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Investigation of Lower and Upper Bounds of a Jump Graph Using Topological Indices

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

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Short Research Article

Abstract

Topological indices are a type of mathematical measure that relate to the atomic composition of any straight forward finite graph. For quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) analyses [1]. The main aim of this paper is to find new bounds of a jump graph using some topological indices like Hyper Zagreb index, Nirmala Index, VL Index and Forgotten topological index. The Topological indices are mathematical techniques used to mathematically correlate the relationship between the chemical structure and various physical attributes, chemical reactivity, or biological activity.

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1 Introduction

A mathematical method termed a topological graph index, also known as a molecular descriptor, can be used to analyse any graph that represents a molecular structure. This index can be used to assess numerical numbers and further look into various physicochemical aspects of a molecule. As a result, it is a good way to eliminate time-consuming and expensive laboratory studies. In particular, in studies of quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR), molecular descriptors play a crucial role in mathematical chemistry. Topological descriptors are a type of molecular descriptor. Numerous topological indices are used nowadays, some of which are in chemistry. They can be categorised based on the structural characteristics of the graphs that were used to calculate them. Here we will discuss some topological indices Let G be a simple graph connected with vertex set V(G) and edge set E(G). Clearly, the number of vertices and the number of edges are the two fundamental parameters in topological indices. Numerous topological indices have been developed and used in recent years for a variety of purposes, including chemical documentation, isomer discrimination, molecular complexity research. In any graph, the number of edges with u as an end vertex is called degree of u and is denoted by $deg_G(u)$ the minimum and maximum degrees of graph are represented as δ_G and Δ_G respectively.

2 Materials and Methods

Many scholars have found bounds for many topological indices[2]. The J-vertex corona product of the graph is a new class of operator graph that will now be defined[3][4]

Hyper Zagreb Index:

In 2013, Shirdel et al introduced distance based Zagreb indices named Hyper zagreb index as[5][6][7]

$$HZ(G) = \sum_{i,j \in E(G)} (d_i + d_j)^2$$

Nirmala Index:

Inspired by the work of Sombor indices, V R Kulli introduces the Nirmala index of a graph G as[8]

$$N(G) = \sum_{i,j \in E(G)} (\sqrt{d_i + d_j})$$

VL Index:

By the work of Zagreb index, Deepika T introduced the VL index of a graph and is defined as[9][10]

$$VL(G) = \frac{1}{2} \sum_{i,j \in E(G)} [d_i + d_j + d_i \cdot d_j]$$

Forgotten Topological index:

Furtula and Gutman introduced Forgotten topological index and established its some properties . This index is defined as [11][12][13]

$$F(G) = \sum_{i,j \in E(G)} [d_i^2 + d_j^2]$$

Definition 2.1. The Jump Graph J(G) of a graph G is the graph defined on E(G) where two vertices are adjacent if and only if their corresponding edges are not adjacent in G[14][15].

Definition 2.2 The corona product of G and H of two graphs are obtained by taking one copy of G and n_1 copies of H and by joining each vertex of the i^{th} copy of H to the i^{th} vertex of G, where $1 \le i \le n_1$.[16][3]

Definition 2.3: The corona product of a Jump graph is obtained from one copy of J(G) λ_1 copies of H and joining a vertex V[J(G)], that is, one of the i^{th} position in J(G) to every vertex in the i^{th} copy of H.[17][18]

3 Properties of Jump Graph

The graph has

 $(i).\lambda_1 + \lambda_1\eta_2$ vertices

$$\begin{array}{ll} (ii).\lambda_1(\lambda_2+\eta_2)+\frac{\lambda_1(\lambda_1-1)}{2}-\sum_{i,j\in E(G)}\frac{[\deg(i)+\deg(j)-2]}{2} & edges\\ (iii).The\ degree\ of\ a\ vertex,\ \ \mathbf{v}\in v(G)\ \text{is\ given\ by} \end{array}$$

$$deg_G(i) = deg_H(i) + 1$$
, if $i \in V(H)$
 $deg_{J(G)}(i) + \eta_2$, if $i \in V[J(G)]$

