

Albertson energy and Albertson-Estrada index of graphs

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Received 7 July 2018; Revised 7 January 2019; Accepted 11 January 2019.

Communicated by Hamidreza Rahimi

Abstract. Let G be a graph of order n with vertices labeled as v_1, v_2, \dots, v_n . Let d_i be the degree of the vertex v_i for $i = 1, 2, \dots, n$. The Albertson matrix of G is the square matrix of order n whose (i, j) -entry is equal to $|d_i - d_j|$ if v_i is adjacent to v_j and zero, otherwise. The main purposes of this paper is to introduce the Albertson energy and Albertson-Estrada index of a graph, both base on the eigenvalues of the Albertson matrix. Moreover, we establish upper and lower bounds for these new graph invariants and relations between them.

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Keywords: Eigenvalue of graph, energy, Albertson-Estrada index, Albertson energy.

2010 AMS Subject Classification: 05C50.

1. Introduction

All graphs considered in this paper are assumed to be simple. Let G be a (molecular) graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. If v_i and v_j are adjacent vertices of G , then the edge connecting them is denoted by $v_i v_j$. For a vertex $v_i \in V(G)$, we denote the degree of v_i by d_i . The *adjacency* matrix of a graph G is the square matrix $A = A(G) = [a_{ij}]$, in which $a_{ij} = 1$ if v_i is adjacent to v_j and $a_{ij} = 0$, otherwise. The eigenvalues of $A(G)$ are the adjacency eigenvalues of G (they are labeled as $\lambda_1, \lambda_2, \dots, \lambda_n$). These form the adjacency spectrum of G [5]. Thus, $\det A = \prod_{i=1}^n \lambda_i$.

A topological index is a real number associated with a graph which characterizes the topology of the graph and is invariant under graph isomorphism. There are many distance or degree based topological indices. Degree based topological indices are of great

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importance and play a vital role in chemical graph theory. Some results on topological indices of chemical graphs have been studied by Gao et al. [14, 15]. The topological index of a molecule structure can be considered as a nonempirical numerical quantity which quantitates the molecular structure and its branching pattern. In mathematical chemistry, there is a large number of topological indices of the form

$$TI = TI(G) = \sum_{v_i, v_j \in E(G)} F(d_i, d_j), \quad (1)$$

where the summation goes over all pairs of adjacent vertices u_i, v_j of the molecular graph G and $F = F(x, y)$ is an appropriately chosen function. In particular, $F(x, y) = \frac{1}{\sqrt{xy}}$ for the Randić (or connectivity) index, $F(x, y) = x + y$ for the first Zagreb index, $F(x, y) = xy$ for the second Zagreb index, $F(x, y) = \frac{1}{\sqrt{x+y}}$ for the sum connectivity index. Also, the logarithms of the two multiplicative Zagreb indices can be presented in the form of (1), namely by choosing $F(x, y) = \ln(x + y)$ for the logarithm of the modified first multiplicative Zagreb index, $F(x, y) = \ln x + \ln y$ for the logarithm of second multiplicative Zagreb index. Note that there are several more indices in [15, 17]. To each of such topological indices, a matrix TI can be associated as

$$(TI)_{ij} = \begin{cases} F(d_i, d_j) & \text{if } v_i v_j \in E(G) \\ 0 & \text{otherwise.} \end{cases}$$

The Albertson index of a graph G is a square matrix $\mathbf{A} = [a_{ij}]$ of order n with

$$a_{ij} = \begin{cases} 0 & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are not adjacent} \\ |d_i - d_j| & \text{if the vertices } v_i \text{ and } v_j \text{ of } G \text{ are adjacent} \\ 0 & \text{if } i = j. \end{cases}$$

The eigenvalues of $\mathbf{A}(G)$ labeled as $\varsigma_1 \geq \varsigma_2 \geq \dots \geq \varsigma_n$ are said to be the Zagreb or \mathbf{A} -eigenvalues of G and their collection is called second Zagreb spectrum or \mathbf{A} -spectrum of G . The Zagreb indices were widely studied degree-based topological indices and were introduced by Gutman and Trinajstić [22]. The first and the second indices of a graph G are respectively defined as

$$M_1(G) = \sum_{u_i \in V(G)} d_i^2 = \sum_{u_i v_j \in E(G)} [d_i + d_j] \text{ and } M_2(G) = \sum_{u_i v_j \in E(G)} [d_i d_j].$$

Recently, there was a vast research on comparing Zagreb indices [25, 26, 28], establishing various upper bounds [6, 8, 38, 40] and relation involving graph invariants [39, 42] and a survey on the first Zagreb index [20].

If all vertices of a graph have the same degree, then the graph is said to be regular. Regularity makes calculations easier in many occasions. A graph which is not regular, that is which has at least two different vertex degrees, is said to be irregular. Irregularity may occur slightly or strongly. As a result of this, several measures for irregularity have some of these measures are in terms been defined and used by some authors [21, 24]. One of such measures was put forward by Albertson [2], who considered the quantity

$$\mathbf{A} = \mathbf{Alb}(G) = \sum_{u_i v_j \in E(G)} |d_i - d_j|.$$

This quantity is sometimes referred to as the Albertson index [21, 23]. In a recent work [13] it was called the third Zagreb index. Another irregularity index was briefly mentioned in [1], but seems that has not been investigated in any detail. Motivated by this fact, we studied this index and its properties, especially the inverse problem for it. We propose that this graph invariant be called sigma index and be denoted by σ in resemblance with the standard deviation in statistics. It is defined as $\sigma(G) = \sum_{u_i v_j \in E(G)} (d_i - d_j)^2$.

