Research Article

Fareeha Jamal, Muhammad Imran*, and Bilal Ahmad Rather

On inverse sum indeg energy of graphs

https://doi.org/10.1515/spma-2022-0175
received June 22, 2022; accepted October 03, 2022

Abstract: For a simple graph with vertex set $\{v_1, v_2, \ldots, v_n\}$ and degree sequence d_{v_i} $i = 1, 2, \ldots, n$, the inverse sum indeg matrix (ISI matrix) $A_{\text{ISI}}(G) = (a_{ij})$ of G is a square matrix of order n, where $a_{ij} = \frac{d_{v_i} d_{v_j}}{d_{v_i} + d_{v_j}}$, if v_i is adjacent to v_j and 0, otherwise. The multiset of eigenvalues $\tau_1 \geq \tau_2 \geq \cdots \geq \tau_n$ of $A_{\text{ISI}}(G)$ is known as the ISI spectrum of G. The ISI energy of G is the sum $\sum_{i=1}^{n} |\tau_i|$ of the absolute ISI eigenvalues of G. In this article, we give some properties of the ISI eigenvalues of graphs. Also, we obtain the bounds of the ISI eigenvalues and characterize the extremal graphs. Furthermore, we construct pairs of ISI equienergetic graphs for each $n \geq 9$.

Keywords: topological indices, adjacency matrix, inverse sum indeg matrix, energy

MSC 2020: 05C50, 05C09, 05C92, 15A18

1 Introduction

A graph $G = G(V, E)$ consists of a vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and an edge set $E(G)$. We consider only simple and undirected graphs, unless otherwise stated. The number of elements in $V(G)$ is the *order* n, and the number of elements in $E(G)$ is the *size* m of G. By $u \sim v$, we mean vertex u is adjacent to vertex v, we also denote an edge by e. The *neighbourhood* $N(v)$ of $v \in V(G)$ is the set of vertices adjacent to v. The *degree* d_{v_i} (or simply d_i) of a vertex v_i is the number of elements in the set $N(v_i)$. A graph G is called *r-regular* if the degree of every vertex is r. For two distinct vertices u and v in a connected graph G, the *distance* $d(u, v)$ between them is the length of a shortest path connecting them. The largest distance between any two vertices in a connected graph is called the *diameter* of G. We denote the complete graph by K_n, the complete bipartite graph by $K_{a,b}$, and the star by $K_{1,n-1}$. We follow the standard graph theory notation, and more graph theoretic notations can be found in [1].

The adjacency matrix $A(G)$ of G is a square matrix of order $n \times n$, with (i, j)th entry equals 1, if v_i and v_j are adjacent and 0 otherwise. Clearly, $A(G)$ is a real symmetric matrix, and its multiset of eigenvalues is known as the spectrum of G. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalue of $A(G)$, where the eigenvalue λ_1 is called the spectral radius of G. More about the adjacency matrix $A(G)$ can be seen in [1–3].

The energy [4] of G is defined as follows:

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|.$$

The energy is intensively studied in both mathematics and theoretical chemistry since it is the trace norm of real symmetric matrices in linear algebra and the total π-electron energy of a molecule, see [5,6]. For more about the energy of G, including the recent development, see [7–9].

*** Corresponding author: Muhammad Imran,** Department of Mathematical Sciences, College of Science, United Arab Emirate University, Al Ain 15551, Abu Dhabi, UAE, e-mail: m.imran658@uaeu.ac.ae
Fareeha Jamal: Department of Mathematical Sciences, College of Science, United Arab Emirate University, Al Ain 15551, Abu Dhabi, UAE, e-mail: 202090514@uaeu.ac.ae
Bilal Ahmad Rather: Department of Mathematical Sciences, College of Science, United Arab Emirate University, Al Ain 15551, Abu Dhabi, UAE, e-mail: bilalahmadrr@gmail.com

The inverse sum indeg index (ISI index) [10] is a topological index defined as follows:

$$\mathrm{ISI}(G) = \sum_{v_iv_j \in E(G)} \frac{d_{v_i} d_{v_j}}{d_{v_i} + d_{v_j}}.$$

The ISI index is a well-studied topological index and has many applications in quantitative structure-activity or structure-property relationships (QSAR/QSPR) [11–13].

