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Graphs with Maximum Laplacian–Energy–Like Invariant and Incidence Energy

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Abstract

The Laplacian–energy–like invariant, LEL, is the sum of the square roots of the Laplacian eigenvalues of the underlying graph G. The incidence energy IE is the sum of the square roots of the signless Laplacian eigenvalues of G. The vertex bipartiteness v_b of a graph G is the minimum number of vertices whose deletion from G results in a bipartite graph. Graphs having maximum LEL and IE values are determined among graphs with a fixed number n of vertices and fixed vertex bipartiteness, $1 \le v_b \le n-3$.

1 Introduction

In this paper we are concerned with simple graphs. For each such graph G, the vertex set is denoted by $\mathcal{V}(G)$ and its edge set by $\mathcal{E}(G)$. The order of G is n, and we label its vertices so that $\mathcal{V}(G) = \{1, \ldots, n\}$. An edge with end vertices i and j is denoted by ij. If two vertices i and j are not adjacent, i.e., if $ij \notin \mathcal{E}(G)$, then we write $i \nsim j$.

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The number of neighbors of a vertex i is its degree.

The complement of the graph G, denoted by \overline{G} , is the graph for which $\mathcal{V}(\overline{G}) = \mathcal{V}(G)$ and $\mathcal{E}(\overline{G}) = \{ij : ij \notin \mathcal{E}(G)\}.$

The subgraph induced by a vertex subset $S \subset \mathcal{V}(G)$, denoted by $\langle S \rangle$, is a graph with vertex set S and edge set $\mathcal{E}(\langle S \rangle) = \{ij : i, j \in S \land ij \in \mathcal{E}(G)\}$.

The spectrum of a matrix M (the multiset of the eigenvalues of M) will be denoted by $\sigma(M)$. If convenient, the multiplicities of the eigenvalues are represented in $\sigma(M)$ as powers in square brackets. For instance, $\sigma(M) = \{\xi_1^{[m_1]}, \xi_2^{[m_2]}, \dots, \xi_q^{[m_q]}\}$ indicates that ξ_1 has multiplicity m_1 , ξ_2 has multiplicity m_2 , and so on. If α is an eigenvalue of M and \mathbf{x} one of its eigenvectors, then the pair (α, \mathbf{x}) is an eigenpair of M.

The adjacency matrix of the graph G is the square matrix $A_G = (a_{ij})$ of order n, such that

$$a_{ij} = \begin{cases} 1 & \text{if } ij \in \mathcal{E}(G) \\ 0 & \text{otherwise.} \end{cases}$$

The spectrum of A_G , namely $\sigma(A_G) = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$, is referred to as the ordinary or A-spectrum of the graph G [7].

The vertex degree matrix D_G is the $n \times n$ diagonal matrix whose i-th diagonal entry is the degree of the i-th vertex of G. Then the Laplacian and the signless Laplacian matrices of G are $L_G = D_G - A_G$ and $Q_G = D_G + A_G$, respectively. Both are positive semidefinite [4,7], and their spectra are called the Laplacian and signless Laplacian spectra of the graph G. The respective eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ and $s_1 \geq s_2 \geq \cdots \geq s_n \geq 0$ are the Laplacian and the signless Laplacian eigenvalues of G.

The Laplacian–energy–like invariant, LEL, was introduced in [26], and is defiend as

$$LEL = LEL(G) = \sum_{i=1}^{n} \sqrt{\mu_i}.$$
 (1)

In [26] it was claimed that the properties of LEL are similar to those of the Laplacian graph energy (hence the name). It was later demonstrated that LEL is much more analogous to the ordinary graph energy, based on the A-spectrum [21]. For more details on LEL see the reviews [25,38], the recent papers [12,28,33–35], and the references cited therein.

The incidence energy, IE(G) was introduced in [22] as the energy of the incidence matrix of the underlying graph G. Eventually [20], it was discovered that IE obeys a relation fully analogous to (1), namely

$$IE = IE(G) = \sum_{i=1}^{n} \sqrt{s_i}$$
.

For details on IE see the review [3], the recent papers [2, 11, 19, 27, 29, 34], and the references cited therein.

Of the numerous results known in the theory of Laplacian and signless Laplacian graph spectra [5, 8, 9, 17, 18, 24, 30–32], we recall the following.

