Dedicated to Professor Mircea Diudea on the Occasion of His 65th Anniversary

ON THE EDGE VERSION OF GEOMETRIC-ARITHMETIC INDEX OF NANOCONES

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ABSTRACT. In this paper, the edge version geometric-arithmetic index of certain nanocones is presented.

Keywords: Geometric-arithmetic (GA) index, GAe index, Nanocones

INTRODUCTION

A numerical quantity that can be used to characterize the structure of a molecular graph is called a Topological Index. The obvious candidates for topological indices are the number of vertices and edges. Topological indices are invariant under the graph isomorphism. The importance of topologically indices is generally related to quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR).

In this article we will consider only simple graphs without loop and multiple edges. Let G be a simple graph, with the vertex set V(G) and edge set E(G). The line graph L(G) of a graph G is the graph whose vertices are the edges of G and two vertices G and G are incident if and only if they have a common end vertex in G. The degree G of a vertex G is the number of vertices adjacent to G. Also, the degree G of an edge G of an edge G of its joining vertices in G. The distance G between two vertices G and G is the length of the shortest path between G and G in G.

For a natural number \dot{k} , we define the partitions

$$V_{k}(G) = \{u \in V(G) | d_{u} = k\} \text{ and } E_{k}(G) = \{e = uv \in E(G) | d_{u} + d_{v} = k\}.$$

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The first member of geometric-arithmetic index class was introduced in [1]:

$$GA_{1}(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_{u} \times d_{v}}}{d_{u} + d_{v}}.$$

The second member of this class was defined in [2]:

$$GA_{2}(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_{u} \times n_{v}}}{n_{u} + n_{v}}$$

where $n_u = \left| \left\{ y \middle| y \in V(G), d(u, y) < d(y, v) \right\} \right|$ and |A| denotes the number of elements of a set A.

The third member of this class was considered in [3]:

$$GA_3(G) = \sum_{uv \in E(G)} \frac{2\sqrt{m_u \times m_v}}{m_u + m_v}$$

where
$$m_u = |\{x | x \in E(G), d(u, x) < d(x, v)\}|$$
.

The fourth member of the class of *GA* index was introduced by M. Ghorbani et al. in [4]:

$$GA_4\left(G\right) = \sum_{uv \in E(G)} \frac{2\sqrt{\epsilon_u \times \epsilon_v}}{\epsilon_u + \epsilon_v}$$

where ϵ_u is the eccentricity of a vertex u and defined as the maximum graph distance between u and any other vertex v of G.

The fifth member of the class of GA index was introduced in [5]:

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u \times S_v}}{S_u + S_v}$$

$$S_{\boldsymbol{u}} = \sum_{\boldsymbol{v} \in N} d_{\boldsymbol{v}} \text{ where } N_{\boldsymbol{u}} = \left\{\boldsymbol{v} \in V\left(G\right) \middle| \boldsymbol{u}\boldsymbol{v} \in E\left(G\right)\right\}.$$

The sixth member of this class, also known as edge version of *GA* index, was launched in [6]:

$$GA_{e}(G) = \sum_{uv \in L(E(G))} \frac{2\sqrt{d_{e} \times d_{f}}}{d_{e} + d_{f}}.$$

For further results on geometric-arithmetic index we address to the articles [7-14]. The aim of this paper is to study the edge version of geometric-arithmetic index GA_e of nanocones $CNC_K[n]$.

RESULTS AND DISCUSSION

The following lemma is useful for finding the degree of a vertex of line graph.