The inverse sum indeg matrix (ISI matrix) of a graph G, introduced by Zangi et al. [14], is a square matrix of order n defined as follows:

$$A_{\mathrm{ISI}}(G) = (a_{ij})_{n \times n} = \begin{cases} \dfrac{d_{v_i} d_{v_j}}{d_{v_i} + d_{v_j}} & \text{if } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise}. \end{cases}$$

The ISI matrix is a real symmetric, and its eigenvalues are also real. We order its eigenvalues from largest to smallest by

$$\tau_1 \geq \tau_2 \geq \cdots \geq \tau_n.$$

The multiset of all eigenvalues of the ISI matrix of G is known as the ISI spectrum of G, and the largest eigenvalue τ_1 is called the ISI- spectral radius of G. If an eigenvalue, say τ, of the ISI matrix occurs with algebraic multiplicity $k \geq 2$, then we denote it by $\tau^{[k]}$. The ISI energy of G is defined as follows:

$$\mathcal{E}_{\mathrm{ISI}}(G) = \sum_{i=1}^{n} |\tau_i|.$$

Zangi et al. [14] gave the basics properties of the ISI matrix including the bounds for the ISI energy of graphs. Hafeez and Farooq [15] obtained ISI spectrum and ISI energy from special graphs. They also gave some bounds on the ISI energy of graphs. Bharali et al. [16] gave some bounds on ISI energy and introduced ISI Estrada index of G. Havare [17] obtained the ISI index and ISI energy of the molecular graphs of Hyaluronic Acid-Paclitaxel conjugates. For some other types of energies and indices, see [18–26].

In Section 2, we characterize graphs with two distinct ISI eigenvalues and three distinct ISI eigenvalues among bipartite graphs and give some sharp bounds on the ISI spectral radius and the ISI energy of graphs, which are better than already known results. In Section 3, we give the ISI spectrum of the join of two graphs, and as a consequence, we construct ISI equienergetic graphs for every integer $n \geq 9$. We end up article with a conclusion for future work.

2 Inverse sum indeg energy of graphs

It is trivial that nK_1 is the only graph with exactly one ISI eigenvalue and its ISI spectrum is $\{0^{[n]}\}$. Next, we have result about graphs whose all ISI eigenvalues are equal in absolute value.

Proposition 2.1. *Let G be a graph of order n. Then, $|\tau_1| = |\tau_2| = \cdots = |\tau_n|$ if and only if $G \cong nK_1$ or $G \cong \frac{n}{2}K_2$.*

Proof. If G is either nK_1 or $\frac{n}{2}K_2$, then the ISI spectrum of nK_1 is $\{0^{[n]}\}$ and ISI spectrum of $\frac{n}{2}K_2$ is $\left\{\left(\frac{1}{2}\right)^{\left[\frac{n}{2}\right]}, \left(-\frac{1}{2}\right)^{\left[\frac{n}{2}\right]}\right\}$. Now, it is clear that $|\tau_1| = |\tau_2| = \cdots = |\tau_n|$.

Conversely, assume that $|\tau_1| = |\tau_2| = \cdots = |\tau_n|$ and let k be the number of isolated vertices in G. If $k \geq 1$, then $\tau_1 = \tau_2 = \cdots = \tau_n = 0$ and $G \cong nK_1$. The other possibility is that $k = 0$, and if maximum degree is 1, then $d_i = 1$, for $i = 1, 2, \ldots, n$. Thus, G must be $\frac{n}{2}K_2$. Now, if maximum degree is greater than or equal to two, then G

contains a connected component G' with order at least 3. By Perron-Frobenius theorem, $\tau_1(G) > \tau_2(G')$, which is not possible. Thus, $G \cong \frac{n}{2}K_2$. □

The following well-known result provides a relationship between the number of distinct eigenvalues in a graph and its diameter. It can be found in [2].

Theorem 2.2. [2] *Let G be a connected graph with diameter D. Then, G has at least $D + 1$ distinct adjacency eigenvalues.*

From the proof of Theorem 2.2 (Proposition 1.3.3, [2]), it follows that Theorem 2.2 is true for any non-negative symmetric matrix $M = (m_{ij})_{n\times n}$ indexed by the order of a graph G, in which $m_{ij} > 0$ if and only if v_i is adjacent to v_j. The following result is the consequence of Theorem 2.2.

Corollary 2.3. *If G is a graph of diameter D and has t distinct ISI eigenvalues, then $D \le t - 1$.*

Another immediate important consequence is given as follows.

Corollary 2.4. *Let G be a connected graph of order $n \ge 2$. Then, G has exactly two distinct ISI eigenvalues if and only if G is the complete graph.*

Proof. Let $G \cong K_n$, then the ISI spectrum of G is $\left\{\frac{(n-1)^2}{2}, \left(-\frac{(n-1)}{2}\right)^{[n-1]}\right\}$, and G has two distinct ISI eigenvalues.