4 Preliminary Results

Theorem 1: Let G and H be two simple connected graphs, then the bounds for the hyper Zagreb index of jump graph given by

$$HZ(G) \ge 4\lambda_1\lambda_2(\Delta+1)^2 + [\Delta_H - 2\Delta_G + 2 + \lambda_1 + \eta_2]^2 +$$

$$\left[\frac{\lambda_{1}(\lambda_{1}-1)}{2} - \lambda_{1}(\Delta_{G}-1)\right]\left[2\lambda_{1} - 4\Delta_{G} - 2 + 2\eta_{2}\right]^{2}$$

and

$$HZ(G) \le 4\lambda_1\lambda_2(\delta+1)^2 + [\delta_H - 2\delta_G + 2 + \lambda_1 + \eta_2]^2 +$$

$$\left[\frac{\lambda_1(\lambda_1 - 1)}{2} - \lambda_1(\delta_G - 1)\right] \left[2\lambda_1 - 4\delta_G - 2 + 2\eta_2\right]^2$$

Proof:

$$HZ(G) = \lambda_1 \sum_{i,j \in E(G)} [(deg_H(i) + 1) + (deg_H(j) + 1)]^2 +$$

$$\sum_{e \in V(J(G))} \sum_{i \in V(H)} \left[\left(deg_H(i) + 1 \right) + \left(deg_{J(G)}(e) + \eta_2 \right) \right]^2$$

$$+ \sum_{e,t \in E(J(G))} \left[(deg_{J(G)}(e) + \eta_2) + (deg_{J(G)}(t) + \eta_2) \right]^2$$

$$= \lambda_1 \lambda_2 [(deg_H(i) + 1) + (deg_H(j) + 1)]^2 + \lambda_1 \eta_2 [(deg_H(i) + 1) + (deg_{J(G)}(e) + \eta_2)]^2 +$$

$$[(\frac{\lambda_1(\lambda_1-1)}{2})-\lambda_1[\frac{deg_G(i)+deg_{J(G)}-2}{2}]][(deg_{J(G)(e)}+\eta_2)+(deg_{J(G)}(t)+\eta_2)]^2$$

$$\begin{split} &=\lambda_1\lambda_2[deg_H(i)+(deg_H(j)+2]^2+\lambda_1\eta_2[(deg_H(i)+1)+[(\lambda_1-1)-(deg_G(i)+deg_G(j)-2)+\eta_2]^2+\\ &\qquad \qquad [\frac{(\lambda_1(\lambda_1-1)}{2})-\lambda_1[\frac{deg_G(i)+deg_G(j)-2}{2}]]\\ &\qquad \qquad [[(\lambda_1-1)-(deg_G(i)+deg_G(j)-2)+\eta_2]+[(\lambda_1-1)-deg_G(i)+deg_G(j)-2)+\eta_2]]^2\\ &\qquad \qquad \geq \lambda_1\lambda_2[\Delta_H+_H+2]^2+\lambda_1\eta_2[(\Delta_H+1)+[(\lambda_1-1)-(\Delta_G+\Delta_G-2)+\eta_2]+\\ &\qquad \qquad [(\frac{\lambda_1(\lambda_1-1)}{2})-\lambda_1(\frac{(\Delta_G+\Delta_G-2)}{2})][[(\lambda_1-1)-(\Delta_G+\Delta_G-2)+\eta_2]+[(\lambda_1-1)-(\Delta_G+\Delta_G-2)+\eta_2]]^2\\ &\qquad \qquad \geq \lambda_1\lambda_24(\Delta_H+1)^2+[\Delta_H-2\Delta_G+2+\lambda_1+\eta_2]^2+\\ &\qquad \qquad [[\frac{\lambda_1(\lambda_1-1)}{2}]-\lambda_1(\Delta_G-1)][\lambda_1-2\Delta_G-3+\eta_2]+[\lambda_1-2\Delta_G+1+\eta_2]]^2\\ &\leq \lambda_1\lambda_24(\delta_H+1)^2+[\delta_H-2\delta_G+2+\lambda_1+\eta_2]^2+\\ &\qquad \qquad [\frac{\lambda_1(\lambda_1-1)}{2}]-\lambda_1(\delta_G-1)][\lambda_1-2\delta_G-3+\eta_2]+[\lambda_1-2\delta_G+1+\eta_2]]^2 \end{split}$$