Lemma 1. [14] Let G be a graph, $u \in V(G)$ and $e = uv \in E(G)$. Then:

$$d_e = d_u + d_v - 2.$$

Theorem 1. Let G be a graph of $CNC_3[n]$ nanocones for $n \ge 1$ with $3(n+1)^2$ vertices and $3\left(\frac{3}{2}n^2 + \frac{5}{2}n + 1\right)$ edges. Then:

$$GA_e(G) = \frac{12}{5}\sqrt{6} + 6n - 3 + \frac{24}{7}n\sqrt{3} + 9n^2.$$

Proof. The edge version of GA index is equivalent to GA_1 index of its line graph. The graph of $CNC_3[n]$ nanocones and its line graph are shown in Fig. 1. Now we will partition the vertex set and edge set of G as follows:

$$V_{2}(G) = \{u \in V(G) | d_{u} = 2\} \Rightarrow |V_{2}(G)| = 3(n+1),$$

$$V_{3}(G) = \{u \in V(G) | d_{u} = 3\} \Rightarrow |V_{3}(G)| = 3(n^{2} + n),$$

$$E_{4}(G) = \{e = uv \in E(G) | d_{u} + d_{v} = 4\} \Rightarrow |E_{4}(G)| = 3,$$

$$E_{5}(G) = \{e = uv \in E(G) | d_{u} + d_{v} = 5\} \Rightarrow |E_{5}(G)| = 6n \text{ and}$$

$$E_{6}(G) = \{e = uv \in E(G) | d_{u} + d_{v} = 6\} \Rightarrow |E_{6}(G)| = \frac{3n(3n+1)}{2}.$$

On the other hand it is easy to see that

 $|V(L(G))| = 3\left(\frac{3}{2}n^2 + \frac{5}{2}n + 1\right)$, so we can partition the V(L(G)) by using

Lemma 1, as follows:

$$\begin{split} V_2\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \big| \, d_e = 2\right\} \Rightarrow \left|V_2\big(L(G)\big)\right| = 3, \\ V_3\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \big| \, d_e = 3\right\} \Rightarrow \left|V_3\big(L(G)\big)\right| = 6n \text{ and} \\ V_4\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \big| \, d_e = 4\right\} \Rightarrow \left|V_4\big(L(G)\big)\right| = \frac{3n(3n+1)}{2}. \end{split}$$

And we get

$$|E(L(G))| = \frac{2 \times 3 + 3 \times 6n + 2 \times 3n(3n+1)}{2} = 3(n+1)(3n+1).$$

Now we split E(L(G)) as follows:

$$\begin{split} E_5\big(L(G)\big) = & \left\{ef \in E\big(L(G)\big) \middle| d_e + d_f = 5\right\} \Rightarrow \left|E_5\big(L(G)\big) \middle| = 2\middle|V_2\big(L(G)\big) \middle| = 6, \\ E_6\big(L(G)\big) = & \left\{ef \in V\big(L(G)\big) \middle| d_e + d_f = 6\right\} \\ \Rightarrow & \left|E_6\big(L(G)\big) \middle| = \middle|V_3\big(L(G)\big) \middle| - \middle|V_2\big(L(G)\big) \middle| = 6n - 3, \\ E_7\big(L(G)\big) = & \left\{ef \in E\big(L(G)\big) \middle| d_e + d_f = 7\right\} \Rightarrow \left|E_7\big(L(G)\big) \middle| = \middle|V_3\big(L(G)\big) \middle| = 6n \\ \text{and } E_8\big(L(G)\big) = & \left\{ef \in E\big(L(G)\big) \middle| d_e + d_f = 8\right\} \\ \Rightarrow & \left|E_8\big(L(G)\big) \middle| = \middle|E\big(L(G)\big) \middle| - \middle|E_5\big(L(G)\big) \middle| - \middle|E_6\big(L(G)\big) \middle| - \middle|E_7\big(L(G)\big) \middle| = 9n^2. \\ \text{Since } GA_e\big(G\big) = & \sum_{uv \in L(E(G))} \frac{2\sqrt{d_e \times d_f}}{d_e + d_f}, \text{ then} \\ GA_e\big(G\big) = & 6\frac{2\sqrt{2\times 3}}{2+3} + 3\big(2n-1\big)\frac{2\sqrt{3\times 3}}{3+3} + 6n\frac{2\sqrt{3\times 4}}{3+4} + 9n^2\frac{2\sqrt{4\times 4}}{4+4} \\ \text{After simplification we get} \\ GA_e\big(G\big) = & \frac{12}{5}\sqrt{6} + 6n - 3 + \frac{24}{7}n\sqrt{3} + 9n^2. \end{split}$$