Conversely, if G has exactly two distinct eigenvalues, from Corollary 2.3, its diameter is 1. Therefore, G is necessarily K_n. □

The following observation states that G has a symmetric ISI spectrum towards the origin if G is bipartite.

Remark 2.5. Clearly, the ISI matrix of the bipartite graph G can be written as follows:

$$\mathrm{ISI}(G) = \begin{pmatrix} \mathbf{0} & B \\ B^T & \mathbf{0} \end{pmatrix}.$$

If τ is an eigenvalue of $\mathrm{ISI}(G)$ with an associated eigenvector $X = (x_1, x_2)^T$, then it is clear that $\mathrm{ISI}(G)X = \tau X$. Also, it is easy to see that $\mathrm{ISI}(G)X' = -\tau X'$, where $X' = (x_1, -x_2)^T$. This implies that the ISI eigenvalues of a bipartite graph are symmetric about the origin.

Proposition 2.6. *Let G be a bipartite graph. Then, G has three distinct ISI eigenvalues if and only if G is the complete bipartite graph.*

Proof. Let $G \cong K_{a,b}$ be the complete bipartite graph with partite cardinality a and b, $(a + b = n)$. Then, the ISI spectrum (see [15]) of G is

$$\left\{\frac{(ab)^{\frac{3}{2}}}{n}, 0^{[n-2]}, -\frac{(ab)^{\frac{3}{2}}}{n}\right\},$$

and clearly G has three distinct ISI eigenvalues. Conversely, if we assume that G has three distinct ISI eigenvalues, then by Corollary 2.3, the diameter of G is at most two. Also, by Corollary 2.4, diameter of G cannot be one as in this case G cannot have three distinct ISI eigenvalues. So, diameter of G is exactly two. As G is a bipartite graph of diameter two, so any two non-adjacent vertices of G must have the same neighbour; otherwise, if a vertex u has neighbour w not adjacent to v, then w along with uv-path induces the path P_4 subgraph, which cannot happen as the diameter of G is two. Thus, any two non-adjacent vertices in G share the common neighbour, and it follows that G is the complete bipartite graph. □

The sum of the squares of the eigenvalues (Frobenius norm of real symmetric matrix) of the ISI matrix (Theorem 5, [14]) is

$$\sum_{i=1}^{n}\tau_i^2 = -2\sum_{1\le i<j\le n}\tau_i\tau_j = 2\sum_{1\le i<j\le n}\left(\frac{d_id_j}{d_i+d_j}\right)^2 = 2B, \tag{1}$$

where $B = \sum_{1\le i<j\le n}\left(\frac{d_id_j}{d_i+d_j}\right)^2$.

The following result gives the bounds for the ISI spectral radius of graphs in terms of the Frobenius norm and ISI index.

Lemma 2.7. *Let G be a graph of order n. Then the following holds*

(i) $\sqrt{\frac{2B}{n}} \le \tau_1 \le \sqrt{\frac{2(n-1)B}{n}}$, *with equality on left if and only if* $G \cong nK_1$ *or* $G \cong \frac{n}{2}K_2$. *While for connected graph, right equality holds if and only if* $G \cong K_n$.

(ii) $\tau_1 \ge \frac{2\mathrm{ISI}(G)}{n}$ *with equality holding if and only if G is a connected regular graph.*

Proof. As $\tau_1^2+\tau_2^2+\cdots+\tau_n^2 = 2B$, so $2B \le n\tau_1^2$, with equality if and only if $|\tau_1| = |\tau_2| = \cdots = |\tau_n|$. By Proposition 2.1, $G \cong nK_1$ or $G \cong \frac{n}{2}K_2$.

Also, by the Cauchy-Schwartz inequality, we have

$$\tau_1^2 = 2B - \sum_{i=2}^{n}\tau_i^2 \le 2B - \frac{1}{n-1}\left(\sum_{i=2}^{n}\tau_i\right)^2 = 2B - \frac{\tau_1^2}{n-1}.$$

Therefore, $\tau_1 \le \sqrt{\frac{2(n-1)B}{n}}$. If equality holds, then all above inequalities are equalities, that is $\tau_2 = \tau_3 = \cdots = \tau_n$. It follows that G has two distinct ISI eigenvalues. By Corollary 2.4, G is the complete graph.