This paper is organized as follows. In Section 3, we state some previously known results. In section 4, we introduce and investigate the Albertson energy and obtain lower and upper bounds for it. In section 5, we put forward the concept of Albertson-Estrada index and obtain lower and upper bounds for it. In section 6, we investigate relations between the Albertson-Estrada index and the Albertson energy.

2. Preliminaries

In this section, we shall list some previously known results that will be needed in the next sections. At the first, we calculate $tr(\mathbf{A}^2)$, $tr(\mathbf{A}^3)$ and $tr(\mathbf{A}^4)$, where tr denotes the Trace of a matrix. Now, let us present the following lemma as the first preliminary result. Denote by \mathbb{N}_k the k-th spectral moment of the Albertson matrix \mathbf{A} , i. e.,

$$\mathbb{N}_k = tr(\mathbf{A})^k = \sum_{i=1}^n (\zeta_i)^k \tag{2}$$

Lemma 2.1 Let G be a graph with n vertices and Albertson matrix \mathbf{A} . Then

$$\mathbb{N}_1 = tr(\mathbf{A}) = 0, \tag{3}$$

$$\mathbb{N}_2 = tr(\mathbf{A}^2) = 2\sigma(G), \tag{4}$$

$$\mathbb{N}_3 = tr(\mathbf{A}^3) = 2 \sum_{i \sim j} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_i - d_k)(d_k - d_j) \right), \tag{5}$$

$$\mathbb{N}_4 = tr(\mathbf{A}^4) = \sum_{i=1}^n \left(\sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \right)^2 + \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_i - d_k)(d_k - d_j) \right)^2, \tag{6}$$

where $\sum_{i \sim j}$ indicates summation over all pairs of adjacent vertices v_i, v_j . Nowadays, \mathbf{A} is referred to as the Albertson index.

Proof. By definition, the diagonal elements of \mathbf{A} are equal to zero. Therefore, the trace of \mathbf{A} is zero. Next, we calculate the matrix $\left(\mathbf{A}\right)^2$. For $i = j$

$$\left(\mathbf{A}\right)_{ii}^2 = \sum_{j=1}^n \mathbf{A}_{ij} \mathbf{A}_{ji} = \sum_{j=1}^n \left(\mathbf{A}_{ij}\right)^2 = \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} \left(\mathbf{Z}_{ij}^{(2)}\right)^2 = \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (|d_i - d_j|)^2.$$

whereas for $i \neq j$

$$\left(\mathbf{A}\right)_{ii}^2 = \sum_{j=1}^n \mathbf{A}_{ij} \mathbf{A}_{ji} = \mathbf{A}_{ii} \mathbf{A}_{ij} + \mathbf{A}_{ij} \mathbf{A}_{jj} + \sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} \mathbf{A}_{ik} \mathbf{A}_{kj} = |d_i - d_j| \sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_k)^2.$$

Therefore,

$$tr\left(\mathbf{A}\right)_{ii}^2 = \sum_{i=1}^n \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 = 2 \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 = 2\sigma(G).$$

Since the diagonal elements of $\left(\mathbf{A}\right)^3$ are

$$tr\left(\left(\mathbf{A}\right)^3\right)_{ii} = \sum_{j=1}^n \mathbf{A}_{ij} \left(\mathbf{A}\right)_{jk}^2 = \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} |(d_i - d_j)| \left(\mathbf{A}\right)_{ij}^2 = \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_k)^2 \right),$$

Thus, We obtain

$$tr\left(\left(\mathbf{A}\right)^3\right) = \sum_{i=1}^n \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_k)^2 \right) = 2 \sum_{i \sim j} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_i - d_k)(d_k - d_j) \right).$$

Now, we calculate $tr(\mathbf{A}^4)$. Because $tr(\mathbf{A}^4) = \left\| \left(\left(\mathbf{A}\right)^2 \right) \right\|_F^2$, where $\left\| \left(\left(\mathbf{A}\right)^2 \right) \right\|_F^2$ denotes the Frobenius norm of \mathbf{A} , we obtain

$$\begin{aligned} tr(\mathbf{A}^4) &= \sum_{i,j=1}^n \left| \left(\mathbf{A}\right)_{ii}^2 \right|^2 = \sum_{i=j} \left| \left(\mathbf{A}\right)_{ii}^2 \right|^2 + \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} \left| \left(\mathbf{A}\right)_{ij}^2 \right|^2 \\ &= \sum_{i=1}^n \left(\sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \right)^2 + \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_k)^2 \right)^2. \end{aligned}$$

■

Remark 1 For any real x , the power-series expansion of e^x is $\sum_{k \geq 0} \frac{x^k}{k!}$.

Lemma 2.2 For any non-negative real x , $e^x \geq 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{4}$. Equality holds if and only if $x = 0$.

Theorem 2.3 [4] (Chebishev’s inequality) Let $a_1 \leq a_2 \leq \dots \leq a_n$ and $b_1 \leq b_2 \leq \dots \leq b_n$ be real numbers. Then we have

$$\left(\sum_{i=1}^n a_i \right) \left(\sum_{i=1}^n b_i \right) \leq n \sum_{i=1}^n a_i b_i,$$

equality occurs if and only if $a_1 = a_2 = \dots = a_n$ or $b_1 = b_2 = \dots = b_n$.

Remark 2 For nonnegative x_1, x_2, \dots, x_n and $k \geq 2$,

$$\sum_{i=1}^n (x_i)^k \leq \left(\sum_{i=1}^n x_i^2 \right)^{\frac{k}{2}}. \tag{7}$$

Lemma 2.4 [41] Let G be a graph with m edges. Then, for $k \geq 4$, $M_{k+2} \geq M_k$ with equality for all even $k \geq 4$ if and only if G consists of m copies of complete graph on two vertices and possibly isolated vertices, and with equality for all odd $k \geq 5$ if and only if G is a bipartite graph.