The Laplacian eigenvalues $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) = 0$ of a graph G and $\mu_1(\overline{G}) \geq \mu_2(\overline{G}) \geq \cdots \geq \mu_n(\overline{G}) = 0$ of its complement \overline{G} are related as $\mu_j(\overline{G}) = n - \mu_{n-j}(G)$ for $j = 1, 2, \ldots, n-1$.

The spectra of L_G and Q_G coincide if and only if the graph G is bipartite.

For $u, w \in \mathcal{V}(G)$ and $u \nsim v$, let G^+ be the graph obtained by adding to G the new edge e = uw. The eigenvalues of L(G) and Q(G) interlace the eigenvalues of $L(G^+)$ and $Q(G^+)$, respectively and

$$trace(L(G^+)) - trace(L(G)) = trace(Q(G^+)) - trace(Q(G)) = 2$$
.

This, in particular, implies

$$\sum_{i=1}^n \sqrt{\mu_i\left(G\right)} < \sum_{i=1}^n \sqrt{\mu_i(G^+)} \qquad \text{ and } \qquad \sum_{i=1}^n \sqrt{s_i(G)} < \sum_{i=1}^n \sqrt{s_i(G^+)}$$

i.e.,

$$LEL(G) < LEL(G^+)$$
 and $IE(G) < IE(G^+)$.

2 Join graph operations

Let G_1 and G_2 be two vertex-disjoint graphs. Their *join* is the graph $G_1 \vee G_2$ such that

$$\mathcal{V}(G_1 \vee G_2) = \mathcal{V}(G_1) \cup \mathcal{V}(G_2)$$

and

$$\mathcal{E}(G_1 \vee G_2) = \mathcal{E}(G_1) \cup \mathcal{E}(G_2) \cup \{ij : i \in \mathcal{V}(G_1) \land j \in \mathcal{V}(G_2)\}.$$

A generalization of the join operation was introduced in [6] as follows:

Consider a family of vertex-disjoint graphs, $\mathcal{F} = \{G_1, \dots, G_k\}$, where G_i has order n_i , for $1 \leq i \leq k$, and a graph H such that $\mathcal{V}(H) = \{1, \dots, k\}$. Each vertex $i \in \mathcal{V}(H)$ is

assigned to the graph $G_i \in \mathcal{F}$. The H-join of G_1, \ldots, G_k is the graph $G = H[G_1, \ldots, G_k]$ such that $\mathcal{V}(G) = \bigcup_{i=1}^k \mathcal{V}(G_i)$ and

$$\mathcal{E}(G) = \left(\bigcup_{i=1}^{k} \mathcal{E}(G_i)\right) \bigcup \left(\bigcup_{uv \in \mathcal{E}(H)} \left\{ ij : i \in \mathcal{V}(G_u) , j \in \mathcal{V}(G_v) \right\} \right).$$

If the graphs G_1, \ldots, G_k are regular, then we can characterize the signless Laplacian spectrum of G. For this, we first need to specify some notation. For $1 \le i \le k$, define

$$N_i = \sum_{ij \in \mathcal{E}(H)} n_j \,.$$

In [14], the generalized composition of symmetric matrices was introduced as follows. By this concept we obtain the following result.

Theorem 1. Let H be a graph such that $A(H) = (a_{ij})_{1 \leq i,j \leq k}$. Let G_1, \ldots, G_k be regular graphs of degrees r_1, \ldots, r_k and with n_1, \ldots, n_k vertices, respectively. Consider $G = H[G_1, \ldots, G_k]$. Moreover, consider the $k \times k$ matrix $\Omega = (\omega_{ij})$, where

$$\omega_{ij} = \begin{cases} 2r_i + N_i & \text{if} \quad i = j \\ a_{ij} \sqrt{n_i n_j} & \text{if} \quad i \neq j \end{cases}.$$

Then

$$\sigma(Q_G) = \sigma(\Omega) \bigcup_{i=1}^{k} \left[\sigma(Q_{G_i} + N_i I_{n_i}) \setminus \{2r_i + N_i\} \right]. \tag{2}$$

In a similar manner, by applying the results to the Laplacian matrix of $H[G_1, \ldots, G_k]$ where G_1, \ldots, G_k are arbitrary graphs (see [6, Theorem 8]), we arrive at:

Theorem 2. Let H be a graph such that $A(H) = (a_{ij})_{1 \le i,j \le k}$. Let G_1, \ldots, G_k be arbitrary graphs. Consider $G = H[G_1, \ldots, G_k]$. Moreover, consider the $k \times k$ matrix $\Upsilon = (\eta_{ij})$, where

$$\eta_{ij} = \begin{cases} N_i & if \quad i = j \\ -a_{ij} \sqrt{n_i n_j} & if \quad i \neq j. \end{cases}$$

Then

$$\sigma(L_G) = \sigma(\Upsilon) \bigcup_{i=1}^k \left[\sigma(L_{G_i} + N_i I_{n_i}) \setminus \{N_i\} \right].$$

Remark 1. Using the Theory of Equitable Partitions (see, [4, Ch. 2]), it is also possible to characterize the full spectrum of Q_G and L_G .

