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New bound for edge spectral radius and edge energy of graphs

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Abstract

Let $X(V,E)$ be a simple graph with n vertices and m edges without isolated vertices. Denote by $B=(b_{ij})_{m\times m}$ the edge adjacency matrix of X. Eigenvalues of the matrix B, $\mu_1,\mu_2,\cdots,\mu_m$, are the edge spectrum of the graph X. An important edge spectrum-based invariant is the graph energy, defined as $E_e(X)=\sum_{i=1}^{m}|\mu_i|$. Suppose B' be an edge subset of $E(X)$ (set of edges of X). For any $e\in B'$ the degree of the edge e_i with respect to the subset B' is defined as the number of edges in B' that are adjacent to e_i. We call it as ε-degree and is denoted by ε_i. Denote $\mu_1(X)$ as the largest eigenvalue of the graph X and s_i as the sum of ε-degree of edges that are adjacent to e_i. In this paper, we give lower bounds of $\mu_1(X)$ and $\mu_1^{D'}(X)$ in terms of ε-degree. Consequently, some existing bounds on the graph invariants $E_e(X)$ are improved.

Keywords: ε-degree, adjacency matrix, spectral radius, dominating set, graph energy, bound of energy.
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1. Introduction

Consider a molecular graph X with n vertices and m edges. It is commonly accepted to represent X by its vertex adjacency matrix A. This is a square, symmetric matrix of order n whose (i,j)-entry is equal to unity if the vertices i and j are adjacent, and is equal to zero otherwise. The edge adjacency matrix B is a square, symmetric matrix of order m, whose (i,j)-entry is equal to unity if the edges i and j are adjacent (Two edges are said to be adjacent if they are incident to a common

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vertex), and is equal to zero otherwise. In other words, matrix A reflects the adjacency of carbon atoms (existence of chemical bonds), whereas B reflects the adjacency of these bonds. The edge adjacency matrix was mentioned in the chemical graph theory [6, 8]. For any $e_i \in E$ (set of edges of X), the degree of e_i denoted by d_i, is the number of edges that are adjacent to e_i. A subset D' of E is called edge dominating set if every edges of $E - D'$ is adjacent to some edges in D'. Any edge dominating set with minimum cardinality is called minimum edge dominating set and this cardinality is called edge domination number (see for instance [16, 12, 1]). For any graph X, let $B(X) = b_{ij}$ be the edge adjacency matrix.

$$b_{ij} = \begin{cases} 1 & \text{if } e_i \text{ and } e_j \text{ are adjacent,} \\ 0 & \text{otherwise} \end{cases}$$

The eigenvalues $\mu_1, \mu_2, \cdots, \mu_m$ of the edge adjacency matrix $B(X)$ are said to be edge eigenvalues of the graph X and assumed in non-increasing order. The largest eigenvalue $\mu_1(X)$ is called spectral radius of the graph. Till now, there are many bounds for $\mu_1(X)$ (see for instance [17, 14, 7]).
The energy of the graph X is defined as

$$E(X) = \sum_{i=1}^{m} |\lambda_i|, \tag{1.1}$$

where λ_i, $i = 1, 2, \cdots, n$, are the eigenvalues of adjacency matrix of graph X.
This concept was put forward by Ivan Gutman and is intensely studied in chemistry, since it can be used to approximate the total π-electron energy of a molecule (see, e.g. [8, 15, 11, 10]). This spectrum-based graph invariant has been much studied in both chemical and mathematical literature. For more details on the mathematical aspects of the theory of graph energy and list of references see [9, 4, 5, 14, 3]. A number of topological indices can be reformulated in terms of the edge degrees instead of the vertex degrees such as the total edge adjacency index and the edge connectivity index. Motivated by the interesting results on energy of a graph, in this paper we define and consider the Edge energy and Bond energy(upper and lower bound) as $E_e(X) = \sum_{i=1}^{m} |\mu_i|$.
where μ_i, $i = 1, 2, \cdots, m$, are the eigenvalues of edge adjacency matrix of graph X.
Here, we present known results that will be needed in the forthcoming theorems.

