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Contra Harmonic Index Of Graphs

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Abstract

Let G be amolecular graph with vertex set V(G) and edge set E(G). We introduce a new topological index namely Contra Harmonic index which is defined as

$$CH(G) = \sum_{uv\in E(G)} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)}$$

where d(u) and d(v) are the degree of the vertices u and v.In this paper, we obtained bounds for contra harmonic index of graphs.

Keywords: *Contra Harmonic index, Contra Harmonic Co-index*

I. INTRODUCTION

Molecular graphs are chemical graphs in which vertices corresponds to individual atoms and edges to chemical bonds between them. Molecular graphs are necessarily connected graphs. A single number that can be used to characterize the graph of a molecule is called a topological index. Such a number is referred to by graph theorists as a graph invariants[8]. The interest in topological indices is in the main related to their use in non-empirical quantitative structure – property relationships (QSPR) and quantitative structure – activity relationships (QSAR).The first and second Zagreb indices $M_1(G)$ and $M_2(G)$ were introduced 30 years ago byGutman and Trinajstic [3]. They are defined as

$$M_1(G) = \sum_{v\epsilon V(G)} d(v)^2$$

$$M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$$

For any real α, the generalisedrandic number $R_\alpha(G)$ is defined in [5]as follows

$$R_\alpha(G) = \sum_{uv\in E(G)} \big(d(u)d(v)\big)^\alpha$$

In 1980, SiemionFajtlowicz introduces harmonic index [6] which are defined as follows

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

The inverse sum indeg index (ISI index) of a graph G is defined in [13] as follows

$$ISI(G) = \sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}$$

In this paper we introduced a topological indices namely Contra Harmonic indexCH(G) is defined as the sum of the term$\frac{d(u)^2+d(v)^2}{d(u)+d(v)}$over all edges uv of graph G.

$$CH(G) = \sum_{uv\in E(G)} \frac{d(u)^2+d(v)^2}{d(u)+d(v)}$$

The Contra Harmonic Co – index is defined as the sum of the term $\frac{d(u)^2+d(v)^2}{d(u)+d(v)}$for every edge not in G.

$$\overline{CH}(G) = \sum_{uv\notin E(G)} \frac{d(u)^2+d(v)^2}{d(u)+d(v)}$$

Theorem 1

Let G be a moleculargraph with n vertices and m edges. Then $CH(G) \geq 2m$.

Proof:

We have $x^2 + y^2 \geq 2(x+y)$, $\forall\, x, y \geq 2$

Put $x = d(u)$ and $y = d(v)$

$$\mathrm{d(u)}^2 + \mathrm{d(v)}^2 \geq 2(\mathrm{d(u)} + \mathrm{d(v)})$$

$$\frac{\mathrm{d(u)}^2 + \mathrm{d(v)}^2}{\mathrm{d(u)} + \mathrm{d(v)}} \geq 2$$

Taking summation over all edges, we get

$$\sum_{uv\in E(G)} \frac{d(u)^2+d(v)^2}{d(u)+d(v)} \geq \sum_{uv\in E(G)} 2 = 2m$$

$$CH(G) \geq 2m$$

Theorem 2

For any molecular graph G, CH(G) ≤ M_1(G)

Proof:

For any non negative integer a and b,we have $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$

Substitute $a = \mathrm{d(u)}^2$ and $b = \mathrm{d(v)}^2$

$$\sqrt{\mathrm{d(u)}^2+\mathrm{d(v)}^2} \le \sqrt{\mathrm{d(u)}^2}+\sqrt{\mathrm{d(v)}^2}$$

$$= \mathrm{d(u)} + \mathrm{d(v)}$$

Squaring on both sides,

$$\mathrm{d(u)}^{\,2}+\mathrm{d(v)}^{\,2} \le (\mathrm{d(u)}+\mathrm{d(v)})^2$$

$$\frac{\mathrm{d(u)}^{\,2}+\mathrm{d(v)}^{\,2}}{\mathrm{d(u)}+\mathrm{d(v)}} \le \mathrm{d(u)} + \mathrm{d(v)}$$