(ii) Let $X = (x_1, x_2, \ldots, x_n)^T$ be an arbitrary vector of $\mathbb{R}^n$ and let J denote the vector with all entries equal to 1, that is $J = (1, 1, \ldots, 1)$. Furthermore, we note that $A_{\mathrm{ISI}}(G)$ is non-negative and an irreducible matrix. Thus, by Perron-Frobenius theorem, $\tau_1 \ge |\tau_i|$ for all i and $\tau_1 > 0$. Therefore, by Rayleigh quotient for Hermitian matrices [27], we have

$$\tau_1 = \max_{X\neq 0}\frac{X^TA_{\mathrm{ISI}}(G)X}{X^TX} \ge \frac{J^TA_{\mathrm{ISI}}(G)J}{X^TX} = \frac{2\mathrm{ISI}(G)}{n}.$$

If G is an r-regular graph, then $A_{\mathrm{ISI}}(G) = \frac{r}{2}A(G)$. Also, it is well known that the largest eigenvalue λ_1 of $A(G)$ is bounded above by the maximum degree Δ with equality if and only if G is regular. So, for regular graphs, we have $\tau_1 = \frac{r^2}{2}$ and $\frac{2\mathrm{ISI}(G)}{n} = \frac{2rm}{2n} = \frac{r^2}{2} = \tau_1$, since $m = \frac{nr}{2}$. □

Next, we have the analogue of the McClelland bound for the ISI energy of a graph. The upper bound of (i) part of Theorem 2.8 is given in [15], but extremal graphs were not characterized.

Theorem 2.8. *Let G be a graph of order n. Then,*

$$2\sqrt{B} \le \mathcal{E}_{\mathrm{ISI}}(G) \le \sqrt{2nB},$$

with equality holding on right if and only if $G \cong nK_1$ *or* $G \cong \frac{n}{2}K_2$ *and equality holding on left if and only if* $G \cong K_{a,b}$, $a+b=n$.

Proof. By applying the Cauchy-Schwarz inequality to vector $(|\tau_1|, |\tau_2|, \ldots, |\tau_n|)$, we have

$$\mathcal{E}_{\mathrm{ISI}}(G) = \sum_{i=1}^{n}|\tau_i| \le \sqrt{n\sum_{i=1}^{n}\tau_i^2} = \sqrt{2nB}, \tag{2}$$

with equality holding if and only if $|\tau_1| = |\tau_2| = \cdots = |\tau_n|$. By Proposition 2.1, G is either nK_1 or $\frac{n}{2}K_2$.

Also, by equation (1), we have

$$(\mathcal{E}_{\mathrm{ISI}}(G))^2 = \sum_{i=1}^{n}\tau_i^2 + 2\sum_{1\le i<j\le n}|\tau_i||\tau_j| \ge \sum_{i=1}^{n}\tau_i^2 + 2\left|\sum_{1\le i<j\le n}\tau_i\tau_j\right| = 2\sum_{i=1}^{n}\tau_i^2 = 4B,$$

with equality holding if and only if $\tau_1 = -\tau_n$ and $\tau_2 = \cdots = \tau_{n-1} = 0$. By Proposition 2.6, G must be the complete bipartite graph, since ISI spectrum is symmetric towards origin and 0 is the ISI eigenvalue of G with multiplicity $n-2$. Conversely, for $G \cong K_{a,b}$, $\sqrt{B} = \frac{(ab)^{\frac{3}{2}}}{n}$, and $\mathcal{E}_{\mathrm{ISI}}(K_{a,b}) = 2\frac{(ab)^{\frac{3}{2}}}{n} = 2\sqrt{B}$. □

The second part of the next result is the analogue of Koolen-Moulton bound for the ISI energy of graphs.

Theorem 2.9. *Let G be a graph of order n. Then, the following hold.*

(i) *If G is connected, then*

$$\mathcal{E}_{\mathrm{ISI}}(G) \ge 2\tau_1 \ge \frac{4\mathrm{ISI}(G)}{n},$$

with equality if and only if G is regular and has only one positive ISI eigenvalue, like the complete regular multipartite graphs, the Peterson graph and its complement.

(ii)

$$\mathcal{E}_{\mathrm{ISI}}(G) \le \frac{2\mathrm{ISI}(G)}{n} + \sqrt{(n-1)\left(2B - \left(\frac{2\mathrm{ISI}(G)}{n}\right)^2\right)}.$$

The bound is achieved if G is either nK_1, $\frac{n}{2}K_2$, K_n or a non-complete connected graph with three distinct ISI eigenvalues $\tau_1 = \frac{2\mathrm{ISI}(G)}{n}$ and the other two distinct eigenvalues with absolute value $\sqrt{\frac{2B-\left(\frac{2\mathrm{ISI}(G)}{n}\right)^2}{(n-1)}}$.