3. Bounds for the Albertson energy

In this section, we consider the Albertson energy of graph G . We also give lower and upper bounds for it. In the 1970s, one of the present authors noticed that practically all results that until then were obtained for the HMO total π -electron energy, in particular those in the papers [36, 37]. The molecular graphs encountered in the HMO theory but hold for all graphs. This observation motivated him to put forward [19] the following: If G is a graph on n vertices and $\lambda_1, \dots, \lambda_n$ are its eigenvalues, then the energy of G is $E = E(G) = \sum_{i=1}^n |\lambda_i|$. This concept was introduced by Gutman and is intensively studied in chemistry, since it can be used to approximate the total π -electron energy of a molecule (see [16, 18]). For details on energy including also its mathematical properties, see [3, 7, 30–35]. The Albertson energy of a graph G is defined as $\mathbf{AE}(G) = \sum_{i=1}^n |\varsigma_i|$, where $\varsigma_1, \varsigma_2, \dots, \varsigma_n$ are eigenvalues of the Albertson matrix. At first, we state the following useful lemma.

Lemma 3.1 Let x_1, \dots, x_n be n positive numbers. Then $\frac{n}{\frac{1}{x_1} + \dots + \frac{1}{x_n}} \leq \sqrt[n]{x_1 x_2 \dots x_n}$.

Proof. By arithmetic-geometric mean inequality we have $\frac{\frac{1}{x_1} + \dots + \frac{1}{x_n}}{n} \geq \sqrt[n]{\frac{1}{x_1} \frac{1}{x_2} \dots \frac{1}{x_n}}$. By inverting both sides of inequality above, we get $\frac{n}{\frac{1}{x_1} + \dots + \frac{1}{x_n}} \leq \sqrt[n]{x_1 x_2 \dots x_n}$. ■

Theorem 3.2 Let G be a graph with n vertices. Then $e^{-\sqrt{2\sigma(G)}} \leq \mathbf{AE}(G) \leq e^{\sqrt{2\sigma(G)}}$.

Proof. Lower bound. By definition of the Albertson energy and by the arithmetic-geometric mean inequality, we have $\mathbf{AE}(G) = \sum_{i=1}^n |\varsigma_i| = n(\frac{1}{n} \sum_{i=1}^n |\varsigma_i|) \geq n(\sqrt[n]{|\varsigma_1| \dots |\varsigma_n|})$. By Lemma 3.1, Theorem 2.3 and relations (4) and (7), we have

$$\begin{aligned} n(\sqrt[n]{|\varsigma_1| |\varsigma_2| \dots |\varsigma_n|}) &\geq n\left(\frac{n}{\sum_{i=1}^n \frac{1}{|\varsigma_i|}}\right) \geq n\left(\frac{n}{\sum_{i=1}^n \frac{1}{|\varsigma_i|} \sum_{i=1}^n |\varsigma_i|}\right) \\ &\geq n\left(\frac{n}{n \sum_{i=1}^n \frac{1}{|\varsigma_i|} |\varsigma_i|}\right) \geq n\left(\frac{n}{n^2 \sum_{i=1}^n |\varsigma_i|}\right) \\ &> n\left(\frac{n}{n^2 \sum_{i=1}^n e^{|\varsigma_i|}}\right) = \frac{1}{\sum_{i=1}^n \sum_{k \geq 0} \frac{(|\varsigma_i|)^k}{k!}} \\ &= \frac{1}{\sum_{k \geq 0} \frac{1}{k!} (\sum_{i=1}^n (|\varsigma_i|)^k)} \geq \frac{1}{\sum_{k \geq 0} \frac{1}{k!} (\sum_{i=1}^n (|\varsigma_i|)^2)^{\frac{k}{2}}} \\ &= \frac{1}{\sum_{k \geq 0} \frac{1}{k!} (\sum_{i=1}^n (\varsigma_i)^2)^{\frac{k}{2}}} = \frac{1}{\sum_{k \geq 0} \frac{1}{k!} \left(\sqrt{2\sigma(G)}\right)^k} \\ &= \frac{1}{e^{\sqrt{2\sigma(G)}}}. \end{aligned}$$

Therefore, we have $\mathbf{AE}(G) \geq e^{-\sqrt{2\sigma(G)}}$.

Upper bound. By definition of the Albertson energy and relations (4) and (7), we have

$$\begin{aligned} \mathbf{AE}(G) &= \sum_{i=1}^n |\varsigma_i| < \sum_{i=1}^n e^{|\varsigma_i|} \\ &= \sum_{i=1}^n \sum_{k \geq 0} \frac{(|\varsigma_i|)^k}{k!} = \sum_{k \geq 0} \frac{1}{k!} \sum_{i=1}^n (|\varsigma_i|)^k \\ &\leq \sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^n (|\varsigma_i|)^2 \right)^{\frac{k}{2}} = \sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^n (\varsigma_i)^2 \right)^{\frac{k}{2}} \\ &= \sum_{k \geq 0} \frac{1}{k!} \left(2\sigma(G) \right)^{\frac{k}{2}} = \sum_{k \geq 0} \frac{1}{k!} \left(\sqrt{2\sigma(G)} \right)^k = e^{\sqrt{2\sigma(G)}}. \end{aligned}$$

■

Theorem 3.3 Let G be a graph with n vertices. Then $\sqrt{2\sigma(G)} \leq \mathbf{AE}(G) \leq \sqrt{2n\sigma(G)}$.

