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Bounds for General Connectivity Indices of Tensor Product of Connected Graphs

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Abstract: Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. In this paper, bounds for the Randić, general Randić, sum-connectivity, the general sum-connectivity and harmonic indices for tensor product of graphs are determined by using the combinatorial inequalities and combinatorial computing.

Keywords: Tensor product of graphs; Randić index; sum-connectivity index; harmonic index.

1. Introduction and Preliminary Results

In molecular graph, we show, atoms and covalent bonds in the molecule by vertices and edges respectively. In computational chemistry, molecular graphs are extensively used for analysis of molecular structures [28]. For correlating and predicting chemical, physical and biological activity (property) from molecular structure is an important problem in computational and theoretical chemistry [26]. The most important step in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) is the representation of chemical structures of various molecules numerically to find out a correlation model between the chemical structures of different chemical compounds and their biological and chemical activities (properties). We can say that a major task in QSAR/QSPR researches is the transformation of the chemical formula (or molecular graph) into numeric form exactly. The topological index is one of the most popular quantification methods used for the molecular structures, because of its direct application on molecular structures and rapid computations when number of molecules is very large [1,5,22,31].

Topological index is a tool that transforms the whole molecular graph into a number that describes the structure and the branching pattern of the molecule [6]. The chemist Harold Wiener used a topological index for the first time in 1947 [29]. We use Wiener index for finding correlation between molecular structure of certain hydrocarbon compounds and their physical and chemical properties. Since 1947, more than hundred topological indices have been defined, from which, Randić connectivity index is listed among the most useful molecular descriptors in structure-activity and structure-property relationships studies [23,27,30]. The Randić index [24] of the graph G , also known as product-connectivity index [21,32] is defined as:

$$R = R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg_G(u) \deg_G(v)}}$$

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It was named as, "branching index" by Randić himself. Soon after it was re-named as, "connectivity index" [18] and [19]. Now it is referred as, "Randić index". It is most often applied and most successful among all the popular topological descriptors [25]. It is the most studied structure descriptor because it is discussed in hundreds of papers and a few books are also written on it. It was proved suitable for drug design [13,24].

Bollobás [8] and Amic et al. [3] independently, proposed general Randić index and defined it as:

$$R_{\alpha}(G) = \sum_{uv \in E(G)} [deg_G(u) deg_G(v)]^{\alpha}, \text{ where } \alpha \text{ is a variable parameter.}$$

Its mathematical properties and generalizations have been studied extensively, that are available in summarized form in the books [14,20]. A number of variants of Randić connectivity index have been proposed in the mathematical literature. The sum-connectivity index is one of the popular variants. It was introduced by Zhou, B. and Trinajstić, N. in 2008 [4], [32] and [33]. They defined it as:

$$\mathcal{X}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg_G(u) + deg_G(v)}}.$$

The general sum-connectivity index was defined as:

$$\mathcal{X}_{\alpha}(G) = \sum_{uv \in E(G)} [deg_G(u) + deg_G(v)]^{\alpha}, \text{ where } \alpha \text{ is a variable parameter.}$$

Another degree based topological index, known as harmonic index, denoted by $H(G)$ is defined as:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{deg_G(u) + deg_G(v)}.$$

In the whole paper, G is a simple, finite and connected graph. The *order* of $G = |V(G)|$, where $V(G)$ denotes set of vertices of G and *size* of $G = |E(G)|$, where $E(G)$ denotes the set of edges of G . An edge $e \in E(G)$ is denoted by uv , where u, v are end vertices of e . Two vertices are called *adjacent* if they have an edge between them. The set consisting of all vertices adjacent to a specific vertex u is known as *neighborhood* of u that is notified as, $N_G(u)$. The *degree* of u in G , is $deg_G(u) = |N_G(u)|$. The distance between u and the vertex farthest from u in G is called the *eccentricity* of u , denoted by $ecc_G(u)$. Radius of G is defined as the minimum eccentricity among the vertices of G and is denoted by $rad(G)$. The maximum eccentricity is known as its *diameter* and is denoted as $diam(G)$. We use the notations from books [9], [10].

Let G and H be simple, finite and connected graphs. The tensor product, $G \times H$ of graphs G and H is the graph having $V(G) \times V(H)$ as its set of vertices, two vertices (x, y) and (u, v) are adjacent in $G \times H$ if and only if $xu \in E(G)$ and $yv \in E(H)$. The tensor product of P_4 and P_5 is illustrated in Figure ??.