Proof. Let $p \ge 1$ be the number of positive ISI eigenvalues. Then,

$$\mathcal{E}_{\mathrm{ISI}}(G) = \sum_{i=1}^{n}|\tau_i| = 2\sum_{i=1}^{p}|\tau_i| \ge 2\tau_1,$$

with equality holding if and only if G has only two non-zero ISI eigenvalues (one positive and one negative as $\sum_{i=1}^{n}\tau_i = 0$). By Lemma 2.7, we obtain

$$\mathcal{E}_{\mathrm{ISI}}(G) \ge \frac{4\mathrm{ISI}(G)}{n},$$

with equality holding if and only if G is a regular connected graph with only one positive ISI eigenvalue.

(ii) By the Cauchy-Schwartz inequality, we have

$$\mathcal{E}_{\mathrm{ISI}}(G) = \tau_1 + \sum_{i=2}^{n}|\tau_i| \le \tau_1 + \sqrt{(n-1)(2B-\tau_1^2)}, \tag{3}$$

with equality if and only if $|\tau_2| = |\tau_3| = \cdots = |\tau_n|$. We can easily verify that $F(x) = x + \sqrt{(n-1)(2B-x^2)}$ is decreasing in the interval $\left(\sqrt{\frac{2B}{n}}, \sqrt{2B}\right)$. Thus, inequality (3) remains valid if on the right side of $F(x)$, the variable is replaced with any lower bound of τ_1. So from Lemma 2.7. we have

$$\mathcal{E}_{\mathrm{ISI}}(G) \le \frac{2\mathrm{ISI}(G)}{n} + \sqrt{(n-1)\left(2B - \left(\frac{2\mathrm{ISI}(G)}{n}\right)^2\right)}.$$

The equality occurs if and only if all inequalities are equalities. By Lemma 2.7, G is a regular graph and by equality in the Cauchy-Schwartz inequality if $|\tau_2| = |\tau_3| = \cdots = |\tau_n| = \sqrt{\frac{2B-\left(\frac{2\mathrm{ISI}(G)}{n}\right)^2}{(n-1)}}$. Thus, we have two cases: first possibility is G has two distinct ISI eigenvalues and by Corollary 2.4, $G \cong K_n$. The second possibility is that G has three distinct ISI eigenvalues, $\tau_1 = \frac{2\mathrm{ISI}(G)}{n}$ and the other two distinct eigenvalues with absolute value $\sqrt{\frac{2B-\left(\frac{2\mathrm{ISI}(G)}{n}\right)^2}{(n-1)}}$. □

Next, lemma is an application of interlacing theorem, it relates the independence number (the cardinality of a largest pairwise non-adjacent vertex set) to the number of positive and non-positive ISI eigenvalues of G.

Lemma 2.10. *Let G be a graph with n vertices, and let p and q be the number of ISI eigenvalues that are greater than and less than equal to* 0*, respectively. Then,*

$$\mu \le \min\{n-p, n-q\},$$

where μ is the independence number of G.

Proof. As G has independence number μ, so the ISI matrix of G has the principal submatrix $M' = \mathbf{0}_{\mu\times\mu}$. By interlacing theorem [27], we obtain $\tau_\mu(A_{\mathrm{ISI}}(G)) \ge \tau_\mu(M') = 0$ and $\tau_{n-\mu+1}(A_{\mathrm{ISI}}(G)) \ge \tau_1(M') = 0$. This completes the proof. □

Theorem 2.11. *Let G be a connected graph with independence number μ, p, and q number of ISI eigenvalues which are greater than and less than equal to* 0*, respectively. Then*

$$\mathcal{E}_{\mathrm{ISI}}(G) \le 2\sqrt{(n-\mu)B}, \tag{4}$$

with equality holding if and only if G is the star graph $K_{1,n-1}$.

Proof. Let $\tau_1 \ge \tau_2 \ge \cdots \ge \tau_p$ and $\tau_1' \ge \tau_2' \ge \cdots \ge \tau_q'$ be the positive and non-positive ISI eigenvalues of G, respectively. Since $\sum_{i=1}^{n}\tau_i = 0$, so $\sum_{i=1}^{p}\tau_i = \sum_{i=1}^{q}|\tau_i'|$ and by the definition of ISI energy, we have

$$\mathcal{E}_{\mathrm{ISI}}(G) = 2\sum_{i=1}^{p}\tau_i = 2\sum_{i=1}^{q}|\tau_i'|.$$

Now, by using the Cauchy-Schwartz inequality, we have

$$\mathcal{E}_{\mathrm{ISI}}(G) = 2\sum_{i=1}^{p}\tau_i \le 2\sqrt{p\sum\nolimits_{i=1}^{p}\tau_i^2},$$

with equality holding if and only if $\tau_1 = \tau_2 = \cdots = \tau_p$.

