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Quadratic-Contraharmonic index of graphs

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A B S T R A C T

Inspired by the definition of Geometric-Arithmetic index of graphs, we defined Quadratic-Contraharmonic index of graphs and investigate its basic mathematical properties.

1 Introduction

Let G be a simple connected graph with n vertices and m edges. d_v is the number of edges incident to the vertex v. A vertex of degree one is said to be a pendent vertex. The graph of order n, in which one vertex has degree $n-1$ and all other vertices are pendent, is the star S_n . The graph of order n,in which all vertices are of degree $n-1$, is the complete graph K_n .We write Δ and δ for the largest and the smallest of all degrees of vertices of G, respectively.
Motivated by Randić index [14], Vukičević and Furtula [1]

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proposed the geometric-arithmetic index as follows;

$$GA(G)=\sum_{uv\in E(G)}\frac{\sqrt{d_ud_v}}{(d_u+d_v)/2}=\sum_{uv\in E(G)}\frac{2\sqrt{d_ud_v}}{d_u+d_v} \tag{1}$$

where summation goes over all edges of graph G, and d_u, d_v are the degrees of vertices u and v that are connected with edge uv. In [1], Vukičević and Furtula gave the lower and upper bounds for the GA index, identified the trees with the minimum and the maximum GA indices, which are the star and the path respectively, and then the path is the unique molecular tree (tree with maximum degree at most four used to model carbon skeletons of acyclic hydrocarbons) with the maximum GA index. After the GA index was defined via Equation (1), other "geometric-arithmetic" indices were defined by to replace in Equation (1) the vertex degrees by some other vertex property. See the references [2–13] for mathematical features and chemical applicability of GA index and these new geometric-arithmetic indices.

Here we are proposing a new index inspired by the definition of geometric-arithmetic index. It is defined as follows:

$$\psi(G)=\sum_{uv\in E(G)}\frac{\sqrt{\left({d_u}^2+{d_v}^2\right)/2}}{\left({d_u}^2+{d_v}^2\right)/(d_u+d_v)}=\sum_{uv\in E(G)}\frac{d_u+d_v}{\sqrt{2\left({d_u}^2+{d_v}^2\right)}}. \tag{2}$$

This index is named as Quadratic-Contraharmonic index ($QC(G)$ or $\psi(G)$) of any graph G because, as it can be seen from the Equation(2), it consists from quadratic mean of end-vertex degrees of an edge uv, ($\sqrt{\left({d_u}^2+{d_v}^2\right)/2}$) as numerator and contraharmonic mean of end-vertex degrees of the edge uv , ($\frac{{d_u}^2+{d_v}^2}{d_u+d_v}$) as denominator.

In this paper we intend to investigate basic mathematical properties of this novel topological index of graphs.

2 Lower and upper bounds of QC index for general graphs and chemical graphs

Now, we will establish exact values of QC index for some well known graphs. By direct calculation we obtain the following proposition.

Proposition 1. *For paths P_n , stars S_n , complete graphs K_n and cycles C_n on $n \geq 3$ vertices holds:*
1.$\psi(P_n) = n - 3 + \frac{3\sqrt{10}}{5}$,
2.$\psi\left(S_n\right) = \frac{n(n-1)}{\sqrt{2n^2-4n+4}}$,
3.$\psi\left(K_n\right) = \frac{n(n-1)}{2}$,
4.$\psi\left(C_n\right) = n$.

And now, we can give lower and upper bounds of QC index for general graphs.

Proposition 2. *Let G be a simple graph with n vertices, then;*

$$0 \leq \psi\left(G\right) \leq \frac{n\left(n-1\right)}{2}.$$

Lower bound is achieved if and only if G is an empty graph and upper bound is achieved if and only if G is a complete graph.

Proof. Note that contribution of each edge is positive. Therefore $\psi\left(G\right) \geq 0$. If G is an empty graph then $\psi\left(G\right) = 0$. Now, let us prove the upper bound. It is well known that quadratic mean is less or equal to contraharmonic mean. Hence,$\psi\left(G\right) \leq 1.m \leq \frac{n(n-1)}{2}$, where m is the number of edges. Moreover, the equality is obtained if and only if G is the complete graph. □

Proposition 3. *Let G be a simple connected graph with n vertices, then;*

$$\frac{n\left(n-1\right)}{\sqrt{2n^2-4n+4}} \leq \psi\left(G\right) \leq \frac{n\left(n-1\right)}{2}.$$

Lower bound is achieved if and only if G is a star and upper bound is achieved if and only if G is a complete graph.