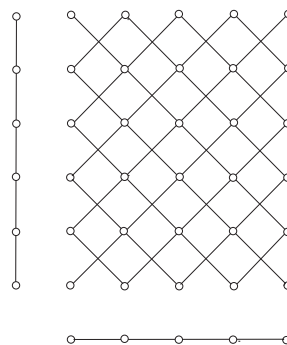


Figure 1: The tensor product $P_4 \times P_5$

The tensor product, as an operation on binary relations was introduced by Alfred North Whitehead and Bertrand Russell in 1912. The tensor product is also known as the direct, categorical, cardinal, relational, Kronecker, weak direct product or conjunction. It is equivalent to the Kronecker product of the adjacency matrices of the graphs [15].

The importance of degree based topological indices can not be denied because they play a significant role in theoretical chemistry and chemical graph theory. For detailed study and outstanding results on important degree-based, connectivity topological indices of various significant graphs and products we recommend to consult [7], [11], [16] and [17]. Some explicit computing formulas for the Randić, sum-connectivity and second sum-connectivity indices of some significant graphs can be studied from [12,25]. Here we discuss some results from [2] which are related to our work.

Theorem 1. [2] Let G and H be graphs of order n_1 and n_2 and size m_1 and m_2 , respectively. Then lower bound for harmonic index of strong product of G and H is:

$$\frac{n_1 m_2 + n_2 m_1 + m_1 m_2}{[n_1 - \text{diam}(G)] + [n_2 - \text{diam}(H)] + [n_1 - \text{diam}(G)][n_2 - \text{diam}(H)]}$$

Theorem 2. [2] Let G and H be graphs of order n_1 and n_2 and size m_1 and m_2 , respectively. Then lower bound for sum-connectivity index of strong product of G and H is:

$$\frac{n_1 m_2 + n_2 m_1 + m_1 m_2}{\sqrt{2} \sqrt{[n_1 - \text{diam}(G)] + [n_2 - \text{diam}(H)] + [n_1 - \text{diam}(G)][n_2 - \text{diam}(H)]}}$$

Now we state the distinct properties of tensor product of graphs in form of the following lemma.

Lemma 1. Let G and H be graphs of order n_1 and n_2 and size m_1 and m_2 , respectively. Then we have:

- (a) $|V(G \times H)| = |V(G)| |E(H)|$ and $|E(G \times H)| = 2|E(G)| |E(H)|$
- (b) $\deg_{G \times H}(u, v) = \deg_G(u) \deg_H(v)$
- (c) The tensor product is commutative and associative.
- (d) The tensor product of connected nontrivial graphs is connected if and only if at least one of the factor graphs is non-bipartite.

The calculation of topological indices from the product of graphs is complicated. So, it is very beneficial and time saving to find out the formulas for product of graphs, in form of their factor graphs. For this purpose, we presented lower bounds for Randić, sum-connectivity and harmonic indices for an important product, called tensor product of graphs in form of its factor graphs. We also presented lower and upper bounds for general Randić and general sum-connectivity indices for the said product in its factor graphs.

2. Main Results and Discussions

In the present section, we determine bounds for Randić (connectivity), general Randić (general connectivity), sum-connectivity, general sum-connectivity and harmonic indices of tensor product of connected graphs in terms of their factor graphs.

In the next theorem we compute the upper and lower bounds for the general Randić (general connectivity) index of tensor product of connected graphs.

Theorem 3. Let G and H be connected graphs of order n_1 and n_2 and size m_1 and m_2 , respectively. Then we have,

- (a) For $\alpha < 0$, $R_\alpha(G \times H) \geq 2m_1 m_2 [n_1 - \text{rad}(G)]^{2\alpha} [n_2 - \text{rad}(H)]^{2\alpha}$
- (b) For $\alpha > 0$, $R_\alpha(G \times H) \leq 2m_1 m_2 [n_1 - \text{rad}(G)]^{2\alpha} [n_2 - \text{rad}(H)]^{2\alpha}$
- (c) For $\alpha = 0$, $\chi_\alpha(G \times H) = 2m_1 m_2$.