Similarly,

$$\mathcal{E}_{\mathrm{ISI}}(G) = 2\sum_{i=1}^{q}|\tau_i'| \le 2\sqrt{q\sum\nolimits_{i=1}^{q}(\tau_i')^2},$$

with equality holding if and only if $|\tau_1'| = |\tau_2'| = \cdots = |\tau_q'|$. Now, by Lemma 2.10, we have

$$\frac{(\mathcal{E}_{\mathrm{ISI}}(G))^2}{2} \le p\sum_{i=1}^{p}\tau_i^2 + q\sum_{i=1}^{q}(\tau_i')^2 \le (n-\mu)\sum_{i=1}^{p}\tau_i^2 + (n-\mu)\sum_{i=1}^{q}(\tau_i')^2 = (n-\mu)\sum_{i=1}^{n}\tau_i^2 = (n-\mu)2B,$$

and the required inequality (4) follows.

If equality holds in (4), then from above, we have $\tau_1 = \tau_2 = \cdots = \tau_p, |\tau_1'| = |\tau_2'| = \cdots = |\tau_q'|$, and $p = q = n-\mu$. But by the Perron-Frobenious theorem, τ_1 is a simple eigenvalue of G, so $p = 1$, and it implies that $q = 1$, $\mu = n-1$, and the ISI eigenvalue 0 has multiplicity $n-2$. By Lemma 2.6, G is the complete bipartite graph, thereby it follows that $G \cong K_{1,n-1}$, since its independence number is $n-1$.

Also, the ISI spectrum ([15], Theorem 8) of $K_{1,n-1}$ is

$$\left\{0^{[n-2]}, \pm\frac{\sqrt{(n-1)^3}}{n}\right\},$$

the independence number is $\alpha = n-1$, and

$$2B = \left(\frac{\sqrt{(n-1)^3}}{n}\right)^2 + \left(-\frac{\sqrt{(n-1)^3}}{n}\right)^2 = 2\frac{(n-1)^3}{n^2}.$$

Therefore, we have

$$2\sqrt{(n-\mu)B} = 2\sqrt{(n-n+1)\frac{(n-1)^3}{n^2}} = 2\frac{\sqrt{(n-1)^3}}{n} = \mathcal{E}_{\mathrm{ISI}}(K_{1,n-1}).$$

This proves the equality case. □

3 ISI equienergetic graphs

Two graphs of the same order are said to be equienergetic (or adjacency equienergetic) if they have the same energy but have a different adjacency spectrum. Likewise, two graphs of order n are said to be ISI equienergetic if they have the same ISI energy but distinct ISI spectrum.

Let G_1 and G_2 be the connected graphs of order n_1 and n_2, respectively. The join of G_1 and G_2, denoted by $G_1 + G_2$, is the graph obtained by joining each vertex of G_1 to every vertex of G_2. If both G_1 and G_2 are complete graphs, then $G_1 + G_2$ is the complete graph, otherwise its diameter is 2.

Suppose we have a matrix M partitioned in some block form, and we form a new matrix Q whose entries are the average row sums of the blocks of the partitioned matrix, then such a matrix is known as the quotient matrix. If the average row sums of blocks are some constant, not necessarily same for all blocks, and this happens for every block we say that the quotient matrix is equitable. In general, the eigenvalues of Q matrix interlace those of M. While for equitable quotient matrix, each of the eigenvalues of Q is the eigenvalue of M [1,2].

The following theorem gives the ISI spectrum of the join of two regular non-complete graphs.

Theorem 3.1. *Let G_1 and G_2 be r_1-regular and r_2-regular graphs of order n_1 and n_2, respectively. Let $\lambda_1 = r_1, \lambda_2, \ldots, \lambda_{n_1}$, and $\lambda_1' = r_2, \lambda_2', \ldots, \lambda_{n_2}'$ be the adjacency eigenvalues of G_1 and G_2, respectively. Then, the ISI spectrum of $G_1 + G_2$ consists of the eigenvalues $\frac{r_1+n_2}{2}\lambda_i$ and $\frac{r_2+n_1}{2}\lambda_j'$, where $i = 2, 3, \ldots, n_1$ and $j = 2, 3, \ldots, n_2$, and the other two eigenvalues are*

$$\frac{1}{2}\left(\frac{1}{2}(r_1^2 + n_2r_1 + r_2^2 + n_1r_2) \pm \sqrt{D}\right),$$

where $D = \left(\frac{r_1^2+n_2r_1+r_2^2+n_1r_2}{2}\right)^2 - 4\left(\frac{r_1r_2(r_1+n_2)(r_2+n_1)}{4} - n_1n_2\left(\frac{(r_1+n_2)(r_2+n_1)}{r_1+r_2+n}\right)^2\right)^2.$