Lemma 1.1. *If X is a connected graph on n vertices with m edges and let $\mu_1, \mu_2, \cdots, \mu_m$ be its edge eigenvalues.Then $\sum_{i=1}^{m} \mu_i = 0$ and $\sum_{i=1}^{m} \mu_i^2 = 2\sum_{1\leq i\leq j\leq m} b_{ij}$.*

Proof . We know $\sum_{i=1}^{m} \mu_i = trace(B(X)) = 0$.
Also $\sum_{i=1}^{m} \mu_i^2 = trace(B(X))^2 = \sum_{i=1}^{m}\sum_{j=1}^{m} b_{ij}^2 = 2\sum_{1\leq i\leq j\leq m} b_{ij}^2$. Since $b_{ij} = 1$ or 0 we have

$$\sum_{i=1}^{m} \mu_i^2 = 2 \sum_{1\leq i\leq j\leq m} b_{ij}.$$

□

Bearing this in mind, we immediately arrive at the following upper and lower bound for edge energy:

Theorem 1.2. *If X is a connected graph on n vertices with m edges then the following inequality hold,*

$$\sqrt{2 \sum_{1\leq i\leq j\leq m} b_{ij}} \leq E_e(X) \leq \sqrt{2m \sum_{1\leq i\leq j\leq m} b_{ij}}.$$

Proof . By the Cauchy-Schwartz inequality

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

we put $a_i = 1$ and $b_i = |\mu_i|$ in the above inequality we have

$$\begin{aligned}
[E_e(X)]^2 &= \left(\sum_{i=1}^{m} |\mu_i|\right)^2 \leq \left(\sum_{i=1}^{m} |1|^2\right)\left(\sum_{i=1}^{m} |\mu_i|^2\right) \\
&= m\left(\sum_{i=1}^{m} |\mu_i|^2\right) = 2m \sum_{1\leq i\leq j\leq m} b_{ij},
\end{aligned}$$

And $[E_e(X)]^2 = \left(\sum_{i=1}^{m} |\mu_i|\right)^2 \geq \sum_{i=1}^{m} |\mu_i|^2 = 2\sum_{1\leq i\leq j\leq m} b_{ij}$ which show the lower bound. □

Theorem 1.3. *If X is a connected graph on n vertices with m edges. then the following inequality hold.*

$$\sqrt{2\sum_{1\leq i\leq j\leq m} b_{ij} + m(m-1)det(B)^{\frac{2}{m}}} \leq E_e(X).$$

Proof . By using inequality between the arithmetic mean and geometric mean, we have,

$$\begin{aligned}
[E_e(X)]^2 &= \left(\sum_{i=1}^{m} |\mu_i|\right)^2 = \sum_{i=1}^{m} |\mu_i|^2 + \sum_{i\neq j} |\mu_i||\mu_j| \\
&= 2\sum_{1\leq i\leq j\leq m} b_{ij} + m(m-1)\mathbf{AM}|\mu_i||\mu_j| \\
&\geq 2\sum_{1\leq i\leq j\leq m} b_{ij} + m(m-1)\mathbf{GM}|\mu_i||\mu_j| \\
&= 2\sum_{1\leq i\leq j\leq m} b_{ij} + m(m-1)det(B)^{\frac{2}{m}}.
\end{aligned}$$

Where AM describes the arithemetic mean and GM the geometric mean, hence the inequality hold. □

In this section, we analyse the bound for $\mu_1(X)$ in terms of ε-degree. The ε-degree is also used to get bounds for the largest eigenvalue $\mu_1^{D'}(X)$ of this matrix.

Definition 1.4. *Let $X(V,E)$ be a simple graph and E' be any edge subset. The degree of an edge e_i of a graph X with respect to E' is the number of edges of E' that are adjacent to e_i. This degree is denoted by $d_{E'}(e_i)$ or ε_i.*

If $E' = \varnothing$ then $\varepsilon_i = 0$ and if $E' = E$ then $\varepsilon_i = d(e_i), \forall e_i \in E$.

Lemma 1.5. *[17]. Let B be a nonnegative symmetric matrix and x be a unit vector of R^n. If $\mu_1(B) = x^T Bx$, then $Bx = \mu_1(B)x$.*

2. BOUNDS FOR EDGE SPECTRAL RADIUS

Theorem 2.1. *Let X be a connected graph with m edges as $e_1, e_2, \cdots, e_m$. If $\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_m$ represent ε-degree sequence of these edges with respect to an edge subset E' of X then*

$$\mu_1(X) \geq \sqrt{\frac{\sum_{i=1}^m s_i^2}{\sum_{i=1}^m \varepsilon_i^2}},$$

Where, s_i is sum of ε-degree edges that are adjacent to e_i.