Proof. (a) Let G and H be the graphs with vertex sets $\{u_1, u_2, \dots, u_{n_1}\}$ and $\{v_1, v_2, \dots, v_{n_2}\}$ respectively. Then by definition,

$$\begin{aligned}
R_\alpha(G \times H) &= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H)} [deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l)]^\alpha \\
R_\alpha(G \times H) &= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} [deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l)]^\alpha
\end{aligned} \quad (1)$$

By using Lemma 1 and part (b), we get

$$deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l) = deg_G(u_i) deg_H(v_j) deg_G(u_k) deg_H(v_l).$$

Since, for a graph G with n vertices, for all $u \in V(G)$

$$deg_G(u) \leq n - ecc_G(u) \text{ and } rad(G) \leq ecc(G).$$

Therefore, using these facts, we have

$$deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l) \leq [n_1 - rad(G)] \cdot [n_2 - rad(H)] \cdot [n_1 - rad(G)] \cdot [n_2 - rad(H)].$$

Which implies the inequality,

$$deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l) \leq [n_1 - rad(G)]^2 \cdot [n_2 - rad(H)]^2. \quad (2)$$

By using inequality (2) in equation (1), we have

$$\begin{aligned}
R_\alpha(G \times H) &= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} [deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l)]^\alpha \\
&= \sum_{u_i u_k \in E(G)} \sum_{v_j v_l \in E(H)} [deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l)]^\alpha \\
&\geq 2m_1 m_2 [n_1 - rad(G)]^{2\alpha} [n_2 - rad(H)]^{2\alpha}, \text{ since } \alpha < 0. \\
R_\alpha(G \times H) &\geq 2m_1 m_2 [n_1 - rad(G)]^{2\alpha} [n_2 - rad(H)]^{2\alpha}, \text{ for } \alpha < 0.
\end{aligned} \quad (3)$$

Which is required inequality.

(b) To prove the inequality given in part (b), we use inequality (2) and equation (1),

$$\begin{aligned}
R_\alpha(G \times H) &= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} [deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l)]^\alpha \\
&= \sum_{u_i u_k \in E(G)} \sum_{v_j v_l \in E(H)} [deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l)]^\alpha \\
&\leq 2m_1 m_2 [n_1 - rad(G)]^{2\alpha} [n_2 - rad(H)]^{2\alpha}, \text{ since } \alpha > 0. \\
R_\alpha(G \times H) &\leq 2m_1 m_2 [n_1 - rad(G)]^{2\alpha} [n_2 - rad(H)]^{2\alpha}, \text{ for } \alpha > 0.
\end{aligned} \quad (4)$$

which is the required inequality.

$$(c) \text{ Now, } R_\alpha(G \times H) = \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} [deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l)]^\alpha$$

$$= \sum_{u_i u_k \in E(G)} \sum_{v_j v_l \in E(H)} [deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l)]^\alpha$$

putting $\alpha = 0$, $R_\alpha(G \times H) = 2m_1 m_2$, which completes the proof. \square

The following theorem shows the lower bound for the Randić (connectivity) index of tensor product of connected graphs.

Theorem 4. Let G and H be connected graphs of order n_1 and n_2 and size m_1 and m_2 , respectively. Then we have

$$R(G \times H) \geq \frac{2m_1 m_2}{[n_1 - rad(G)][n_2 - rad(H)]}.$$

Proof. Let G and H be the graphs with vertex sets $\{u_1, u_2, \dots, u_{n_1}\}$ and $\{v_1, v_2, \dots, v_{n_2}\}$ respectively. Then by definition,

$$R(G \times H) = \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H)} \frac{1}{\sqrt{deg_{G \times H}(u_i, v_j) deg_{G \times H}(u_k, v_l)}}$$

$$\begin{aligned}
&= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} \frac{1}{\sqrt{\deg_{G \times H}(u_i, v_j) \deg_{G \times H}(u_k, v_l)}} \\
R(G \times H) &= \sum_{u_i u_k \in E(G)} \sum_{v_j v_l \in E(H)} \frac{1}{\sqrt{\deg_{G \times H}(u_i, v_j) \deg_{G \times H}(u_k, v_l)}} \quad (5)
\end{aligned}$$

Now we use inequality (2) in equation (5) as under,

$$R(G \times H) \geq \frac{2m_1 m_2}{\sqrt{[n_1 - \text{rad}(G)]^2 [n_2 - \text{rad}(H)]^2}}$$

Which leads us to the required result,

$$R(G \times H) \geq \frac{2m_1 m_2}{[n_1 - \text{rad}(G)][n_2 - \text{rad}(H)]}. \quad (6)$$

□

In the following theorem, we compute the lower and upper bounds for the general sum-connectivity index of tensor product of connected graphs.