Proof. By Cauchy-Schwarz inequality, we have

$$\left(\sum_{i=1}^n a_i b_i \right)^2 \leq \left(\sum_{i=1}^n a_i^2 \right) \left(\sum_{i=1}^n b_i^2 \right)$$

for real numbers a_i and b_i . Let $a_i = 1$, $b_i = |\varsigma_i|$. Then we have

$$\left(\sum_{i=1}^n |\varsigma_i| \right)^2 \leq n \left(\sum_{i=1}^n |\varsigma_i|^2 \right) = n \sum_{i=1}^n (\varsigma_i)^2 = 2\sigma(G).$$

Therefore, $\mathbf{AE}(G) \leq \sqrt{2n\sigma(G)}$. This gives the upper bound for $\mathbf{AE}(G)$. Now, for the lower bound of $\mathbf{AE}(G)$, we can easily obtain the inequality

$$\left(\mathbf{AE}(G) \right)^2 = \left(\sum_{i=1}^n |\varsigma_i| \right)^2 \geq \sum_{i=1}^n |\varsigma_i|^2 = 2\sigma(G).$$

■

Theorem 3.4 Let G be a connected graph with n vertices. Then

$$\mathbf{AE}(G) \geq \sqrt{2\sigma(G) + n(n-1) |\det \mathbf{A}|^{\frac{2}{n}}}.$$

Proof. By definition of the Albertson energy, we have

$$\begin{aligned} \left(\mathbf{AE}(G) \right)^2 &= \left(\sum_{i=1}^n |\varsigma_i| \right)^2 = \sum_{i=1}^n |\varsigma_i|^2 + 2 \sum_{1 \leq i < j \leq n} |\varsigma_i| |\varsigma_j| \\ &= 2\sigma(G) + 2 \sum_{1 \leq i < j \leq n} |\varsigma_i| |\varsigma_j| \\ &= 2\sigma(G) + 2 \sum_{i \neq j} |\varsigma_i| |\varsigma_j|. \end{aligned}$$

For nonnegative numbers, since the arithmetic mean is not smaller than the geometric mean, then we have

$$\frac{1}{n(n-1)} \sum_{i \neq j} |s_i| |s_j| \geq \left(\prod_{i \neq j} |s_i| |s_j| \right)^{\frac{1}{n(n-1)}} = \left(\prod_{i=1}^n |s_i|^{2(n-1)} \right)^{\frac{1}{n(n-1)}} = \prod_{i=1}^n |s_i|^{\frac{2}{n}} = |\det \mathbf{A}|^{\frac{2}{n}}.$$

■

Remark 3 Let G be a graph with n vertices. Then $\mathbf{AE}(G) \geq n \sqrt[n]{|\det \mathbf{A}|}$.

By definition of the Albertson energy and the arithmetic-geometric mean inequality, we have

$$\mathbf{AE}(G) = \sum_{i=1}^n |s_i| = n \left(\frac{1}{n} \sum_{i=1}^n |s_i| \right) \geq n \left(\sqrt[n]{|s_1| |s_2| \cdots |s_n|} \right) = n \sqrt[n]{\prod_{i=1}^n |s_i|} = n \sqrt[n]{|\det \mathbf{A}|}.$$

Theorem 3.5 Let G be a non-empty graph with n vertices. Then $\mathbf{AE}(G) \geq \frac{1}{2\sigma(G)}$.

Proof. By definition of the Albertson energy and by the arithmetic-geometric mean inequality, we have

$$\mathbf{AE}(G) = \sum_{i=1}^n |s_i| = n \left(\frac{1}{n} \sum_{i=1}^n |s_i| \right) \geq n \left(\sqrt[n]{|s_1| |s_2| \cdots |s_n|} \right).$$

By Lemma 3.1, Theorem 2.3, and relations (4) and (7), we get

$$\begin{aligned} n \left(\sqrt[n]{|s_1| |s_2| \cdots |s_n|} \right) &\geq n \left(\frac{n}{\sum_{i=1}^n \frac{1}{|s_i|}} \right) \geq n \left(\frac{n}{\sum_{i=1}^n \frac{1}{|s_i|} \sum_{i=1}^n |s_i|} \right) \\ &\geq n \left(\frac{n}{n \sum_{i=1}^n \frac{1}{|s_i|} |s_i|} \right) \geq n \left(\frac{n}{n^2 \sum_{i=1}^n |s_i|} \right) \\ &\geq \frac{1}{\sum_{i=1}^n (|s_i|)^k} \geq \frac{1}{(\sum_{i=1}^n (|s_i|)^2)^{\frac{k}{2}}} \\ &= \frac{1}{(\sum_{i=1}^n (s_i)^2)^{\frac{k}{2}}} = \frac{1}{(2\sigma(G))^{\frac{k}{2}}}. \end{aligned}$$

Hence, $\mathbf{A}(G) \geq \frac{1}{2\sigma(G)}$ for $k = 2$.

■

4. Bounds for the Albertson Estrada index of graphs

In this section, we consider the Albertson Estrada index of graph G . We also give lower and upper bounds for it. As a new direction for the studying on indexes and their bounds, we will introduce and investigate Albertson Estrada index and its bounds.

The Estrada index of the graph G is defined by Estrada [12] as $EE = EE(G) = \sum_{i=1}^n e^{\lambda_i}$.

Although invented in the year 2000, the Estrada index has already found numerous applications in Physics, Chemistry and complex networks, for details see [11, 12]. Also, for the recent work of the mathematical properties on Estrada index, see [9, 10, 27, 29].