3 An application to incidence energy

We approach towards our application of Theorem 1 by means some external definitions and results.

The algebraic connectivity of a graph, denoted by μ , is the second smallest Laplacian eigenvalue [16]. It is among the most important and most studied Laplacian eigenvalues. In recent years, it received much attention, see [1,10,13,23,36,37] and the references cited therein. A graph is connected if and only if $\mu > 0$.

The vertex connectivity (or just connectivity) of a connected graph G, denoted by $\gamma(G)$, is the minimum number of vertices of G whose deletion disconnects G.

The minimum number of vertices whose deletion yields a bipartite graph from G is called the *vertex bipartiteness* of G and is denoted by $v_b(G)$, see [15].

Let a be a natural number such that $a \leq n-3$. Let

$$\Sigma_a(n) = \{G = (\mathcal{V}(G), \mathcal{E}(G)) : |\mathcal{V}(G)| = n \text{ and } v_b(G) \le a\}.$$

If $i, j \in \mathcal{V}(G)$ are such that $i \nsim j$, let G^+ be the graph obtained from G by adding to it a new edge ij. We have earlier shown that $IE(G^+) > IE(G)$ and $LEL(G^+) > LEL(G)$.

Let $\widehat{G} \in \Sigma_a(n)$ such that $IE(\widehat{G}) > IE(G)$ for all $G \in \Sigma_a(n)$. Let $\widetilde{b} \leq a$ and consider $i_1, \ldots, i_{\widetilde{b}} \in \mathcal{V}(\widehat{G})$ such that $\widehat{G} \setminus \left\{i_1, \ldots, i_{\widetilde{b}}\right\}$ is a bipartite graph with bipartition $\{X, Y\}$. Let s = |X| and r = |Y|. Thus, $n = s + r + \widetilde{b}$.

Suppose that there exist vertices $i \in X$ and $j \in Y$ such that $i \nsim j$. If we consider the graph $\widehat{G}^+ = \widehat{G} + ij$, then $\widehat{G}^+ \in \Sigma_a(n)$, and

$$IE(\widehat{G}^+) > IE(\widehat{G})$$

which is a contradiction. This implies

$$\widehat{G}\setminus\{i_1,\ldots,i_{\widetilde{b}}\}=K_{r,s}=\overline{K}_r\vee\overline{K}_s$$
.

On the other hand, suppose that that there exist vertices $i, j \in \{i_1, \dots, i_{\tilde{b}}\}$ such that $i \nsim j$. Then $\widehat{G}^+ = \widehat{G} + ij \in \Sigma_a(n)$ and $IE(\widehat{G}^+) > IE(\widehat{G})$, which again is a contradiction. This implies

$$\langle \{i_1,\ldots,i_{\tilde{b}}\}\rangle = K_{\tilde{b}}.$$

By the same kind of reasoning we obtain

$$\widehat{G} = K_{\widetilde{b}} \vee (\overline{K}_r \vee \overline{K}_s) =: K_3 \left[K_{\widetilde{b}}, \overline{K}_r, \overline{K}_s \right]. \tag{3}$$

We now prove that $\widetilde{b}=a$. Assume the opposite, namely that $\widetilde{b}\leq a-1$ and $s+r=n-\widetilde{b}>n-a\geq 3$. Thus $s+r\geq 3$, implying $r\geq 2$ or $s\geq 2$. We suppose that $r\geq 2$. Then the graph $K_{\widetilde{b}}\vee (\overline{K}_r\vee \overline{K}_s)$ has the subgraph $K_{\widetilde{b}+1}=K_1\vee K_{\widetilde{b}}$, formed by a vertex of \overline{K}_r and the vertices of $K_{\widetilde{b}}$. It is easy to check that $G=K_{\widetilde{b}+1}\vee (\overline{K}_{r-1}\vee \overline{K}_s)\in \Sigma_a(n)$ and it has $r-1\geq 1$ edges more than our graph \widehat{G} in (3), implying that

$$IE(G) > IE(\widehat{G})$$

which obviously is again a contradiction. Therefore

$$\widehat{G} = K_a \vee (\overline{K}_r \vee \overline{K}_s) =: K_3 \left[K_a, \overline{K}_r, \overline{K}_s \right]. \tag{4}$$

