

COMPUTING SOME TOPOLOGICAL INDICES OF NANO STRUCTURES OF BRIDGE GRAPH

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Let $G=(V,E)$ be a graph, where V is a non-empty set of vertices and E is a set of edges. If $x,y \in V(G)$ then the distance $d_G(x,y)$ between x and y is defined as the length of any shortest path in G connecting x and y . In this paper we compute Randić, Zagreb, ABC and geometric arith- metic indices of nano structures of bridge graph

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1. Introduction

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted [1]. Topological indices of nanotubes are numerical descriptors that are derived from graph of chemical compounds. Such indices based on the distances in graph are widely used for establishing relationships between the structure of nanotubes and their physicochemical properties. Usage of topological indices in biology and chemistry began in 1947 when chemist Harold Wiener [2,3,5] introduced Wiener index to demonstrate correlations between physicochemical properties of organic compounds and the index of their molecular graphs.

If $x,y \in V(G)$ then the distance $d_G(x,y)$ between x and y is defined as the length of any shortest path in G connecting x and y . The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [2]. They are defined as $ZG_2(G) = \sum_{uv \in E(G)} d_u d_v$ where d_u and

d_v are the degrees of u and v . The connectivity index introduced in 1975 by Milan Randić [3, 4, 5], who has shown this index to reflect molecular branching. Randić index (Randić molecular

connectivity index) was defined as follows $\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$. Recently Furtula et al. [1]

introduced atom-bond connectivity (ABC) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}}$$

and the geometric arithmetic index of G is defined as $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u) \cdot d(v)}}{d(u) + d(v)}$. Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs with $v_i \in V(G_i)$.

The bridge graph $B(G_1, G_2, \dots, G_d) = B(G_1, G_2, \dots, G_d; v_1, v_2, \dots, v_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is the graph obtained from the graphs G_1, G_2, \dots, G_d by connecting the vertices v_i and v_{i+1} by an edge for all $i = 1, 2, \dots, d - 1$. About this subject in [15,16] computed PI index,

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vertex PI index and Szeged index of bridge graphs, and the main result of this paper is an explicit formula for the geometric arithmetic index of the bridge graph of G_1, G_2, \dots, G_d , (Fig.1). In special case of bridge graphs, we defined $G_d(H, v) = B(H, H, \dots, H; v, v, \dots, v)$.

In this paper we compute Randić, Zagreb, geometric arithmetic and *ABC* indices for bridge graphs.

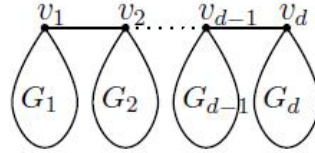


Fig 1: The bridge graph

2. Results and discussion

The aim of this section is to compute some topological indices for an infinite family of nano structures of bridge graphs. We compute this topological indices for three case of bridge graphs. First we consider bridge graphs over path graph, in continue consider bridge graphs over cycle and Complete graph.

Case 1. Let P_n be the path graph on n vertices. For Bridge graph $G_d(P_n, v_1)$ we have dn vertices and $dn-1$ edges and the edge set of graph can be dividing to fore partitions, e. g. $[E_1], [E_2], [E_3]$ and $[E_4]$. For every $e = uv$ belong to $[E_1], du = 3, dv = 2$. Similarly, for every $e = uv$ belong to $[E_2], du = dv = 3$. For every $e = uv$ belong to $[E_3], du = dv = 2$. Finally, if $e = uv$ be an edge of $[E_4]$, then $du = 2$ and $dv = 1$. Then $|E(P_n)| = n-1, |E_1| = d, |E_2| = d-3, |E_3| = d(n-3)+2, |E_4| = d$ and we have

$$M_2(G_d(P_n, v_1)) = \sum_{E_1} 6 + \sum_{E_2} 9 + \sum_{E_3} 4 + \sum_{E_4} 2 = 4dn + 5d - 35$$

$$\begin{aligned} \chi(G_d(P_n, v_1)) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} = \sum_{E_1} \frac{1}{\sqrt{2 \times 3}} + \sum_{E_2} \frac{1}{\sqrt{3 \times 3}} + \sum_{E_3} \frac{1}{\sqrt{2 \times 2}} + \sum_{E_4} \frac{1}{\sqrt{2 \times 1}} \\ &= \frac{d}{\sqrt{6}} + \frac{d-3}{3} + \frac{d(n-3)}{2} + \frac{d}{\sqrt{2}} + 1 \end{aligned}$$