Let $M_k = M_k(G) = \sum_{i=1}^n (\lambda_i)^k$ be the k th spectral moment of a graph G . Bearing in mind

the power-series expansion of e^x , we have $EE = \sum_{i=1}^{\infty} \frac{M_k(G)}{k!}$. It is well known that $M_k(G)$

is equal to the number of closed walks of length k of the graph G . In fact, Estrada index of graphs has an important role in Chemistry and Physics, and there exists a vast literature that studies this special index. Thus, let G be a graph of order n whose Albertson eigenvalues are $s_1 \geq s_2 \geq \cdots \geq s_n$. Then the Albertson-Estrada index of G ,

denoted by $\mathbf{AEE}(G)$, is defined to be $\mathbf{AEE} = \mathbf{AEE}(G) = \sum_{i=1}^n e^{s_i}$. Recalling (2), it follows that $\mathbf{AEE}(G) = \sum_{i=1}^{\infty} \frac{\mathbb{N}_k}{k!}$. We begin this section with theorem as follows:

Theorem 4.1 Let G be a graph with n vertices. Then

$$\begin{aligned} \mathbf{AEE}(G) &\geq n + 2\sigma(G) + 2 \sum_{i \sim j} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_i - d_k)(d_k - d_j) \right) (\sinh(1) - 1) \\ &+ \left(\cosh(1) - 1 \right) \sum_{i=1}^n \left(\sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \right)^2 \\ &+ \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_i - d_k)(d_k - d_j) \right)^2. \end{aligned}$$

Proof. Note that $\mathbb{N}_2 = 2\sigma(G)$. By Lemma 2.4,

$$\begin{aligned} \mathbf{AEE}(G) &= n + 2\sigma(G) + \sum_{k \geq 1} \frac{\mathbb{N}_{2k+1}}{(2k+1)!} + \sum_{k \geq 1} \frac{\mathbb{N}_{2k+2}}{(2k+2)!} \\ &\geq n + 2\sigma(G) + \sum_{k \geq 1} \frac{\mathbb{N}_3}{(2k+1)!} + \sum_{k \geq 1} \frac{\mathbb{N}_4}{(2k+2)!} \\ &= n + 2\sigma(G) + 2 \sum_{i \sim j} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_i - d_k)(d_k - d_j) \right) (\sinh(1) - 1) \\ &+ \left(\cosh(1) - 1 \right) \sum_{i=1}^n \left(\sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \right)^2 \\ &+ \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_i - d_k)(d_k - d_j) \right)^2. \end{aligned}$$

Therefore, we have

$$\begin{aligned} \mathbf{AEE}(G) &\geq n + 2\sigma(G) + 2 \sum_{i \sim j} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_i - d_k)(d_k - d_j) \right) (\sinh(1) - 1) \\ &+ \left(\cosh(1) - 1 \right) \sum_{i=1}^n \left(\sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \right)^2 \\ &+ \sum_{\substack{j \in \{1, \dots, n\} \\ i \sim j}} (d_i - d_j)^2 \left(\sum_{\substack{k \in \{1, \dots, n\} \\ i \sim k \sim j}} (d_i - d_k)(d_k - d_j) \right)^2. \end{aligned}$$

■

Theorem 4.2 Let G be a graph with n vertices. Then $\mathbf{AEE}(G) \leq n - 1 + e^{\sqrt{2\sigma(G)-1}}$.

Proof. Let the number of positive eigenvalues of G be n_+ . Since $f(x) = e^x$ monotonically increases in the interval $(-\infty, +\infty)$ and $m \neq 0$, we get

$$\begin{aligned}
 \mathbf{AEE} &= \sum_{i=1}^n e^{\varsigma_i} < n - n_+ \sum_{i=1}^{n_+} e^{\varsigma_i} \\
 &= n - n_+ \sum_{i=1}^{n_+} \sum_{k \geq 0} \frac{(\varsigma_i)^k}{k!} \\
 &= n + \sum_{k \geq 1} \frac{1}{k!} \sum_{i=1}^{n_+} (\varsigma_i)^k \tag{8} \\
 &\leq n + \sum_{k \geq 1} \frac{1}{k!} \left[\sum_{i=1}^{n_+} \varsigma_i^2 \right]^{\frac{k}{2}} \\
 &= n + \sum_{k \geq 1} \frac{1}{k!} \left[\sum_{i=1}^{n_+} \varsigma_i^2 \right]^{\frac{k}{2}}.
 \end{aligned}$$

Since every (n, m) -graph with $m \neq 0$ has K_2 as its induced subgraph and the spectrum of K_2 is $1, -1$ it follows from the interlacing inequalities that $\varsigma_n \leq -1$, which implies that $\sum_{i=n_++1}^n (\varsigma_i)^2 \geq 1$. Consequently, $\mathbf{AEE} \geq n + \sum_{k \geq 1} \frac{1}{k!} [2\sigma(G) - 1]^{\frac{k}{2}} = n - 1 + e^{\sqrt{2\sigma(G)-1}}$. ■

Theorem 4.3 Let G be a graph with n vertices. Then

$$\mathbf{AEE}(G) \geq \sqrt{n^2(1 + \sigma) + 2n\sigma(G) + \frac{\mathbb{N}_3}{3} + \frac{1}{12}n\mathbb{N}_4}.$$

Proof. Suppose that $\varsigma_1, \varsigma_2, \dots, \varsigma_n$ is the spectrum of G . Using Lemma 2.2, we have

$$\begin{aligned}
 (\mathbf{AEE}(G))^2 &= \sum_{i=1}^n \sum_{j=1}^n e^{\varsigma_i + \varsigma_j} \geq \sum_{i=1}^n \sum_{j=1}^n \left(1 + \varsigma_i + \varsigma_j + \frac{(\varsigma_i + \varsigma_j)^2}{2} + \frac{(\varsigma_i + \varsigma_j)^3}{6} + \frac{(\varsigma_i + \varsigma_j)^4}{24} \right) \\
 &= \sum_{i=1}^n \sum_{j=1}^n \left(1 + \varsigma_i + \varsigma_j + \frac{\varsigma_i^2}{2} + \frac{\varsigma_j^2}{2} + \varsigma_i \varsigma_j + \frac{\varsigma_i^3}{6} + \frac{\varsigma_j^3}{6} + \frac{\varsigma_i^2 \varsigma_j}{2} + \frac{\varsigma_i \varsigma_j^2}{2} \right. \\
 &\quad \left. + \frac{\varsigma_i^4}{24} + \frac{\varsigma_j^4}{24} + \frac{\varsigma_i^2 \varsigma_j^2}{4} + \frac{\varsigma_i^3 \varsigma_j}{6} + \frac{\varsigma_i \varsigma_j^3}{6} \right).
 \end{aligned}$$