Theorem 5. Let G and H be graphs of order n_1 and n_2 and size m_1 and m_2 , respectively. Then we have:

- (a) For $\alpha < 0$, $\mathcal{X}_\alpha(G \times H) \geq 2^{\alpha+1} m_1 m_2 (n_1 - \text{rad}(G))^\alpha (n_2 - \text{rad}(H))^\alpha$
- (b) For $\alpha > 0$, $\mathcal{X}_\alpha(G \times H) \leq 2^{\alpha+1} m_1 m_2 (n_1 - \text{rad}(G))^\alpha (n_2 - \text{rad}(H))^\alpha$
- (c) For $\alpha = 0$, $\mathcal{X}_\alpha(G \times H) = 2m_1 m_2$.

Proof. (a) Let G and H be the graphs with vertex sets $\{u_1, u_2, \dots, u_{n_1}\}$ and $\{v_1, v_2, \dots, v_{n_2}\}$ respectively. Then by definition,

$$\begin{aligned}
\mathcal{X}_\alpha(G \times H) &= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H)} [\deg_{G \times H}(u_i, v_j) + \deg_{G \times H}(u_k, v_l)]^\alpha \\
\mathcal{X}_\alpha(G \times H) &= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} [\deg_{G \times H}(u_i, v_j) + \deg_{G \times H}(u_k, v_l)]^\alpha \quad (7)
\end{aligned}$$

By using part (b) of Lemma. 1, we get

$$\deg_{G \times H}(u_i, v_j) + \deg_{G \times H}(u_k, v_l) = \deg_G(u_i) \deg_H(v_j) + \deg_G(u_k) \deg_H(v_l).$$

Since, for a graph G with n vertices, for all $u \in V(G)$

$$\deg_G(u) \leq n - \text{ecc}_G(u), \text{diam}(G) \geq \text{ecc}(G) \text{ and } \text{rad}(G) \leq \text{ecc}(G).$$

Therefore,

$$\deg_{G \times H}(u_i, v_j) + \deg_{G \times H}(u_k, v_l) \leq [n_1 - \text{rad}(G)][n_2 - \text{rad}(H)] + [n_1 - \text{rad}(G)][n_2 - \text{rad}(H)].$$

Which implies the inequality,

$$\deg_{G \times H}(u_i, v_j) + \deg_{G \times H}(u_k, v_l) \leq 2[n_1 - \text{rad}(G)][n_2 - \text{rad}(H)]. \quad (8)$$

By using inequality (8) in equation (7), we have

$$\begin{aligned}
\mathcal{X}_\alpha(G \times H) &= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} [\deg_{G \times H}(u_i, v_j) + \deg_{G \times H}(u_k, v_l)]^\alpha \\
&= \sum_{u_i u_k \in E(G)} \sum_{v_j v_l \in E(H)} [\deg_{G \times H}(u_i, v_j) + \deg_{G \times H}(u_k, v_l)]^\alpha \\
&\geq 2m_1 m_2 2^\alpha [n_1 - \text{rad}(G)]^\alpha [n_2 - \text{rad}(H)]^\alpha, \text{ since } \alpha < 0.
\end{aligned}$$

$$\mathcal{X}_\alpha(G \times H) \geq 2^{1+\alpha} m_1 m_2 [n_1 - \text{rad}(G)]^\alpha [n_2 - \text{rad}(H)]^\alpha, \text{ for } \alpha < 0. \quad (9)$$

Hence proof of part (a) is completed.

(b) To prove the inequality given in part (b), we use inequality (8) and equation (7) and get

$$\mathcal{X}_\alpha(G \times H) = \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} [\deg_{G \times H}(u_i, v_j) + \deg_{G \times H}(u_k, v_l)]^\alpha$$

$$\begin{aligned}
&= \sum_{u_i u_k \in E(G)} \sum_{v_j u_l \in E(H)} [deg_{G \times H}(u_i, v_j) + deg_{G \times H}(u_k, v_l)]^\alpha \\
&\leq 2m_1 m_2 2^\alpha [n_1 - rad(G)]^\alpha [n_2 - rad(H)]^\alpha, \text{ since } \alpha > 0.
\end{aligned}$$

$$\mathcal{X}_\alpha(G \times H) \leq 2^{1+\alpha} m_1 m_2 [n_1 - rad(G)]^\alpha [n_2 - rad(H)]^\alpha, \text{ for } \alpha > 0. \quad (10)$$