Proof. Let $G = G_1 + G_2$ be the join of r_1-regular graph G_1 and r_2-regular graph G_2. Clearly, G is of order $n = n_1 + n_2$. We first index the vertices of G_1 and then the vertices G_2. With this indexing, the ISI matrix is

$$M = \begin{pmatrix} \frac{r_1+n_2}{2}A(G_1) & \frac{(r_1+n_2)(r_2+n_1)}{r_1+r_2+n}J_{n_1\times n_2} \\ \frac{(r_1+n_2)(r_2+n_1)}{r_1+r_2+n}J_{n_2\times n_1} & \frac{r_2+n_1}{2}A(G_2) \end{pmatrix}, \tag{5}$$

where $J_{n_1\times n_2}$ and $J_{n_2\times n_1}$ are the matrices whose each entry equals 1, and $A(G_i)$ is the adjacency matrix of G_i, for $i = 1, 2$. Since G_1 is r_1 regular, it follows that r_1 is an eigenvalue of $A(G_1)$ with the corresponding eigenvector J (whose all entries are equal to 1), and J is orthogonal to all other eigenvectors of G_1. Let x be a non-zero column vector satisfying $A(G_1)x = \lambda_i x$ and $J^Tx = 0$. Noting that $J_{n_1\times n_2}x = 0$ and taking $X = \binom{x}{0}$, we obtain

$$MX = \frac{r_1+n_2}{2}\lambda_i X.$$

This implies that if λ_i is the eigenvalue of $A(G_1)$, $\lambda \neq r_1$, then $\frac{r_1+n_2}{2}\lambda_i$ is the eigenvalue of the ISI matrix of $G_1 + G_2$. In this way, we obtain $n_1 - 1$ eigenvalues $\frac{r_1+n_2}{2}\lambda_i$, $i = 2, 3, \ldots, n$ of matrix (5).

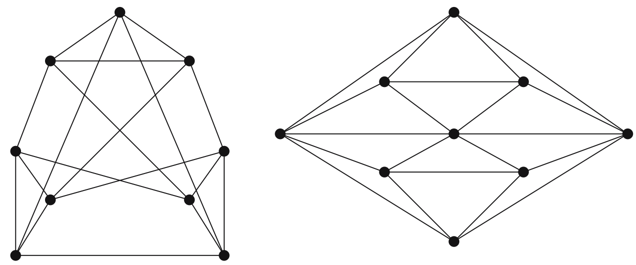

Figure 1: Two equienergetic graphs on none vertices.

Similarly as above, we can verify that $\frac{r_2+n_1}{2}\lambda_i'$, $i = 2, 3, \ldots, n_2$, are $n_2 - 1$ eigenvalues of the ISI matrix of G. The other two ISI eigenvalues of $G_1 + G_2$ are those of the quotient matrix

$$\begin{pmatrix} r_1\frac{r_1+n_2}{2} & n_2\frac{(r_1+n_2)(r_2+n_1)}{r_1+r_2+n} \\ n_1\frac{(r_1+n_2)(r_2+n_1)}{r_1+r_2+n} & r_2\frac{r_2+n_1}{2} \end{pmatrix}. \tag{6}$$

Clearly, the characteristic polynomial of (6) is

$$\lambda^2 - \frac{\lambda}{2}(r_1(r_1+n_2) + r_2(r_2+n_1)) + \frac{r_1r_2(r_1+n_2)(r_2+n_1)}{4} - n_1n_2\left(\frac{(r_1+n_2)(r_2+n_1)}{r_1+r_2+n}\right)^2$$

and its zeros are

$$\frac{1}{2}\left(\frac{1}{2}(r_1^2 + n_2r_1 + r_2^2 + n_1r_2) \pm \sqrt{D}\right),$$

where $D = \left(\frac{r_1^2+n_2r_1+r_2^2+n_1r_2}{2}\right)^2 - 4\left(\frac{r_1r_2(r_1+n_2)(r_2+n_1)}{4} - n_1n_2\left(\frac{(r_1+n_2)(r_2+n_1)}{r_1+r_2+n}\right)^2\right)^2$. This completes the proof. □

The following result gives the ISI energy of $G_1 + G_2$ in terms of the adjacency energy of G_1 and G_2, when both G_1 and G_2 are regular.