By equalities (3)-(6), we have the following equations:

$$\begin{aligned}
 \sum_{i=1}^n \sum_{j=1}^n (\varsigma_i + \varsigma_j) &= n \sum_{i=1}^n \varsigma_i + n \sum_{j=1}^n \varsigma_j = 0. \\
 \sum_{i=1}^n \sum_{j=1}^n \varsigma_i \varsigma_j &= \left(\sum_{i=1}^n \varsigma_i \right)^2 = 0. \\
 \sum_{i=1}^n \sum_{j=1}^n \left(\frac{\varsigma_i^2}{2} + \frac{\varsigma_j^2}{2} \right) &= \frac{n}{2} \sum_{i=1}^n \varsigma_i^2 + \frac{n}{2} \sum_{j=1}^n \varsigma_j^2 = 2n\sigma(G).
 \end{aligned}$$

$$\begin{aligned} \sum_{i=1}^n \sum_{j=1}^n \left(\frac{\varsigma_i^3}{6} + \frac{\varsigma_j^3}{6} \right) &= \frac{n}{6} \sum_{i=1}^n \varsigma_i^3 + \frac{n}{6} \sum_{j=1}^n \varsigma_j^3 = \frac{\mathbb{N}_3}{3}. \\ \sum_{i=1}^n \sum_{j=1}^n \left(\frac{\varsigma_i^4}{24} + \frac{\varsigma_j^4}{24} \right) &= \frac{n}{24} \sum_{i=1}^n \varsigma_i^4 + \frac{n}{24} \sum_{j=1}^n \varsigma_j^4 = \frac{1}{12} n\mathbb{N}_4. \\ \sum_{i=1}^n \sum_{j=1}^n \frac{\varsigma_i^2 \varsigma_j^2}{4} &= n^2 \sigma. \\ \sum_{i=1}^n \sum_{j=1}^n \frac{\varsigma_i \varsigma_j^3}{6} &= \frac{1}{6} \sum_{i=1}^n \varsigma_i \sum_{j=1}^n \varsigma_j^3 = 0. \\ \sum_{i=1}^n \sum_{j=1}^n \frac{\varsigma_i^3 \varsigma_j}{6} &= \frac{1}{6} \sum_{i=1}^n \varsigma_i^3 \sum_{j=1}^n \varsigma_j = 0. \\ \sum_{i=1}^n \sum_{j=1}^n \frac{\varsigma_i \varsigma_j^2}{2} &= \frac{1}{2} \sum_{i=1}^n \varsigma_i \sum_{j=1}^n \varsigma_j^2 = 0. \\ \sum_{i=1}^n \sum_{j=1}^n \frac{\varsigma_i^2 \varsigma_j}{2} &= \frac{1}{2} \sum_{i=1}^n \varsigma_i^2 \sum_{j=1}^n \varsigma_j = 0. \end{aligned}$$

Combining the above relations, we get $\mathbf{AEE}(G) \geq \sqrt{n^2(1 + \sigma) + 2n\sigma(G) + \frac{\mathbb{N}_3}{3} + \frac{1}{12}n\mathbb{N}_4}$. ■

Theorem 4.4 Let G be an graph with n vertices. Then the Albertson-Estrada index of G is bounded as

$$\sqrt{n^2 + 4\sigma(G)} \leq \mathbf{AEE}(G) \leq n - 1 + e^{\sqrt{2\sigma(G)}}. \tag{9}$$

Proof. Lower bound. Directly from the definition of the Albertson-Estrada index, we get

$$(\mathbf{AEE}(G))^2 = \sum_{i=1}^n e^{2\varsigma_i} + 2 \sum_{i < j} e^{\varsigma_i} e^{\varsigma_j}. \tag{10}$$

In view of the inequality between the arithmetic and geometric means and by $\sum_{i=1}^n \varsigma_i = 0$, we have

$$\begin{aligned} 2 \sum_{i < j} e^{\varsigma_i} e^{\varsigma_j} &\geq n(n-1) \left(\prod_{i < j} e^{\varsigma_i} e^{\varsigma_j} \right)^{\frac{2}{n(n-1)}} \\ &= n(n-1) \left[\left(\prod_{i=1}^n e^{\varsigma_i} \right)^{n-1} \right]^{\frac{2}{n(n-1)}} = n(n-1) \left(e^{\sum_{i=1}^n \varsigma_i} \right)^{\frac{2}{n}} = n(n-1). \end{aligned} \tag{11}$$

By means of a power-series expansion and bearing in mind the properties of \mathbb{N}_0 , \mathbb{N}_1 and \mathbb{N}_2 , we get

$$\sum_{i=1}^n e^{2\varsigma_i} = \sum_{i=1}^n \sum_{k \geq 0} \frac{(2\varsigma_i)^k}{k!} = n + 4\sigma(G) + \sum_{i=1}^n \sum_{k \geq 3} \frac{(2\varsigma_i)^k}{k!}.$$