Theorem 2: Let G and H be two simple connected graphs, then the bounds for the Nirmala index of a Jump graph is given by

$$N(G) \ge \sqrt{2\lambda_1\lambda_2(\Delta_H + 1)} + \lambda_1\lambda_2\sqrt{\Delta_H - 2\Delta_G + \lambda_1 + 2 + \eta_2} +$$

 $\left[\left[\frac{\lambda_1(\lambda_1-1)}{2}\right] - \lambda_1(\Delta_G-1)\right]\sqrt{2}\sqrt{\lambda_1-2\Delta_G+1+\eta_2}$

and

$$N(G) \le \sqrt{2\lambda_1\lambda_2(\delta_H + 1)} + \lambda_1\lambda_2\sqrt{\delta_H - 2\delta_G + \lambda_1 + 2 + \eta_2} +$$

$$[[\frac{\lambda_1(\lambda_1-1)}{2}] - \lambda_1(\delta_G-1)]\sqrt{2}\sqrt{\lambda_1-2\delta_G+1+\eta_2}$$

proof:

$$N(G) = \sum_{i,j \in E(G)} \sqrt{d_i + d_j}$$

$$N(G) = \lambda_1 \sum_{i,j \in E(G)} \sqrt{[(deg_H(i) + 1) + (deg_H(j) + 1)]} + \frac{1}{2} \frac{1}{2$$

Theorem 3: Let G and H be two simple connected graphs, then the bounds for VL index is given by

$$VL(G) \ge \frac{1}{2} [[\lambda_1 \lambda_2 (4\Delta_H + \Delta_H^2 + 3) + \lambda_1 \eta_2 (\lambda_1 - \Delta_H + \eta_2 + 2) +$$

$$(\Delta_H + 1)[\lambda_1 - 2\Delta_H + 1 + \eta_2] + [[\frac{\lambda_1(\lambda_1 - 1)}{2}] - \lambda_1(\Delta_G - 1)][2\lambda_1 - 4\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_H + 1 + \eta_2] + [(\Delta_G + 1)(\Delta_G - 1)][2\lambda_1 - 2\Delta_H + 1 + \eta_2] + [(\Delta_G + 1)(\Delta_G - 1)][2\lambda_1 - 2\Delta_H + 1 + \eta_2] + [(\Delta_G + 1)(\Delta_G - 1)][2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 1)[2\lambda_1 - 2\Delta_G + 2\eta_2 + 2] + (\Delta_G + 2\eta_2 + 2\eta_2$$

$$[(\lambda_1 - 1)^2 - 4(\lambda_1 - 1)(\Delta_G - 1) + 4(\Delta_G - 1)^2 + 2\eta_2(\lambda_1 - 1) - 2\eta_2(\Delta_G - 1) + \eta_2^2]]$$

$$VL(G) \le \frac{1}{2}[\lambda_1\lambda_2(4\delta_H + \delta_H^2 + 3) + \lambda_1\eta_2(\lambda_1 - \delta_H + \eta_2 + 2) +$$

