\Gamma_1})^\beta\Big(\frac{M_1(\Gamma_1)}{2} - e_1\Big) = 2088.$$

$$\gamma_1 = 2^\beta(n_1e_2 + n_2e_1)\big(2\Delta_{\Gamma_1} + \Delta_{\Gamma_2}\big)^\beta + 2n_2e_1\big(4\Delta_{\Gamma_1} + \Delta_{\Gamma_2}\big)^\beta + 4^\beta n_2(\Delta_{\Gamma_1})^\beta\Big(\frac{M_1(\Gamma_1)}{2} - e_1\Big) = 5208.$$

Here, we compute GSCI using formula derived in theorem 4

$$\begin{aligned} L_T &= 4M^2(\Gamma_1)\chi_0(\Gamma_2) + 2M^2(\Gamma_2)\chi_0(\Gamma_1) + 3\chi_0(\Gamma_1) \\ &\quad + 2\big(4M(\Gamma_1)\chi(\Gamma_2) + 4M(\Gamma_2)\chi(\Gamma_1) + 6\chi(\Gamma_1)\big) \\ &\quad + \big(M^0(\Gamma_1)\chi_2(\Gamma_2) + 4M^0(\Gamma_2)\chi_2(\Gamma_1) + 12\chi_2(\Gamma_1)\big) \\ &\quad + 2P_{1,0,1}\big(M^0(\Gamma_2)\chi(\Gamma_1)\big) + 2P_{1,1,0}\big(M(\Gamma_2)\chi_0(\Gamma_1)\big) \\ &\quad + 2P_{0,1,1}\big(M(\Gamma_2)\chi(\Gamma_1)\big) + 2P_{2,0,0}\big(M^0(\Gamma_2)\chi_0(\Gamma_1)\big) \\ &\quad + 2P_{0,2,0}\big(M^2(\Gamma_2)\chi_0(\Gamma_1)\big) + 2P_{0,0,2}\big(M^0(\Gamma_2)\chi_0(\Gamma_1)\big) \\ &= 4(10)(3) + 4(12)(3) + 3(3) + 4(6)(12) + 8(6)(10) \\ &\quad + 12(10) + 4(48) + 4(3)(34) + 12(34) + 12(10) + 24(3) \\ &\quad + 24(10) + 2(3(3) + 12(3) + 3(34)) = 2895. \end{aligned}$$

Similarly, using required values from Example 1 to compute U_T, we have $U_T = 4692$. In graph $P_4 +_T C_3$, we observe 6 edges each with end vertex degrees $(4,4)$ and $(3,6)$, 12 edges each having end vertex degrees $(3,4)$ and $(4,6)$, and 9 edges with end vertex degrees $(6,6)$. Now, we compute exact value of GSCI of $P_4 +_T C_3$ for $\beta = 2$. $\chi_2(P_4 +_T C_3) = \sum_{vw \in E(P_4 +_T C_3)} (d_{P_4}(v) + d_{C_3}(w))^2 = 3954$. It is evident that our bounds $L_T = 2895 \leq 3954 \leq 4692 = U_T$ are tighter than the sharp bounds $\gamma_2 = 2088 \leq 3954 \leq 5208 = \gamma_1$, offered in [36].

III. APPLICATIONS AND CONCLUSIONS

Results for cycles C_r and C_s

Let C_r and C_s be two cycle graphs with vertices r and s, respectively. Then GSCI of F-sum graphs $C_r +_S C_s$, $C_r +_R C_s$, $C_r +_Q C_s$, and $C_r +_T C_s$ are given as

1. $\chi_\beta(C_r +_S C_s) = \sum_{i=0}^{\beta}\binom{\beta}{i} rs2^{2\beta}\big(1 + 2^{1-i}\big).$

2. $\chi_\beta(C_r +_R C_s) = \sum_{i=0}^{\beta}\binom{\beta}{i} rs2^{2\beta-i}\big(1 + 2^{2i}\big) + \sum_{\substack{a,b,c \\ a+b+c=\beta}} P_{a,b,c}2^{2a+b+c+1}s = L_R = U_R.$

3. $\chi_\beta(C_r +_Q C_s) = \sum_{i=0}^{\beta}\binom{\beta}{i} rs2^{2\beta+1} + \sum_{\substack{a,b,c \\ a+b+c=\beta}} P_{a,b,c}2^{a+b+c+1}rs = L_Q = U_Q.$

4. $\chi_\beta(C_r +_T C_s) = \sum_{i=0}^{\beta}\binom{\beta}{i} rs2^{\beta}\big(2^{\beta+1} + 2^{2i}\big) + \sum_{\substack{a,b,c \\ a+b+c=\beta}} P_{a,b,c}2^{a+b+c+1}rs = L_T = U_T.$

Note that equality in lower and upper bounds for graphs $C_r +_F C_s$, $F \in \{R, Q, T\}$ holds due to the reason that $\Gamma_1 = C_r$ is regular graph with regularity 2.