Because we are aiming at a (as good as possible) lower bound, it may look plausible to replace $\sum_{k \geq 3} \frac{(2\varsigma_i)^k}{k!}$ by $8 \sum_{k \geq 3} \frac{(\varsigma_i)^k}{k!}$. However, instead of $8 = 2^3$ we shall use a multiplier

$\Upsilon \in [0, 8]$. So as to arrive at

$$\sum_{i=1}^n e^{2s_i} \geq n + 4\sigma(G) + \Upsilon \sum_{i=1}^n \sum_{k \geq 3} \frac{(s_i)^k}{k!} = n + 4\sigma(G) - \Upsilon n - \Upsilon \sigma + \Upsilon \sum_{i=1}^n \sum_{k \geq 0} \frac{(s_i)^k}{k!}$$

i.e.,

$$\sum_{i=1}^n e^{2s_i} \geq (1 - \Upsilon)n + (4 - \omega)\sigma + \Upsilon \mathbf{AEE}(G). \tag{12}$$

By substituting (11) and (12) back into (10) and solving for \mathbf{AEE} , we obtain

$$\mathbf{AEE} \geq \frac{\Upsilon}{2} + \sqrt{\left(n - \frac{\Upsilon}{2}\right)^2 + (4 - \Upsilon)\sigma}. \tag{13}$$

It is elementary to show that for $n \geq 2$ and $\sigma \geq 1$ the function

$$f(x) := \frac{x}{2} + \sqrt{\left(n - \frac{x}{2}\right)^2 + (4 - x)\sigma}$$

monotonically decreases in the interval $[0, 8]$. Consequently, the best lower bound for \mathbf{AEE} is attained not for $\Upsilon = 8$. Set $\Upsilon = 0$ into (13). We arrive at the first half of Theorem 4.4.

Upper bound. By definition of the Albertson-Estrada index,

$$\begin{aligned} \mathbf{AEE} &= n + \sum_{i=1}^n \sum_{k \geq 1} \frac{(s_i)^k}{k!} \leq n + \sum_{i=1}^n \sum_{k \geq 1} \frac{(|s_i|)^k}{k!} \\ &= n + \sum_{k \geq 1} \frac{1}{k!} \sum_{i=1}^n [(s_i)^2]^{\frac{k}{2}} \leq n + \sum_{k \geq 1} \frac{1}{k!} \left[\sum_{i=1}^n (s_i)^2 \right]^{\frac{k}{2}} \\ &= n + \sum_{k \geq 1} \frac{1}{k!} \left(2\sigma(G) \right)^{\frac{k}{2}} = n - 1 + \sum_{k \geq 0} \frac{\left(\sqrt{2\sigma(G)} \right)^k}{k!} \\ &= n - 1 + e^{\sqrt{2\sigma(G)}}, \end{aligned}$$

which directly leads to the right-hand side inequality in (9). By the proof of Theorem 4.4, this is completed. ■

Theorem 4.5 Let G be a graph with n vertices. Then $\mathbf{AEE}(G) \leq n - 1 + e^{\sqrt[4]{\mathbb{N}_4}}$.

Proof. By definition of the Albertson-Estrada index, we have

$$\begin{aligned} \mathbf{AEE}(G) &= \sum_{i=1}^n e^{s_i} = \sum_{i=1}^n \sum_{k=0}^{\infty} \frac{s_i^k}{k!} \leq n + \sum_{i=1}^n \sum_{k=1}^{\infty} \frac{|s_i|^k}{k!} = n + \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{i=1}^n (s_i^4)^{\frac{k}{4}} \\ &\leq n + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{i=1}^n s_i^4 \right)^{\frac{k}{4}} = n + \sum_{k=1}^{\infty} \frac{1}{k!} (\mathbb{N}_4)^{\frac{k}{4}} = n - 1 + \sum_{k=0}^{\infty} \frac{\sqrt[4]{\mathbb{N}_4^k}}{k!} \\ &= n - 1 + e^{\sqrt[4]{\mathbb{N}_4}}. \end{aligned}$$

Therefore, we have $\mathbf{AEE}(G) \leq n - 1 + e^{\sqrt[4]{\mathbb{N}_4}}$. ■

Theorem 4.6 Let G be a graph with n vertices. Then $\mathbf{AEE}(G) \leq e^{\sqrt{2\sigma(G)}}$.

Proof. By definition of the Albertson-Estrada index and relations (4) and (7), we have

$$\begin{aligned} \mathbf{AEE}(G) &= \sum_{i=1}^n e^{\varsigma_i} \leq \sum_{i=1}^n e^{|\varsigma_i|} = \sum_{i=1}^n \sum_{k \geq 0} \frac{(|\varsigma_i|)^k}{k!} \\ &= \sum_{k \geq 0} \frac{1}{k!} \sum_{i=1}^n (|\varsigma_i|)^k \leq \sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^n (|\varsigma_i|)^2 \right)^{\frac{k}{2}} \\ &= \sum_{k \geq 0} \frac{1}{k!} \left(\sum_{i=1}^n (\varsigma_i)^2 \right)^{\frac{k}{2}} = \sum_{k \geq 0} \frac{1}{k!} (2\sigma(G))^{\frac{k}{2}} \\ &= \sum_{k \geq 0} \frac{1}{k!} (\sqrt{2\sigma(G)})^k = e^{\sqrt{2\sigma(G)}}. \end{aligned}$$

■

5. Bound for the Albertson-Estrada index involving the Albertson energy

In this section, we investigate the relations between the Albertson-Estrada index and the Albertson energy.