Theorem 3.2. *Let G_1 and G_2 be r_1 and r_2 regular graphs of orders n_1 and n_2, respectively. The ISI energy of $G_1 + G_2$ is*

$$\frac{r_1+n_2}{2}\mathcal{E}(G_1) + \frac{r_2+n_1}{2}\mathcal{E}(G_2) - r_1\left(\frac{r_1+n_2}{2}\right) - r_2\left(\frac{r_2+n_1}{2}\right) + \sqrt{D},$$

where $D = \left(\frac{r_1^2+n_2r_1+r_2^2+n_1r_2}{2}\right)^2 - 4\left(\frac{r_1r_2(r_1+n_2)(r_2+n_1)}{4} - n_1n_2\left(\frac{(r_1+n_2)(r_2+n_1)}{r_1+r_2+n}\right)^2\right)^2$.

Proof. By Theorem 3.1, the ISI spectrum of $G_1 + G_2$ consists of $\frac{r_1+n_2}{2}$ times the adjacency eigenvalues of G_1 except r_1, $\frac{r_2+n_1}{2}$ times the adjacency eigenvalues of G_2, except that r_2 and the eigenvalues of Matrix (6). By the definition of ISI energy, we have

$$\begin{aligned}\mathcal{E}_{\text{ISI}}(G_1+G_2) &= \frac{r_1+n_2}{2}\sum_{i=2}^{n_1}|\lambda_i(G_1)| + \frac{r_2+n_1}{2}\sum_{i=2}^{n_2}|\lambda_i(G_2)| + \sqrt{D} \\ &= \frac{r_1+n_2}{2}\left(\sum_{i=2}^{n_1}|\lambda_i(G_1)| + r_1 - r_1\right) + \frac{r_2+n_1}{2}\left(\sum_{i=2}^{n_1}|\lambda_i(G_1)| + r_2 - r_2\right) + \sqrt{D} \\ &= \frac{r_1+n_2}{2}\mathcal{E}(G_1) + \frac{r_2+n_1}{2}\mathcal{E}(G_2) - r_1\left(\frac{r_1+n_2}{2}\right) - r_2\left(\frac{r_2+n_1}{2}\right) + \sqrt{D}.\end{aligned}$$ □

Theorem 3.3. *For every $n > 8$, there exists a pair of ISI equienergetic graphs of order n.*

Proof. Consider two 4-regular equienergetic graphs (Example 4.1, [28]) as in Figure 1. Also, $\mathcal{E}(G_1) = \mathcal{E}(G_2) = 16$ and $\mathcal{E}_{\mathrm{ISI}}(G_1) = \mathcal{E}_{\mathrm{ISI}}(G_1) = 32$. Let $H_1 = G_1 + K_\omega$ and $H_2 = G_2 + K_\omega$ be two new graphs. Then, by applying Theorem 3.2, we have

$$\mathcal{E}_{\mathrm{ISI}}(H_1) = \mathcal{E}_{\mathrm{ISI}}(H_2) = 24 + \frac{(t-1)^2}{2} + \frac{\sqrt{D'}}{4(2w+7)},$$

where $D' = 4\omega^6 + 196\omega^5 + 3{,}517\omega^4 + 28{,}578\omega^3 + 106{,}953\omega^2 + 156{,}528\omega + 28{,}224$. Therefore, H_1 and H_2 are the ISI equienergetic graphs. □

4 Conclusion

The extremal energy (ISI energy) problem is long standing, and it is very non-trivial to explicitly characterize the graphs with maximum and minimum energy (ISI energy) among general graphs. The problem of maximal (minimal) ISI energy of arbitrary graphs remains open. Besides, new concepts like the Estrada index, sum of k largest ISI eigenvalues (Ky Fan k-norm), Laplacian ISI matrices, distribution of ISI eigenvalues, spectral radius, and application of ISI spectra in chemical theory are yet to be introduced/investigated (like in [5,26,25]). The more important is relating the spectral parameters of the ISI matrix to the underlying graph structure and the relation of the ISI matrix to the adjacency matrix for irregular graphs remains challenging.

Funding information: This research is supported by UPAR Grant of United Arab Emirates University (UAEU),Al Ain, UAE via Grants No. G00003739.

Conflict of interest: The authors state no conflict of interest.

Data availability statement: All data generated or analysed during this study are included in this published article.

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