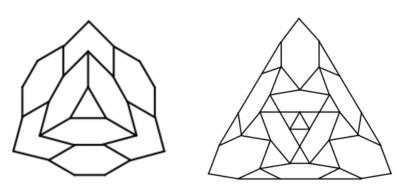


Figure 1. Graph of CNC₃[2] nanocone (left); Graph of L(CNC₃[2]) (right)

Theorem 2. Let G be a graph of $CNC_4[n]$ nanocones for $n \ge 1$ with $4(n+1)^2$ vertices and $4\left(\frac{3}{2}n^2+\frac{5}{2}n+1\right)$ edges. Then $GA_e\left(G\right) = \frac{16}{5}\sqrt{6}+8n-4+\frac{32}{7}n\sqrt{3}+12n^2.$

Proof. The graph of $CNC_4[n]$ nanocones and its line graph are shown in Fig. 2. Now we will partition the vertex set and edge set of G as follows:

$$V_{2}(G) = \{u \in V(G) | d_{u} = 2\} \Rightarrow |V_{2}(G)| = 4(n+1),$$

$$V_{3}(G) = \{u \in V(G) | d_{u} = 3\} \Rightarrow |V_{3}(G)| = 4(n^{2} + n),$$

$$E_{4}(G) = \{e = uv \in E(G) | d_{u} + d_{v} = 4\} \Rightarrow |E_{4}(G)| = 4,$$

$$E_{5}(G) = \{e = uv \in E(G) | d_{u} + d_{v} = 5\} \Rightarrow |E_{5}(G)| = 8n \text{ and}$$

$$E_{6}(G) = \{e = uv \in E(G) | d_{u} + d_{v} = 6\} \Rightarrow |E_{6}(G)| = \frac{4n(3n+1)}{2}.$$

On the other hand it is easy to see that

$$|V(L(G))| = 4\left(\frac{3}{2}n^2 + \frac{5}{2}n + 1\right),$$

so we can partition the V(L(G)) by using Lemma 1, as follows:

$$\begin{split} V_2\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \big| \, d_e = 2\right\} \Rightarrow \left|V_2\big(L(G)\big)\right| = 4, \\ V_3\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \big| \, d_e = 3\right\} \Rightarrow \left|V_3\big(L(G)\big)\right| = 8n \text{ and} \\ V_4\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \big| \, d_e = 4\right\} \Rightarrow \left|V_4\big(L(G)\big)\right| = \frac{4n(3n+1)}{2}. \end{split}$$

And it is easy to see that:

$$\left|E(L(G))\right| = 4(n+1)(3n+1).$$

Now we split E(L(G)) as follows:

$$\begin{split} E_5 \big(L(G) \big) = & \Big\{ ef \in E \big(L(G) \big) \Big| \, d_e + d_f = 5 \Big\} \Rightarrow \Big| E_5 \big(L(G) \big) \Big| = 2 \Big| V_2 \big(L(G) \big) \Big| = 8, \\ E_6 \big(L(G) \big) = & \Big\{ ef \in V \big(L(G) \big) \Big| \, d_e + d_f = 6 \Big\} \\ \Rightarrow & \Big| E_6 \big(L(G) \big) \Big| = \Big| V_3 \big(L(G) \big) \Big| - \Big| V_2 \big(L(G) \big) \Big| = 8n - 4, \\ E_7 \big(L(G) \big) = & \Big\{ ef \in E \big(L(G) \big) \Big| \, d_e + d_f = 7 \Big\} \Rightarrow \Big| E_7 \big(L(G) \big) \Big| = \Big| V_3 \big(L(G) \big) \Big| = 8n \\ & \text{and } E_8 \big(L(G) \big) = \Big| \Big\{ ef \in E \big(L(G) \big) \Big| \, d_e + d_f = 8 \Big\} \\ \Rightarrow & \Big| E_8 \big(L(G) \big) \Big| = \Big| E \big(L(G) \big) \Big| - \Big| E_5 \big(L(G) \big) \Big| - \Big| E_6 \big(L(G) \big) \Big| - \Big| E_7 \big(L(G) \big) \Big| = 12n^2 \,. \end{split}$$
 Since $GA_e \big(G \big) = \sum_{uv \in L(E(G))} \frac{2\sqrt{d_e \times d_f}}{d_e + d_f}, \text{ then}$