and

$$\begin{split} (\delta_H+1)[\lambda_1-2\delta_H+1+\eta_2]+&[[\frac{\lambda_1(\lambda_1-1)}{2}]-\lambda_1(\delta_G-1)][2\lambda_1-4\delta_G+2\eta_2+2]+\\ &[[(\lambda_1-1)^2-4(\lambda_1-1)(\delta_G-1)+4(\delta_G-1)^2+2\eta_2(\lambda_1-1)-2\eta_2(\delta_G-1)+\eta_2^2]] \end{split}$$
 Proof:
$$VL(G)=\frac{1}{2}\sum_{i,j\in E(G)}[d_i+d_j+d_i*d_j]\\ &=\frac{1}{2}[\lambda_1\sum_{i,j\in E(H)}[deg_H(i)+1+(deg_H(j)+1)+(deg_H(j)+1)+(deg_H(i)+1)*(deg_H(i)+1)+(deg_$$

$$= \frac{1}{2} [\lambda_1 \lambda_2 [4\Delta_H + \Delta_H^2 + 3] + \lambda_1 \eta_2 [(\Delta_H + 1)((\lambda_1 - 1) - 2\Delta_H + 2) + \eta_2] +$$

$$[[\frac{\lambda_1 (\lambda_1 - 1)}{2}] - \lambda_1 (\Delta_G - 1)] [(\lambda_1 - 1) - (2\Delta_G - 2) + \eta_2] + [(\lambda_1 - 1) - 2\Delta_G + 2 + \eta_2] +$$

$$[(\lambda_1 - 1) - 2(\Delta_G - 1) + \eta_2)((\lambda_1 - 1) - 2(\Delta_G - 1) + \eta_2)]$$

$$\geq \frac{1}{2} [\lambda_1 \lambda_2 [4\Delta_H + \Delta_H^2 + 3] + \lambda_1 \eta_2 (\lambda_1 - \Delta_H + \eta_2) + [(\Delta_H + 1)(\lambda_1 - 2\Delta_H + 1) + \eta_2] +$$

$$[[\frac{\lambda_1 (\lambda_1 - 1)}{2}] - \lambda_1 (\Delta_G - 1)] [2\lambda_1 - 4\Delta_G + 2\eta_2 + 2] +$$

$$[(\lambda_1 - 1)^2 - 4(\lambda_1 - 1)(\Delta_G - 1) + 4(\Delta_G - 1)^2 + 2\eta_2 (\lambda_1 - 1) - 2\eta_2 (\Delta_G - 1) + \eta_2^2]]$$

$$\leq \frac{1}{2} [\lambda_1 \lambda_2 [4\delta_H + \delta_H^2 + 3] + \lambda_1 \eta_2 (\lambda_1 - \delta_H + \eta_2) + [(\delta_H + 1)(\lambda_1 - 2\delta_H + 1) + \eta_2] +$$

$$[[\frac{\lambda_1 (\lambda_1 - 1)}{2}] - \lambda_1 (\delta_G - 1)] [2\lambda_1 - 4\delta_G + 2\eta_2 + 2] +$$

$$[(\lambda_1 - 1)^2 - 4(\lambda_1 - 1)(\delta_G - 1) + 4(\delta_G - 1)^2 + 2\eta_2(\lambda_1 - 1) - 2\eta_2(\delta_G - 1) + \eta_2^2]]$$

Theorem 4: Let G and H be two simple connected graphs the bounds for the forgotten index of a Jump graph is given by [11], [12]

$$F(G) \ge 2\lambda_1\lambda_2(\Delta_H + 1)^2 + \lambda_1\eta_2[\Delta_H^2 + 2\Delta_H - 2\Delta_G + 3\lambda_1 + \eta_2]^2 +$$

$$\left[\left[\frac{\lambda_{1}(\lambda_{1}-1)}{2}\right] - \lambda_{1}(\Delta_{G}-1)\right]\left[\lambda_{1}-2\Delta_{G}+\eta_{2}+1\right]^{2} + \left[\lambda_{1}-2\Delta_{G}+\eta_{2}+1\right]^{2}$$

and

$$F(G) \le 2\lambda_1\lambda_2(\delta_H + 1)^2 + \lambda_1\eta_2[\delta_H^2 + 2\delta_H - 2\delta_G + 3\lambda_1 + \eta_2]^2 +$$

$$[[\frac{\lambda_{1}(\lambda_{1}-1)}{2}] - \lambda_{1}(\delta_{G}-1)][\lambda_{1}-2\delta_{G}+\eta_{2}+1]^{2} + [\lambda_{1}-2\delta_{G}+\eta_{2}+1]^{2}$$