Proof . Let $\chi = (x_1, x_2, \cdots, x_m)^T$ be the unit positive eigenvector of E' corresponding to $\mu_1(X)$. Take

$$C = \frac{1}{\sqrt{\sum_{i=1}^m \varepsilon_i^2}}(\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_m)^T$$

Noting that C is a unit positive vector, we have

$$\begin{aligned} BC &= \frac{1}{\sqrt{\sum_{i=1}^m \varepsilon_i^2}}(\sum_{j=1}^m b'_{1j}\varepsilon_j, \sum_{i=1}^m b'_{2j}\varepsilon_j, \cdots, \sum_{i=1}^m b'_{mj}\varepsilon_j)^T \\ &= \frac{1}{\sqrt{\sum_{i=1}^m \varepsilon_i^2}}(s_1 + \sum_{j=1}^m d_{1j}\varepsilon_j, s_2 + \sum_{j=1}^m d_{2j}\varepsilon_j, \cdots, s_m + \sum_{j=1}^m d_{mj}\varepsilon_j)^T \end{aligned}$$

Similarly,

$$\begin{aligned} C^T B &= \frac{1}{\sqrt{\sum_{i=1}^m \varepsilon_i^2}}(s_1, s_2, \cdots, s_m), \\ C^T B^2 C &= \frac{1}{\sum_{i=1}^m \varepsilon_i^2}(s_1^2, s_2^2, \cdots, s_m^2) \end{aligned}$$

we have

$$\mu_1(X) = \sqrt{\mu_1(B^2)} = \sqrt{\chi^T B^2 \chi} \geq \sqrt{C^T B^2 C}$$

Hence

$$\mu_1(X) \geq \sqrt{\frac{\sum_{i=1}^m s_i^2}{\sum_{i=1}^m \varepsilon_i^2}}.$$

□

Definition 2.2. *Let D is a minimum edge dominating set, the minimum edge dominating adjacency matrix $B_D(X)$ is defined by $B_D(X) = D'(X) + B(X)$, where $B(X)$ is the edge adjacency matrix and $D'(X) = (d'_{ij})$ is $m \times m$ matrix with*

$$d'_{ij} = \begin{cases} 1 & \text{if } i = j \text{ and } e_i \in D \text{ ,} \\ 0 & \text{otherwise.} \end{cases}$$

Theorem 2.3. *Let X be a connected graph with m edges and D be a minimum edge dominating set. If $\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_m$ represents ε-degree sequence of these edges with respect to an edge subset D of X and $B_D(X)$ is minimum dominating matrix then*

$$\mu_1^{D'}(X) \geq \sqrt{\frac{\sum_{i=1}^m s_i^2 + \sum_{i=1}^k \varepsilon_i^2}{\sum_{i=1}^m \varepsilon_i^2}},\ k = |D|$$

Where, s_i is sum of ε-degree edges that are adjacent to e_i.

Proof . Let $\chi = (x_1, x_2, \cdots, x_m)^T$ be the unit positive eigenvector of $B_D(X)$ corresponding to $\mu_1^{D'}(X)$. Take

$$C = \sqrt{\frac{1}{\sum_{i=1}^m \varepsilon_i^2}}(\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_m)^T$$

Noting that C is a unit positive vector, we have

$$\begin{aligned}(D' + B)C &= \frac{1}{\sqrt{\sum_{i=1}^m \varepsilon_i^2}}\left(\sum_{j=1}^m (d'_{1j} + b_{1j})\varepsilon_j, \cdots, \sum_{j=1}^m (d'_{mj} + b_{mj})\varepsilon_j\right)^T \\ &= \frac{1}{\sqrt{\sum_{i=1}^m \varepsilon_i^2}}(s_1 + \sum_{j=1}^m d'_{1j}\varepsilon_j, \cdots, s_m + \sum_{j=1}^m d'_{mj}\varepsilon_j)^T,\end{aligned}$$

Similarly,

$$C^T(D' + B) = \frac{1}{\sqrt{\sum_{i=1}^m \varepsilon_i^2}}(s_1 + \sum_{j=1}^m d'_{1j}\varepsilon_j, \cdots, s_m + \sum_{j=1}^m d'_{mj}\varepsilon_j),$$

there for

$$\begin{aligned}C^T(D' + B)^2 C &= \frac{1}{\sqrt{\sum_{i=1}^m \varepsilon_i^2}}\left[\left(s_1 + \sum_{j=1}^m d'_{1j}\varepsilon_j\right)^2, \cdots, \left(s_m + \sum_{j=1}^m d'_{mj}\varepsilon_j\right)^2\right] \\ &\geq \frac{1}{\sqrt{\sum_{i=1}^m \varepsilon_i^2}}\left[s_1^2 + \cdots + s_m^2 + (\sum_{j=1}^m d'_{1j}\varepsilon_j)^2 + \cdots + (\sum_{j=1}^m d'_{mj}\varepsilon_j)^2\right],\end{aligned}$$