Taking summation for all edges, we have

$$\sum_{uv\in E(G)} \frac{d(u)^2+d(v)^2}{d(u)+d(v)} \le \sum_{uv\in E(G)} \mathrm{d(u)} + \mathrm{d(v)}$$

$$\mathrm{CH(G)} \le M_1(G)$$

Theorem 3

For any molecular graph G, $\mathrm{CH(G)} = M_1(G) - 2\,ISI(G)$

Proof:

$$\begin{aligned}\mathrm{CH(G)} &= \sum_{uv\in E(G)} \frac{d(u)^2+d(v)^2}{d(u)+d(v)}\\ &= \sum_{uv\in E(G)} \frac{[d(u)+d(v)]^2-2d(u)d(v)}{d(u)+d(v)}\\ &= \sum_{uv\in E(G)} [d(u)+d(v)] - 2\sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}\\ &= M_1(G) - 2\,ISI(G)\end{aligned}$$

Note

The arithmetic geometric inequality

Let $x_1, x_2, \dots, x_n$ be positive numbers. Thenwe have $\frac{n}{\frac{1}{x_1}+\frac{1}{x_2}+\cdots+\frac{1}{x_n}} \le \sqrt[n]{x_1 x_2 \dots x_n}$.

Theorem 4

For any molecular graph G, $M_1(G) - R_{\frac{1}{2}}(G) \le CH(G)$.

Proof:

From the above note, for n = 2, put $x_1 = d(u)$and $x_2 = d(v)$, then

$$\frac{2}{\frac{1}{d(u)}+\frac{1}{d(v)}} \leq \sqrt[2]{d(u)d(v)}$$

$$\sqrt[2]{d(u)d(v)} \geq \frac{2d(u)d(v)}{d(u)+d(v)}$$

$$= \frac{[d(u)+d(v)]^2-[d(u)^2+d(v)^2]}{d(u)+d(v)}$$

$$= \frac{[d(u)+d(v)]^2}{d(u)+d(v)} - \frac{d(u)^2+d(v)^2}{d(u)+d(v)}$$

$$= [d(u)+d(v)] - \frac{d(u)^2+d(v)^2}{d(u)+d(v)}$$

Taking summation for all edges

$$\sum_{uv\in E(G)} \sqrt[2]{d(u)d(v)} \geq \sum_{uv\in E(G)} [d(u)+d(v)] - \sum_{uv\in E(G)} \frac{d(u)^2+d(v)^2}{d(u)+d(v)}$$

$$R_{\frac{1}{2}}(G) \geq M_1(G) - CH(G)$$

Theorem 5

For any molecular graph G with n vertices and m edges, the inequality

$$\mathrm{CH}(\bar{G}) \leq (n-1)^2\overline{H}(G) + \overline{CH}(G) - n(n-1)^2 + 2(n-1)m$$

holds if $\mathrm{d(u)} + \mathrm{d(v)} \leq \mathrm{n} - 1$ for every edge not in G.

Proof:

$$\mathrm{CH}(\bar{G}) = \sum_{uv\in E(\bar{G})} \frac{d\left(\frac{u}{\bar{G}}\right)^2 + d\left(\frac{v}{\bar{G}}\right)^2}{d\left(\frac{u}{\bar{G}}\right) + d\left(\frac{v}{\bar{G}}\right)}$$

$$= \sum_{uv\in E(\bar{G})} \frac{[n-1-d\left(\frac{u}{G}\right)]^2 + [n-1-d\left(\frac{v}{G}\right)]^2}{\left[n-1-d\left(\frac{u}{G}\right)\right] + \left[n-1-d\left(\frac{v}{G}\right)\right]}$$