Theorem 5.1 The Albertson Estrada index $\mathbf{AEE}(G)$ and the graph Albertson energy $\mathbf{AE}(G)$ satisfy the following inequality:

$$\frac{1}{2}\mathbf{AE}(G)(e-1) + n - n_+ \leq \mathbf{AEE}(G) \leq n - 1 + e^{\frac{\mathbf{AE}(G)}{2}}.$$

Proof. Lower bound. since $e^x \geq 1 + x$, equality holds if and only if $x = 0$ and $e^x \geq ex$, equality holds if and only if $x = 1$, we have

$$\begin{aligned} \mathbf{AEE}(G) &= \sum_{i=1}^n e^{\varsigma_i} = \sum_{\varsigma_i > 0} e^{\varsigma_i} + \sum_{\varsigma_i \leq 0} e^{\varsigma_i} \geq \sum_{\varsigma_i > 0} e^{\varsigma_i} + \sum_{\varsigma_i \leq 0} (1 + \varsigma_i) \\ &= e(\varsigma_1 + \varsigma_2 + \cdots + \varsigma_{n_+}) + (n - n_+) + (\varsigma_{n_++1} + \cdots + \varsigma_n) \\ &= (e-1)(\varsigma_1 + \varsigma_2 + \cdots + \varsigma_{n_+}) + (n - n_+) + \sum_{i=1}^n \varsigma_i = \frac{1}{2}\mathbf{AE}(G)(e-1) + n - n_+. \end{aligned}$$

Upper bound. from (8), we have

$$\mathbf{AEE}(G) \leq n + \sum_{k \geq 1} \frac{1}{k!} \sum_{i=1}^{n_+} (\varsigma_i)^k \leq n + \sum_{k \geq 1} \frac{1}{k!} \left(\sum_{i=1}^{n_+} \varsigma_i \right)^k = n - 1 + e^{\frac{\mathbf{AE}(G)}{2}}.$$

■

Theorem 5.2 Let G be a graph with largest eigenvalue ς_1 and p , τ and q be the number of positive, zero and negative eigenvalues of G , respectively. Then

$$\mathbf{AEE}(G) \geq e^{\varsigma_1} + \tau + (p-1)e^{\frac{\mathbf{AE}(G)-2\varsigma_1}{2(p-1)}} + qe^{-\frac{\mathbf{AE}(G)}{2q}}.$$

Proof. Let $\varsigma_1 \geq \cdots \geq \varsigma_p$ be the positive and $\varsigma_{n-q+1}, \dots, \varsigma_n$ be the negative eigenvalues of G . As the sum of eigenvalues of a graph is zero, one has $\mathbf{AE}(G) = 2 \sum_{i=1}^n \varsigma_i = -2 \sum_{i=n-q+1}^n \varsigma_i$.

By the arithmetic-geometric mean inequality, we have

$$\sum_{i=2}^p e^{s_i} \geq (p-1)e^{\frac{(s_2+\dots+s_p)}{(p-1)}} = (p-1)e^{\frac{\mathbf{AE}(G)-2s_1}{2(p-1)}}.$$

Similarly, $\sum_{i=n-q+1}^n e^{s_i} \geq qe^{-\frac{\mathbf{AE}(G)}{2q}}$. For the zero eigenvalues, we also have $\sum_{i=p+1}^{n-q} e^{s_i} = \tau$. So, we obtain

$$\mathbf{AEE}(G) \geq e^{s_1} + \tau + (p-1)e^{\frac{\mathbf{AE}(G)-2s_1}{2(p-1)}} + qe^{-\frac{\mathbf{AE}(G)}{2q}}.$$

■

Theorem 5.3 Let G be a graph with n vertices. Then

$$\mathbf{AEE}(G) - \mathbf{AE}(G) \leq n - 1 - \sqrt{2\sigma(G)} + e^{\sqrt{2\sigma(G)}}.$$

Proof. By definition of the Albertson-Estrada index, we have

$$\mathbf{AEE}(G) = n + \sum_{i=1}^n \sum_{k \geq 1} \frac{(s_i)^k}{k!} \leq n + \sum_{i=1}^n \sum_{k \geq 1} \frac{|s_i|^k}{k!}.$$

Moreover, by considering the Albertson energy, we get

$$\mathbf{AEE}(G) \leq n + \mathbf{AE}(G) + \sum_{i=1}^n \sum_{k \geq 2} \frac{|s_i|^k}{k!}.$$

Hence,

$$\mathbf{AEE}(G) - \mathbf{AE}(G) \leq n + \sum_{i=1}^n \sum_{k \geq 2} \frac{|s_i|^k}{k!} \leq n - 1 - \sqrt{2\sigma(G)} + e^{\sqrt{2\sigma(G)}}.$$

■

Theorem 5.4 Let G be a graph with n vertices. Then, $\mathbf{AEE}(G) \leq n - 1 + e^{\mathbf{AE}(G)}$.

Proof. By definition of the Albertson-Estrada index, we have

$$\mathbf{AEE}(G) \leq n + \sum_{i=1}^n \sum_{k \geq 1} \frac{|s_i|^k}{k!} \leq n + \sum_{k \geq 1} \frac{1}{k!} \left(\sum_{i=1}^n |s_i|^k \right) = n + \sum_{k \geq 1} \frac{(\mathbf{AE}(G))^k}{k!},$$

which implies $\mathbf{AEE}(G) \leq n - 1 + e^{\mathbf{AE}(G)}$.

■

6. Conclusion

In this paper, in section 3, we state some previously known results. In section 4, we introduce and investigate the Albertson energy and obtain lower and upper bounds for it. In section 5, we put forward the concept of Albertson-Estrada index, and obtain lower and upper bounds for it. In section 6, we investigate relations between the Albertson-Estrada index and the Albertson energy.

Acknowledgements

The author wish to record their sincere thanks to the anonymous referees for carefully reading the manuscript and making suggestions that improve the content and presentation of the paper.

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