Results for paths P_r and P_s

Let P_r and P_s be two cycle graphs with vertices r and s, respectively. Then GSCI of F-sum graphs $P_r +_S P_s$ and lower and upper bounds of GSCI for $P_r +_R P_s$, $P_r +_Q P_s$, and $P_r +_T$

P_s are given as

1. $\chi_\beta(P_r +_S P_s)$

$$= \sum_{i=0}^{\beta}\binom{\beta}{i}\big((2+(r-2)2^{\beta-i})(2(3)^i+(s-3)2^{2i}) + (2(3)^i+(r-3)2^{i+1})(2+(s-2)2^{\beta-i})\big).$$

2. $L_R \leq \chi_\beta(P_r +_R P_s) \leq U_R$, where

$$L_R = \sum_{i=0}^{\beta}\binom{\beta}{i}\big(4^{\beta-i}(2+(r-2)2^{\beta-i})(2(3)^i+(s-3)4^i) + 2^\beta(2(3)^i+(r-3)4^i)(2+(s-2)2^{\beta-i})\big) + \sum_{\substack{a,b,c\\ a+b+c=\beta}} P_{a,b,c}2^{a+c+1}(r-1)(2+(s-2)2^b),$$

$$U_R = \sum_{i=0}^{\beta}\binom{\beta}{i}\big(4^{\beta-i}(2+(r-2)2^{\beta-i})(2(3)^i+(s-3)4^i) + 2^\beta(2(3)^i+(r-3)4^i)(2+(s-2)2^{\beta-i})\big) + \sum_{\substack{a,b,c\\ a+b+c=\beta}} P_{a,b,c}2^{2a+c+1}(r-1)(2+(s-2)2^b).$$

3. $L_Q \leq \chi_\beta(P_r +_Q P_s) \leq U_Q$, where

$$L_Q = \sum_{i=0}^{\beta}\binom{\beta}{i}\Big(2^{\beta-i}(2+(r-2)2^{\beta-i})(2(3)^i+(s-3)4^i) + 2^i(2(3)^{\beta-i}+(r-3)4^{\beta-i})s\Big) + \sum_{\substack{a,b,c\\ a+b+c=\beta}} 2P_{a,b,c}(2+(s-2)2^b)(2(3)^c+(r-3)4^c),$$

$$U_Q = \sum_{i=0}^{\beta}\binom{\beta}{i}\Big(2^{\beta-i}(2+(r-2)2^{\beta-i})(2(3)^i+(s-3)4^i) + 4^i(2(3)^{\beta-i}+(r-3)4^{\beta-i})s\Big) + \sum_{\substack{a,b,c\\ a+b+c=\beta}} P_{a,b,c}2^{a+1}(2+(s-2)2^b)(2(3)^c+(r-3)4^c).$$

4. $L_T \leq \chi_\beta(P_r +_T P_s) \leq U_T$, where

$$L_T = \sum_{i=0}^{\beta}\binom{\beta}{i}\Big(2^{\beta-i}(2+(r-2)2^{\beta-i})(2(3)^i+(s-3)4^i) + 2^\beta(2(3)^i+(r-3)4^i)(2+(s-2)2^{\beta-i})\Big) + 2^i(2(3)^{\beta-i}+(r-3)4^{\beta-i})s + \sum_{\substack{a,b,c\\ a+b+c=\beta}} 2P_{a,b,c}(2+(s-2)2^b)(2(3)^c+(r-3)4^c),$$

$$U_T = \sum_{i=0}^{\beta}\binom{\beta}{i}\Big(2^{\beta-i}(2+(r-2)2^{\beta-i})(2(3)^i+(s-3)4^i) + 2^\beta(2(3)^i+(r-3)4^i)(2+(s-2)2^{\beta-i})\Big) + 4^i(2(3)^{\beta-i}+(r-3)4^{\beta-i})s + \sum_{\substack{a,b,c\\ a+b+c=\beta}} P_{a,b,c}2^{a+1}(2+(s-2)2^b)(2(3)^c+(r-3)4^c).$$

IV. CONCLUSION

To find sharp bounds, for certain topological index, is always an intricate and interesting problem. In [36], sharp bounds for GSCI of four operations on graphs $(\Gamma_1 +_S \Gamma_2, \Gamma_1 +_R \Gamma_2, \Gamma_1 +_Q \Gamma_2, \Gamma_1 +_T \Gamma_2)$ are presented. In this paper, we proposed improved as well as persuasive version of lower and upper bounds of GSCI for F-sum graphs, where $F \in \{R, Q, T\}$, and $\beta \in \mathbb{N}$. In addition, we derived exact formula for GSCI of graph $\Gamma_1 +_S \Gamma_2$ and presented some examples. To conclude, we elaborated and compared our improved bounds with the sharp bounds presented in [36] by taking tiny examples, when $\beta = 2$ and $\beta = 3$. Our bounds involve order, size, smallest degree, largest degree of Γ, and certain eminent TI's of the base graphs, whereas sharp bounds involve order, size, smallest degree, and largest degree of Γ, only. As a consequence, one can observe and analyze that our results perform equally well for any kind of parameters, while the sharp bounds deviate from exact value for large values of β, $\Delta(\Gamma)$ or small value of $\delta(\Gamma)$.

LIST OF ABBREVIATIONS

Abbreviation	Meaning
TI	Topological Index
QSAR	Quantitative Structure Activity Relationships
QSPR	Quantitative Structure Property Relationships
FGZI	First General Zagreb Index
GRI	general Randić index
GSCI	general sum-connectivity index

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