$$= \sum_{uv\in E(\bar{G})} \frac{2(n-1)^2 + d\left(\frac{u}{G}\right)^2 + d\left(\frac{v}{G}\right)^2 - 2(n-1)\left[d\left(\frac{u}{G}\right) + d\left(\frac{v}{G}\right)\right]}{2[n-1] - \left[d\left(\frac{u}{G}\right) + d\left(\frac{v}{G}\right)\right]}$$

$$\leq \sum_{uv\in E(\bar{G})} \frac{2(n-1)^2 + d\left(\frac{u}{G}\right)^2 + d\left(\frac{v}{G}\right)^2 - 2(n-1)\left[d\left(\frac{u}{G}\right) + d\left(\frac{v}{G}\right)\right]}{\left[d\left(\frac{u}{G}\right) + d\left(\frac{v}{G}\right)\right]}$$

$$= \sum_{uv\in E(\bar{G})} \frac{2(n-1)^2}{\left[d\left(\frac{u}{G}\right) + d\left(\frac{v}{G}\right)\right]} + \sum_{uv\in E(\bar{G})} \frac{d\left(\frac{u}{G}\right)^2 + d\left(\frac{v}{G}\right)^2}{\left[d\left(\frac{u}{G}\right) + d\left(\frac{v}{G}\right)\right]} + \sum_{uv\in E(\bar{G})} \frac{-2(n-1)\left[d\left(\frac{u}{G}\right) + d\left(\frac{v}{G}\right)\right]}{\left[d\left(\frac{u}{G}\right) + d\left(\frac{v}{G}\right)\right]}$$

$$= (n-1)^2 \sum_{uv\notin E(G)} \frac{2}{\left[d\left(\frac{u}{G}\right) + d\left(\frac{v}{G}\right)\right]} + \sum_{uv\notin E(G)} \frac{d\left(\frac{u}{G}\right)^2 + d\left(\frac{v}{G}\right)^2}{\left[d\left(\frac{u}{G}\right) + d\left(\frac{v}{G}\right)\right]} - 2(n-1) \sum_{uv\notin E(G)} 1$$

$$= (n-1)^2 \overline{H}(G) + \overline{CH}(G) - 2(n-1)\left[\frac{n(n-1)}{2} - m\right]$$

$$= (n-1)^2 \overline{H}(G) + \overline{CH}(G) - n(n-1)^2 + 2(n-1)m$$

Theorem 6

For any molecular graph G with n vertices and m edges and let p be the number of pendant vertices in graph G, then $\mathrm{CH}(\bar{G}) \leq \left(\frac{1+\Delta^2}{1+\delta^2}\right)p + \frac{\Delta^2}{\delta^2}(m-p)$.

Proof:

$$\begin{aligned}
\mathrm{CH(G)} &= \sum_{uv\in E(G)} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)} \\
&= \sum_{\substack{uv\in E(G)\\ d(u)=1}} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)} + \sum_{\substack{uv\in E(G)\\ d(u),d(v)\neq 1}} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)} \\
&= \sum_{\substack{uv\in E(G)\\ d(u)=1}} \frac{1 + d(v)^2}{1 + d(v)} + \sum_{\substack{uv\in E(G)\\ d(u),d(v)\neq 1}} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)} \\
&\leq \sum_{\substack{uv\in E(G)\\ d(u)=1}} \frac{1 + \Delta^2}{1 + \delta} + \sum_{\substack{uv\in E(G)\\ d(u),d(v)\neq 1}} \frac{\Delta^2 + \Delta^2}{\delta^2 + \delta^2} \\
&= \left(\frac{1 + \Delta^2}{1 + \delta}\right)p + \frac{\Delta^2}{\delta^2}(m-p)
\end{aligned}$$

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In this paper, author introduced a new topological index namely Contra Harmonic Index and obtained some bounds. The further research is going on the topic “Contra Harmonic Index for molecular structure”.

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