Let f(z, w) = zw. Note that f(z, w) is the number of edges of $K_{z,w}$. The solution of the optimum problem

$$zw = \text{maximum}, \quad \text{provided } z + w = n - a$$

is reached whenever z=w. Therefore, if n-a is even, for \widehat{G} specified by Eq. (4) we conclude that $r=s=\frac{n-a}{2}$. If n-a is odd, then $r=\left\lfloor \frac{n-a}{2}\right\rfloor$ and $s=\left\lfloor \frac{n+1-a}{2}\right\rfloor$.

If $r = s = \frac{n-a}{2}$, then by Theorem 1,

$$\sigma(Q_{\widehat{G}}) = \left\{ (n-2)^{[a-1]} \, , \left(\frac{n+a}{2}\right)^{[n-a-2]} \right\} \cup \sigma(\Omega)$$

where

$$\Omega = \begin{pmatrix} n + a - 2 & \sqrt{\frac{(n-a)a}{2}} & \sqrt{\frac{(n-a)a}{2}} \\ \sqrt{\frac{(n-a)a}{2}} & \frac{n+a}{2} & \frac{n-a}{2} \\ \sqrt{\frac{(n-a)a}{2}} & \frac{n-a}{2} & \frac{n+a}{2} \end{pmatrix}.$$

We have that

$$\sigma(\Omega) = \left\{ a \,,\, \frac{a + 2n - 2 - \sqrt{4 - 4a + 4an - 3a^2}}{2} \,,\, \frac{a + 2n - 2 + \sqrt{4 - 4a + 4an - 3a^2}}{2} \right\}$$

resulting in

$$\begin{split} IE(\widehat{G}) &= \sqrt{a} + (a-1)\sqrt{n-2} + (n-a-2)\sqrt{\frac{n+a}{2}} \\ &+ \sqrt{\frac{a+2n-2-\sqrt{4-4a+4an-3a^2}}{2}} \end{split}$$

$$+ \sqrt{\frac{a+2n-2+\sqrt{4-4a+4an-3a^2}}{2}}.$$
 (5)

If $r=\left\lfloor \frac{n-a}{2} \right\rfloor$ and $s=\left\lfloor \frac{n+1-a}{2} \right\rfloor$, then by Theorem 1,

$$\sigma(Q_{\widehat{G}}) = \left\{ (n-2)^{[a-1]} \, , \left(\frac{n+a}{2}\right)^{[n-a-2]} \right\} \cup \sigma(\widetilde{\Omega})$$

where

$$\widetilde{\Omega} = \begin{pmatrix} n + a - 2 & \sqrt{ar} & \sqrt{as} \\ \sqrt{ar} & a + s & \sqrt{rs} \\ \sqrt{as} & \sqrt{rs} & a + r \end{pmatrix}.$$

Note that s = r + 1, implying

$$\widetilde{\Omega} = \begin{pmatrix} 2r + 2a - 1 & \sqrt{ar} & \sqrt{a\left(r+1\right)} \\ \sqrt{ar} & a + r + 1 & \sqrt{r\left(r+1\right)} \\ \sqrt{a\left(r+1\right)} & \sqrt{r\left(r+1\right)} & a + r \end{pmatrix}.$$

If $\mathcal{D} = diag\left(a^{-\frac{1}{2}}, r^{-\frac{1}{2}}, (r+1)^{-\frac{1}{2}}\right)$, then we have that

$$S = \mathcal{D}\widetilde{\Omega}\mathcal{D}^{-1} = \begin{pmatrix} 2r + 2a - 1 & r & r+1 \\ a & a+r+1 & r+1 \\ a & r & a+r \end{pmatrix}$$
(6)

resulting in

$$IE(\hat{G}) = \sqrt{\gamma_1} + (a-1)\sqrt{n-2} + (n-a-2)\sqrt{\frac{n+a}{2}} + \sqrt{\gamma_2} + \sqrt{\gamma_3}$$
 (7)

where γ_1 , γ_2 , γ_3 are the eigenvalues of the matrix S in Eq. (6). Thus we have proven:

Theorem 3. Let $1 \le a \le n-3$. Then the following holds.