Proof:

$$F(G) = \sum_{i,j \in E(G)} [d_i^2 + d_j^2]$$

$$\begin{split} F(G) &= \lambda_1 \sum_{i,j \in E(G)} [(\deg_H(i)+1)^2 + (\deg_H(j)+1)^2] + \\ &= \sum_{e,i \in E(G)} [(\deg_H(i)+1)^2 + (\deg_{J(G)}(t)+\eta_2)^2] + \\ &= \sum_{e \in v(i,j)} \sum_{i \in v(G)} [(\deg_H(i)+1)^2 + (\deg_{J(G)}(e)+\eta_2)^2] \\ &= \lambda_1 \lambda_2 [(\deg_H(i)+1)^2 + (\deg_H(j)+1)^2] + \\ &= \lambda_1 \eta_2 [(\deg_H(i)+1)^2 + (\deg_{J(G)}(e)+\eta_2)^2] + \\ &= [\frac{\lambda_1 (\lambda_1-1)}{2}] - \lambda_2 [\frac{\deg_G(i)+\deg_G(j)-2}{2}]][(\deg_{J(G)}(e)+\eta_2)^2 + (\deg_{J(G)}(t)+\eta_2)^2] \\ &= \lambda_1 \lambda_2 [(\deg_G(i)+1)^2 + (\deg_H(j)+1)^2] + \\ &= \lambda_1 \eta_2 [(\deg_H(i)+1)^2 + [(\lambda_1-1)-(\deg_G(i)+\deg_G(j)-2)+\eta_2]^2 + \\ &= [\frac{\lambda_1 (\lambda_1-1)}{2}] - \lambda_1 [\frac{\deg_G(i)+\deg_G(j)-2}{2}]] \\ &= [(\lambda_1-1)-[\deg_G(i)+\deg_G(j)-2]+\eta_2]^2 + [(\lambda_1-1)-[\deg_G(i)+\deg_G(j)-2]+\eta_2]^2 + \\ &= [\frac{\lambda_1 (\lambda_1-1)}{2}] - \lambda_1 [\frac{\Delta_G+\Delta_G-2}{2}]][(\lambda_1-1)-(\Delta_G+\Delta_G-2)+\eta_2]^2 + \\ &= [(\lambda_1-1)-(\Delta_G+\Delta_G-2)+\eta_2]^2 \\ &\geq 2\lambda_1 \lambda_2 (\Delta_H+1)^2 + \lambda_1 \eta_2 [\Delta_H^2 + 2\Delta_H+3\lambda_1-2\Delta_G+\eta_2]^2 + \\ [[\frac{\lambda_1 (\lambda_1-1)}{2}] - \lambda_1 (\Delta_G-1) [\lambda_1-2\Delta_G-1)][\lambda_1-2\Delta_G+\eta_2+1]^2 + [\lambda_1-2\Delta_G+\eta_2+1]^2 \end{split}$$

$$\leq 2\lambda_1\lambda_2(\delta_H + 1)^2 + \lambda_1\eta_2[\delta_H^2 + 2\delta_H + 3\lambda_1 - 2\delta_G + \eta_2]^2 +$$

$$[[\frac{\lambda_1(\lambda_1-1)}{2}] - \lambda_1(\delta_G-1)][\lambda_1-2\delta_G-1)][\lambda_1-2\delta_G+\eta_2+1]^2 + [\lambda_1-2\delta_G+\eta_2+1]^2$$

5 Conclusions

Four topological indices were taken into account to establish the lower and upper boundaries in this article. Researchers can also take into account additional topological indices and calculate their bounds for the graph in a similar manner.

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Competing Interests

Authors have declared that no competing interests exist.

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