$$GA_{e}(G) = 8\frac{2\sqrt{2\times3}}{2+3} + 4(2n-1)\frac{2\sqrt{3\times3}}{3+3} + 8n\frac{2\sqrt{3\times4}}{3+4} + 12n^{2}\frac{2\sqrt{4\times4}}{4+4}$$

After simplification we get

$$GA_e(G) = \frac{16}{5}\sqrt{6} + 8n - 4 + \frac{32}{7}n\sqrt{3} + 12n^2.$$

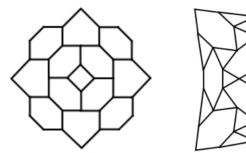


Figure 2. Graph of CNC₄[2] nanocone (left); Graph of L(CNC₄[2]) (right)

Theorem 3. Let G be a graph of $CNC_5[n]$ nanocones for $n \ge 1$ with $5(n+1)^2$ vertices and $5(\frac{3}{2}n^2 + \frac{5}{2}n + 1)$ edges. Then

$$GA_e(G) = 4\sqrt{6} + 10n - 5 + \frac{40}{7}n\sqrt{3} + 15n^2.$$

Proof. The graph of $CNC_5[n]$ nanocones and its line graph are shown in Fig. 3. At first we will partition the vertex set and edge set of G as follows:

$$\begin{split} V_2\left(G\right) = & \left\{u \in V\left(G\right) \middle| d_u = 2\right\} \Rightarrow \left|V_2\left(G\right) \middle| = 5\left(n+1\right), \\ V_3\left(G\right) = & \left\{u \in V\left(G\right) \middle| d_u = 3\right\} \Rightarrow \left|V_3\left(G\right) \middle| = 5\left(n^2 + n\right), \\ E_4\left(G\right) = & \left\{e = uv \in E\left(G\right) \middle| d_u + d_v = 4\right\} \Rightarrow \left|E_4\left(G\right) \middle| = 5, \\ E_5\left(G\right) = & \left\{e = uv \in E\left(G\right) \middle| d_u + d_v = 5\right\} \Rightarrow \left|E_5\left(G\right) \middle| = 10n \text{ and} \\ E_6\left(G\right) = & \left\{e = uv \in E\left(G\right) \middle| d_u + d_v = 6\right\} \Rightarrow \left|E_6\left(G\right) \middle| = \frac{5n\left(3n+1\right)}{2}. \end{split}$$

On the other hand it is easy to see that

$$|V(L(G))| = 5\left(\frac{3}{2}n^2 + \frac{5}{2}n + 1\right),$$

so we can partition the V(L(G)) by using Lemma 1, as follows:

$$\begin{split} V_2\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \big| \, d_e = 2\right\} \Rightarrow \left|V_2\big(L(G)\big)\right| = 5, \\ V_3\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \big| \, d_e = 3\right\} \Rightarrow \left|V_3\big(L(G)\big)\right| = 10n \text{ and } \\ V_4\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \big| \, d_e = 4\right\} \Rightarrow \left|V_4\big(L(G)\big)\right| = \frac{5n(3n+1)}{2}. \end{split}$$
 And we can obtained

$$|E(L(G))| = 5(n+1)(3n+1)$$

Now we split E(L(G)) as follows:

$$\begin{split} E_5 \left(L(G) \right) = & \left\{ ef \in E \left(L(G) \right) \middle| d_e + d_f = 5 \right\} \Rightarrow \left| E_5 \left(L(G) \right) \middle| = 2 \middle| V_2 \left(L(G) \right) \middle| = 10, \\ E_6 \left(L(G) \right) = & \left\{ ef \in V \left(L(G) \right) \middle| d_e + d_f = 6 \right\} \\ \Rightarrow & \left| E_6 \left(L(G) \right) \middle| = \middle| V_3 \left(L(G) \right) \middle| - \middle| V_2 \left(L(G) \right) \middle| = 10n - 5, \\ E_7 \left(L(G) \right) = & \left\{ ef \in E \left(L(G) \right) \middle| d_e + d_f = 7 \right\} \Rightarrow \left| E_7 \left(L(G) \right) \middle| = \middle| V_3 \left(L(G) \right) \middle| = 10n \right. \\ E_8 \left(L(G) \right) = & \left\{ ef \in E \left(L(G) \right) \middle| d_e + d_f = 8 \right\} \text{ and } \\ \Rightarrow & \left| E_8 \left(L(G) \right) \middle| = \middle| E \left(L(G) \right) \middle| - \middle| E_5 \left(L(G) \right) \middle| - \middle| E_6 \left(L(G) \right) \middle| - \middle| E_7 \left(L(G) \right) \middle| = 15n^2. \\ \text{Since } GA_e \left(G \right) = & \sum_{uv \in L(E(G))} \frac{2\sqrt{d_e \times d_f}}{d_e + d_f}, \text{ then } \\ GA_e \left(G \right) = & 10 \frac{2\sqrt{2 \times 3}}{2 + 3} + 5 \left(2n - 1 \right) \frac{2\sqrt{3 \times 3}}{3 + 3} + 10n \frac{2\sqrt{3 \times 4}}{3 + 4} + 15n^2 \frac{2\sqrt{4 \times 4}}{4 + 4} \\ \text{After simplification we get} \end{split}$$

 $GA_e(G) = 4\sqrt{6} + 10n - 5 + \frac{40}{7}n\sqrt{3} + 15n^2.$

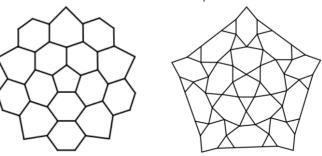


Figure 3. Graph of CNC₅[2] nanocone (left); Graph of L(CNC₅[2]) (right)

Theorem 4. Let G be a graph of $CNC_k[n]$ nanocones for $n \ge 1$ and $k \ge 3$

with
$$5(n+1)^2$$
 vertices and $5\left(\frac{3}{2}n^2 + \frac{5}{2}n + 1\right)$ edges. Then
$$GA_e(G) = 3kn^2 + n\left(2k + \frac{8}{7}k\sqrt{3}\right) + \frac{4}{5}k\sqrt{6} - k.$$

Proof. The graph of $CNC_k[n]$ nanocones and its line graph are shown in Fig. 4 (a) and (b) respectively. At first we will partition the vertex set and edge set of G as follows:

$$V_{2}(G) = \{u \in V(G) | d_{u} = 2\} \Rightarrow |V_{2}(G)| = k(n+1),$$

$$V_{3}(G) = \{u \in V(G) | d_{u} = 3\} \Rightarrow |V_{3}(G)| = k(n^{2} + n),$$

$$E_{4}(G) = \{e = uv \in E(G) | d_{u} + d_{v} = 4\} \Rightarrow |E_{4}(G)| = k,$$

$$E_{5}(G) = \{e = uv \in E(G) | d_{u} + d_{v} = 5\} \Rightarrow |E_{5}(G)| = 2kn \text{ and}$$

$$E_{6}(G) = \{e = uv \in E(G) | d_{u} + d_{v} = 6\} \Rightarrow |E_{6}(G)| = \frac{kn(3n+1)}{2}.$$