$$\begin{aligned} ABC(G_d(P_n, v_1)) &= \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} = \sum_{E_1} \sqrt{\frac{3}{5}} + \sum_{E_2} \sqrt{\frac{7}{6}} + \sum_{E_3} \sqrt{\frac{2}{4}} + \sum_{E_4} \sqrt{\frac{1}{3}} \\ &= \sqrt{\frac{3}{5}}d + \sqrt{\frac{7}{6}}(d-3) + \frac{\sqrt{2}}{2}d(n-3) + \frac{\sqrt{3}}{3}d + \sqrt{2} \end{aligned}$$

$$\begin{aligned} GA(G_d(P_n, v_1)) &= \sum_{uv \in E(G)} \frac{2\sqrt{d(u) \cdot d(v)}}{d(u) + d(v)} = \sum_{E_1} \frac{2\sqrt{2 \times 3}}{2+3} + \sum_{E_2} \frac{2\sqrt{3 \times 3}}{3+3} + \sum_{E_3} \frac{2\sqrt{2 \times 2}}{2+2} + \sum_{E_4} \frac{2\sqrt{2 \times 1}}{2+1} \\ &= \frac{2\sqrt{6}}{5}d + d - 3 + d(n-3) + 2 + \frac{2\sqrt{2}}{3}d = nd + \left(\frac{2\sqrt{2}}{3} + \frac{2\sqrt{6}}{5} - 2\right)d - 1 \end{aligned}$$

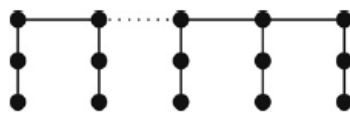


Fig2. The nano structures bridge graph $G_d(P_n, v_1)$

Case 2. Let C_n be the cycle graph on n vertices. For Bridge graph $G_d(C_n, v)$ we have dn vertices and $dn+d-1$ edges and the edge set of graph can be dividing to 5 partitions, e. g. $[E_1], [E_2], [E_3], [E_4]$ and $[E_5]$. For every $e = uv$ belong to $[E_1], du = 2, dv = 2$. Similarly, for every $e = uv$ belong to

$[E_2]$, $du = dv = 4$. For every $e = uv$ belong to $[E_3]$, $du = 3$, $dv = 2$ and for every $e = uv$ belong to $[E_5]$, $du = 3$, $dv = 4$. Finally, if $e = uv$ be an edge of $[E_4]$, then $du = 4$ and $dv = 2$. Then $|E(C_n)| = n$, $|E_1| = d(n-2)$, $|E_2| = d-3$, $|E_3| = 4$, $|E_4| = 2d-4$ and $|E_5| = 2$. Then we have

$$M_2(G_d(C_n, v)) = \sum_{E_1} 4 + \sum_{E_2} 16 + \sum_{E_3} 6 + \sum_{E_4} 8 + \sum_{E_5} 12 = 4dn + 32d - 40$$

$$\begin{aligned} \chi(G_d(C_n, v)) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} = \sum_{E_1} \frac{1}{\sqrt{2 \times 2}} + \sum_{E_2} \frac{1}{\sqrt{4 \times 4}} + \sum_{E_3} \frac{1}{\sqrt{3 \times 2}} + \sum_{E_4} \frac{1}{\sqrt{2 \times 4}} \\ &+ \sum_{E_5} \frac{1}{\sqrt{3 \times 4}} = \frac{1}{2} d(n-2) + \frac{1}{4} (d-3) + \frac{1}{\sqrt{8}} (2d-4) + \frac{4}{\sqrt{6}} + \frac{1}{\sqrt{3}} \end{aligned}$$

$$\begin{aligned} ABC(G_d(C_n, v)) &= \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} = \sum_{E_1} \frac{1}{\sqrt{2}} + \sum_{E_2} \sqrt{\frac{3}{4}} + \sum_{E_3} \sqrt{\frac{3}{5}} + \sum_{E_4} \sqrt{\frac{1}{2}} + \sum_{E_5} \sqrt{\frac{5}{7}} \\ &= \frac{\sqrt{2}}{2} d(n-2) + \sqrt{\frac{3}{4}} (d-3) + 4\sqrt{\frac{3}{5}} + \frac{\sqrt{2}}{2} (2d-4) + 2\sqrt{\frac{5}{7}} \end{aligned}$$

$$\begin{aligned} GA(G_d(C_n, v)) &= \sum_{uv \in E(G)} \frac{2\sqrt{d(u) \cdot d(v)}}{d(u) + d(v)} = \sum_{E_1} 1 + \sum_{E_2} 1 + \sum_{E_3} \frac{2\sqrt{6}}{5} + \sum_{E_4} \frac{2\sqrt{2}}{3} + \sum_{E_5} \frac{4\sqrt{3}}{7} \\ &= dn - d - 3 + \frac{\sqrt{2}}{3} (d-2) + \frac{8\sqrt{6}}{5} + \frac{8\sqrt{3}}{7} \end{aligned}$$