Hence proof of part (b) is completed.

$$\begin{aligned}
(c) \text{ Now, } \mathcal{X}_\alpha(G \times H) &= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} [deg_{G \times H}(u_i, v_j) + deg_{G \times H}(u_k, v_l)]^\alpha \\
&= \sum_{u_i u_k \in E(G)} \sum_{v_j u_l \in E(H)} [deg_{G \times H}(u_i, v_j) + deg_{G \times H}(u_k, v_l)]^\alpha \\
&\text{putting } \alpha = 0, \mathcal{X}_\alpha(G \times H) = 2m_1 m_2, \text{ completes the proof. } \square
\end{aligned}$$

In the following theorem, we compute the lower bound for the general connectivity index of tensor product of graphs.

Theorem 6. Let G and H be graphs of order n_1 and n_2 and size m_1 and m_2 , respectively. Then we have

$$\mathcal{X}(G \times H) \geq \frac{\sqrt{2m_1 m_2}}{\sqrt{[n_1 - rad(G)][n_2 - rad(H)]}}$$

Proof. Let G and H be the graphs with vertex sets $\{u_1, u_2, \dots, u_{n_1}\}$ and $\{v_1, v_2, \dots, v_{n_2}\}$ respectively.

$$\begin{aligned}
\mathcal{X}(G \times H) &= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H)} \frac{1}{\sqrt{deg_{G \times H}(u_i, v_j) + deg_{G \times H}(u_k, v_l)}} \\
&= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} \frac{1}{\sqrt{deg_{G \times H}(u_i, v_j) + deg_{G \times H}(u_k, v_l)}} \\
\mathcal{X}(G \times H) &= \sum_{u_i u_k \in E(G)} \sum_{v_j u_l \in E(H)} \frac{1}{\sqrt{deg_{G \times H}(u_i, v_j) + deg_{G \times H}(u_k, v_l)}} \quad (11)
\end{aligned}$$

By using inequality (8) in equation (11), we have

$$\mathcal{X}(G \times H) \geq \frac{2m_1 m_2}{\sqrt{2[n_1 - rad(G)][n_2 - rad(H)]}}$$

Which leads us to the required result,

$$\mathcal{X}(G \times H) \geq \frac{\sqrt{2m_1 m_2}}{\sqrt{[n_1 - rad(G)][n_2 - rad(H)]}}. \quad (12)$$

□

In the following theorem, we compute the lower bound for the harmonic index of tensor product of graphs.

Theorem 7. Let G and H be graphs of order n_1 and n_2 and size m_1 and m_2 , respectively. Then we have

$$H(G \times H) \geq \frac{2m_1 m_2}{[n_1 - rad(G)][n_2 - rad(H)]}$$

Proof. Let G and H be the graphs with vertex sets $\{u_1, u_2, \dots, u_{n_1}\}$ and $\{v_1, v_2, \dots, v_{n_2}\}$ respectively.

$$\begin{aligned}
H(G \times H) &= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H)} \frac{2}{d_{G \times H}(u_i, v_j) + d_{G \times H}(u_k, v_l)} \\
&= \sum_{(u_i, v_j)(u_k, v_l) \in E(G \times H), i \neq k, j \neq l} \frac{2}{d_{G \times H}(u_i, v_j) + d_{G \times H}(u_k, v_l)} \\
H(G \times H) &= \sum_{u_i u_k \in E(G)} \sum_{v_j u_l \in E(H)} \frac{2}{d_{G \times H}(u_i, v_j) + d_{G \times H}(u_k, v_l)} \quad (13)
\end{aligned}$$

By using inequality (8) in equation (13), we have

$H(G \times H) \geq \frac{2 \times 2m_1m_2}{2[n_1 - rad(G)][n_2 - rad(H)]}$
Which leads us to the required result,

$$H(G \times H) \geq \frac{2m_1m_2}{[n_1 - rad(G)][n_2 - rad(H)]}. \quad (14)$$

□

3. Conclusions

In this paper, we conducted the study of product-connectivity, sum-connectivity and harmonic indices of tensor product of graphs. We presented the exact formulas for lower and upper bounds of Randić, general Randić, sum-connectivity, general sum-connectivity and harmonic indices of tensor product of connected graphs in form of its factor graphs, for the first time. Some other products and topological indices can be considered for future study.

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