On the other hand it is easy to see that $|V(L(G))| = k\left(\frac{3}{2}n^2 + \frac{5}{2}n + 1\right)$,

so we can partition the V(L(G)) by using Lemma 1, as follows:

$$\begin{split} V_2\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \middle| \, d_e = 2\right\} \Rightarrow \left|V_2\big(L(G)\big)\right| = k, \\ V_3\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \middle| \, d_e = 3\right\} \Rightarrow \left|V_3\big(L(G)\big)\right| = 2kn \text{ and } \\ V_4\big(L(G)\big) = & \left\{e \in V\big(L(G)\big) \middle| \, d_e = 4\right\} \Rightarrow \left|V_4\big(L(G)\big)\right| = \frac{kn(3n+1)}{2}. \end{split}$$

And we can obtained

$$\left| E\left(L\left(G\right)\right) \right| = \frac{2 \times k + 3 \times 2kn + 2 \times kn\left(3n+1\right)}{2} = k\left(n+1\right)\left(3n+1\right)$$

Now we split E(L(G)) as follows:

$$E_{5}(L(G)) = \{ef \in E(L(G)) | d_{e} + d_{f} = 5\} \Rightarrow |E_{5}(L(G))| = 2|V_{2}(L(G))| = 2k,$$

$$E_{6}(L(G)) = \{ef \in V(L(G)) | d_{e} + d_{f} = 6\}$$

$$\Rightarrow |E_{6}(L(G))| = |V_{3}(L(G))| - |V_{2}(L(G))| = k(2n-1),$$

$$\begin{split} E_7 \big(L(G) \big) = & \Big\{ ef \in E \big(L(G) \big) \Big| \, d_e + d_f = 7 \Big\} \Rightarrow \Big| E_7 \big(L(G) \big) \Big| = \Big| V_3 \big(L(G) \big) \Big| = 2kn \\ & \text{and } E_8 \big(L(G) \big) = \Big\{ ef \in E \big(L(G) \big) \Big| \, d_e + d_f = 8 \Big\} \\ \Rightarrow & \Big| E_8 \big(L(G) \big) \Big| = \Big| E \big(L(G) \big) - \Big| E_5 \big(L(G) \big) \Big| - \Big| E_6 \big(L(G) \big) \Big| - \Big| E_7 \big(L(G) \big) \Big| = 3kn^2 \\ & \text{Since } GA_e \big(G \big) = \sum_{uv \in L(E(G))} \frac{2\sqrt{d_e \times d_f}}{d_e + d_f}, \text{ then} \\ & GA_e \big(G \big) = 2k \frac{2\sqrt{2 \times 3}}{2 + 3} + k \big(2n - 1 \big) \frac{2\sqrt{3 \times 3}}{3 + 3} + k \big(2n \big) \frac{2\sqrt{3 \times 4}}{3 + 4} + k \big(3n^2 \big) \frac{2\sqrt{4 \times 4}}{4 + 4} \\ & \text{After simplification we get} \\ & GA_e \big(G \big) = 3kn^2 + n \bigg(2k + \frac{8}{7}k\sqrt{3} \, \bigg) + \frac{4}{5}k\sqrt{6} - k. \end{split}$$

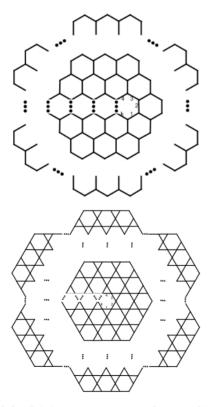


Figure 4. Graph of $CNC_k[n]$ nanocone (top) Graph of $L(CNC_k[n])$ (bottom)

CONCLUSION

In this article the edge version of geometric-arithmetic (GA) index was studied for the case of nanocones, $CNC_k[n]$. In future, we will pay attention to some new classes of nanostructures and study their topological indices which will be practically helpful to identify their underlying topologies.

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