Therefore

$$C^T(D' + B)^2 C = \frac{1}{\sqrt{\sum_{i=1}^m \varepsilon_i^2}}\left[s_1^2 + \cdots + s_m^2 + \sum_{j=1}^m \varepsilon_j^2\right].$$

we have

$$\mu_1^{D'}(X) = \sqrt{\mu_1^{D'}(D' + B)^2} = \sqrt{\chi^T(D' + B)^2\chi} \geq \sqrt{C^T(D' + B)^2 C}.$$

Hence

$$\mu_1^{D'}(X) \geq \sqrt{\frac{\sum_{i=1}^m s_i^2 + \sum_{i=1}^k \varepsilon_i^2}{\sum_{i=1}^m \varepsilon_i^2}}.$$

□

3. An upper bound for the energy of a graph

The eigenvalues of edge adjacency matrix or adjacency of carbon bonds have wide applications in chemical graph. For instance, it can be used to present the edge energy level of specific electrons [2, 13]. In this section, we consider the edge energy of a graph X respect to edge subset of E, and give upper bound for it.

Theorem 3.1. *Let X be a graph with m edges, then*

$$E_e(X) \leq \sqrt{\frac{\sum_{i=1}^{m} s_i^2}{\sum_{i=1}^{m} \varepsilon_i^2}} + \sqrt{(m-1)\Big(T - \frac{\sum_{i=1}^{m} s_i^2}{\sum_{i=1}^{m} \varepsilon_i^2}\Big)}. \tag{3.1}$$

Note that $T = 2\sum_{1\leq i<j\leq m} b_{ij}$.

Proof . Suppose that $\mu_1, \mu_2, \cdots, \mu_m$ is the edge spectrum of X. Using Lemma 1.1 and applying the Cauchy–Schwartz inequality to the vectors $(|\mu_2||\mu_3||\mu_m|)$ and $(1, 1, \cdots, 1)$, we have

$$\begin{aligned} \left(\sum_{i=1}^{m} |\mu_i|\right)^2 &\leq (m-1)\sum_{i=1}^{m} |\mu_i^2 \\ (E_e(X) - \mu_1)^2 &\leq (m-1)(2\sum_{1\leq i<j\leq m} b_{ij} - \mu_1^2), \\ E_e(X) &\leq \mu_1 + \sqrt{(m-1)(2\sum_{1\leq i<j\leq m} b_{ij} - \mu_1^2)}. \end{aligned} \tag{3.2}$$

We define $f(x) = x + \sqrt{(m-1)(2\sum_{1\leq i<j\leq m} b_{ij} - x^2)}$, It is elementary to show that the function is monotonically decreases in for $\sqrt{\frac{2}{m}\sum_{1\leq i<j\leq m} b_{ij}} \leq x \leq \sqrt{2\sum_{1\leq i<j\leq m} b_{ij}}$. since, we consider $x^2 = \mu_1^2 \leq \sum_{i=1}^{m} \mu_i^2 \leq 2\sum_{1\leq i<j\leq m} b_{ij}$. so, $x \leq \sqrt{2\sum_{1\leq i<j\leq m} b_{ij}}$. By computing $F'(x) = 0$, we have $x = \sqrt{\frac{2}{m}\sum_{1\leq i<j\leq m} b_{ij}}$.

By theorem 2.1, $\mu_1(X) \geq \sqrt{\frac{\sum_{i=1}^{m} s_i^2}{\sum_{i=1}^{m} \varepsilon_i^2}}$ and the fact that f is monotonically decreasing, we have

$$f(\mu_1) \leq f\left(\sqrt{\frac{\sum_{i=1}^{m} s_i^2}{\sum_{i=1}^{m} \varepsilon_i^2}}\right),$$

According to inequality (3.2),

$$\begin{aligned} E_e(X) &\leq \mu_1 + \sqrt{(m-1)(2\sum_{1\leq i<j\leq m} b_{ij} - \mu_1^2)} = f(\mu_1) \\ &\leq f(\sqrt{\frac{\sum_{i=1}^{m} s_i^2}{\sum_{i=1}^{m} \varepsilon_i^2}}) = \sqrt{\frac{\sum_{i=1}^{m} s_i^2}{\sum_{i=1}^{m} \varepsilon_i^2}} + \sqrt{(m-1)\Big(T - \frac{\sum_{i=1}^{m} s_i^2}{\sum_{i=1}^{m} \varepsilon_i^2}\Big)}. \end{aligned}$$

□

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