Proof. Assume that $n \geq 2$, because otherwise the claim is trivial. Upper bound follows from Proposition 2. Now, let us prove that for contribution of each edge uv holds:

$$\frac{d_u + d_v}{\sqrt{2\left(d_u{}^2 + d_v{}^2\right)}} \leq \frac{n}{\sqrt{2n^2 - 4n + 4}}.$$

Without loss of generality, we may assume that $d_u \leq d_v$. Denote $x = \frac{d_u}{d_v}$ and note that $\frac{1}{n-1} \leq x \leq 1$. Thus:

$$\frac{d_u + d_v}{\sqrt{2\left(d_u{}^2 + d_v{}^2\right)}} = \frac{x+1}{\sqrt{2\left(x^2+1\right)}}.$$

Simple differential calculation shows that the right hand-side is ascending on the interval $\left[\frac{1}{n-1}, 1\right)$ hence it achieves minimum at $x = \frac{1}{n-1}$. Hence indeed $\frac{d_u+d_v}{\sqrt{2\left(d_u{}^2+d_v{}^2\right)}} \leq \frac{n}{\sqrt{2n^2-4n+4}}$. Since, graph is connected, it has at least $n-1$ edges. Therefore,

$$\psi\left(G\right) \geq \left(n-1\right)\frac{n}{\sqrt{2n^2 - 4n + 4}} = \frac{n\left(n-1\right)}{\sqrt{2n^2 - 4n + 4}}.$$

Moreover, the equality is obtained if and only if graph has $n-1$ edges each connecting vertices of degrees 1 and n. The only such graph is a star. □

Proposition 4. *Let T be tree with $n \geq 3$ vertices, then;*

$$\frac{n\left(n-1\right)}{\sqrt{2n^2 - 4n + 4}} \leq \psi(G) \leq n - 3 + \frac{3\sqrt{10}}{5}$$

Lower bound is achieved if and only if T is a star and upper bound is achieved if and only if T is a path.

Proof. The lower bound follows from Proposition 2. Let us prove the upper bound. Let u be a pendent vertex in T and v its only neighbor. Then;

$$\frac{d_u + d_v}{\sqrt{2\left(d_u{}^2 + d_v{}^2\right)}} = \frac{d_v + 1}{\sqrt{2\left(d_v{}^2 + 1\right)}}.$$

Simple calculation shows that right hand-side is descending on the segment $[1, n-1]$. Hence,

$$\frac{d_u + d_v}{\sqrt{2\left({d_u}^2 + {d_v}^2\right)}} = \frac{d_v + 1}{\sqrt{2\left({d_v}^2 + 1\right)}} \leq \frac{3\sqrt{10}}{10}$$

. Taking into account that contribution of every edge with end-degrees ≥ 2 is at most one, it holds:$\psi\left(T\right) \leq \frac{3\sqrt{10}}{10}.l + \left(n-1-l\right).1,$ where l is the number of leaves in tree T . Since, every tree has at least two leaves, it holds:

$$\psi\left(T\right) \leq \frac{3\sqrt{10}}{10}.l + \left(n-1-l\right).1 \leq \frac{3\sqrt{10}}{5} + \left(n-3\right).$$

Moreover, the equality holds if and only if tree has exactly two edges connecting vertices of degrees 1 and 2; and all other edges connect vertices of the same degree. The only such graph is path. □

3 Conlusion

In this paper we studied Quadratic-Contraharmonic(QC) index index on graphs and trees. Firstly we computed exact values of QC index for some well known graphs. Secondly we established that general simple connected graphs on vertices, maximal graphs with respect to QC index are complete graphs, while minimal graphs are stars. Minimal trees with respect to QC index are stars while maximal tree are paths. There are many open questions for further study. One could try to establish extremal unicyclic graphs, chemical trees and chemical unicyclic graphs with respect to QC index. Deriving exact formulas for the value of QC index on some special kinds of graphs would also be interesting just as studying of how QC index behaves with respect to graph operations.

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