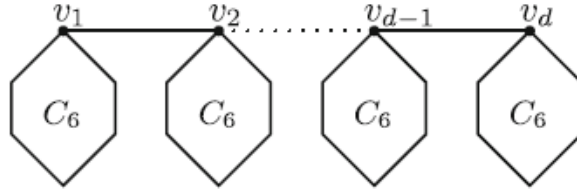


Fig. 3. The nano structures bridge graph $G_d(C_6, v)$

Case 3. Let K_n be the Complete graph on n vertices such that $n > 2$. For Bridge graph $G_d(K_n, v)$ we have dn vertices and $dn(n-1)/2 + d - 1$ edges and the edge set of graph can be dividing to 5 partitions, e. g. $[E_1]$, $[E_2]$, $[E_3]$, $[E_4]$ and $[E_5]$. For every $e = uv$ belong to $[E_1]$, $du = dv = 5$. Similarly, for every $e = uv$ belong to $[E_2]$, $du = 5$, $dv = 4$. For every $e = uv$ belong to $[E_3]$, $du = n-1$, $dv = 4$ and for every $e = uv$ belong to $[E_4]$, $du = n-1$, $dv = 5$. Finally, if $e = uv$ be an edge of $[E_5]$, then $du = dv = n-1$. So $|E(K_n)| = n(n-1)/2$, $|E_1| = d-2$, $|E_2| = 2$, $|E_3| = 2$, $|E_4| = d-2$ and $|E_5| = d(n-1)(n-2)/3$. Then we have

$$\begin{aligned} M_2(G_d(K_n, v)) &= \sum_{E_1} 25 + \sum_{E_2} 20 + \sum_{E_3} 4(n-1) + \sum_{E_4} 5(n-1) + \sum_{E_5} (n-1)^2 \\ &= \frac{1}{3} d(n-2)(n-1)^3 + 5nd + 20d - 2n - 8 \end{aligned}$$

$$\begin{aligned} \chi(G_d(K_n, v)) &= \sum_{E_1} \frac{1}{5} + \sum_{E_2} \frac{1}{\sqrt{20}} + \sum_{E_3} \frac{1}{\sqrt{4(n-1)}} + \sum_{E_4} \frac{1}{\sqrt{5(n-1)}} + \sum_{E_5} \frac{1}{n-1} \\ &= \frac{d-2}{5} + \frac{d(n-2)}{3} + \frac{1}{\sqrt{n-1}} + \frac{d-2}{\sqrt{5n-5}} + \frac{1}{\sqrt{5}} \end{aligned}$$

$$\begin{aligned} ABC(G_d(K_n, v)) &= \sum_{E_1} \frac{2}{\sqrt{5}} + \sum_{E_2} \frac{\sqrt{7}}{3} + \sum_{E_3} \sqrt{\frac{n+1}{n+3}} + \sum_{E_4} \sqrt{\frac{n+2}{n+4}} + \sum_{E_5} \sqrt{\frac{n-2}{n-1}} \\ &= \sqrt{\frac{n-2}{n-1}} \cdot \frac{d(n-1)(n-2)}{3} \end{aligned}$$

$$\begin{aligned}
& + \sqrt{\frac{n+2}{n+4}}(d-2) + 2\sqrt{\frac{n+1}{n+3}} + \frac{2d-4}{\sqrt{5}} + \frac{2\sqrt{7}}{3} \\
GA(G_d(K_n, v)) &= \sum_{E_1} 1 + \sum_{E_2} \frac{4\sqrt{5}}{9} + \sum_{E_3} \frac{4\sqrt{n-1}}{n+3} + \sum_{E_4} \frac{2\sqrt{5n-5}}{n+4} + \sum_{E_5} 1 \\
&= \frac{d(n-1)(n-2)}{3} + \frac{2\sqrt{5n-5}(d-2)}{n+4} + \frac{8\sqrt{n-1}}{n+3} + d-2 + \frac{8\sqrt{5}}{9}
\end{aligned}$$



Fig. 4. The nano structures bridge graph $G_d(K_3, v)$

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