(a) If n-a is even, then $IE(\widehat{G}) \geq IE(G)$ holds for all graphs $G \in \Sigma_a(n)$, where

$$\widehat{G} = K_a \vee \left(\overline{K}_{\frac{n-a}{2}} \vee \overline{K}_{\frac{n-a}{2}}\right) \in \Sigma_a(n)$$
.

Equality holds if and only if $G \cong \widehat{G}$. The expression for $IE(\widehat{G})$ is given by Eq. (5).

(b) If n-a is odd, then $IE(\widehat{G}) \geq IE(G)$ holds for all graphs $G \in \Sigma_a(n)$, where

$$\widehat{G} = K_a \vee \left(\overline{K}_{\lfloor \frac{n-a}{2} \rfloor} \vee \overline{K}_{\lfloor \frac{n+1-a}{2} \rfloor}\right) \in \Sigma_a(n)$$
.

Equality holds if and only if $G \cong \widehat{G}$. The expression for $IE(\widehat{G})$ is given by Eq. (7).

4 An application to Laplacian–energy–like invariant

The aim of this section is to prove that the graph \widehat{G} , specified in Theorem 3, has also maximum Laplacian–energy–like invariant in $\Sigma_a(n)$. Because the considerations are fully analogous to those in the preceding section, we outline only the differences.

The search for the graph $\widehat{G} \in \Sigma_a(n)$ satisfying the condition

$$LEL(\widehat{G}) \ge LEL(G)$$
 for all $G \in \Sigma_a(n)$

leads to $\widehat{G}=K_a\vee(\overline{K}_r\vee\overline{K}_s)$ where $r=s=\frac{n-a}{2}$ if n-a is even, and $r=\left\lfloor\frac{n-a}{2}\right\rfloor$, $s=\left\lfloor\frac{n+1-a}{2}\right\rfloor$ if n-a is odd.

If $r = s = \frac{n-a}{2}$, then by Theorem 2,

$$\sigma(L_{\widehat{G}}) = \left\{ n^{[a-1]}, \left(\frac{n+a}{2} \right)^{[n-a-2]} \right\} \cup \sigma(\Upsilon)$$

where

$$\Upsilon = \begin{pmatrix} n - a & -\sqrt{\frac{(n-a)a}{2}} & -\sqrt{\frac{(n-a)a}{2}} \\ -\sqrt{\frac{(n-a)a}{2}} & \frac{n+a}{2} & -\frac{n-a}{2} \\ -\sqrt{\frac{(n-a)a}{2}} & -\frac{n-a}{2} & \frac{n+a}{2} \end{pmatrix}.$$

We have that

$$\sigma(\Upsilon) = \left\{0\,,\, n^{[2]}\right\}$$

resulting in

$$LEL(\widehat{G}) = 1 + (a+1)\sqrt{n} + (n-a-2)\sqrt{\frac{n+a}{2}}.$$
 (8)

If $r = \lfloor \frac{n-a}{2} \rfloor$ and $s = \lfloor \frac{n+1-a}{2} \rfloor$, then by Theorem 2,

$$\sigma(L_{\widehat{G}}) = \left\{ n^{[a-1]} \,,\, (a+s)^{[r-1]} \,,\, (a+r)^{[s-1]} \right\} \cup \sigma(\widetilde{\Upsilon})$$

where

$$\widetilde{\Upsilon} = \begin{pmatrix} n - a & -\sqrt{ar} & -\sqrt{as} \\ -\sqrt{ar} & a + s & -\sqrt{rs} \\ -\sqrt{as} & -\sqrt{rs} & a + r \end{pmatrix}.$$

We have that

$$\sigma(\widetilde{\Upsilon}) = \left\{0 \,,\, n^{[2]}\right\}$$

resulting in

$$LEL(\widehat{G}) = 1 + (a+1)\sqrt{n} + (r-1)\sqrt{a+s} + (s-1)\sqrt{a+r}$$
.

By using the condition s = r + 1, we obtain

$$LEL(\widehat{G}) = 1 + (a+1)\sqrt{n} + (r-1)\sqrt{a+r+1} + r\sqrt{a+r}.$$
 (9)

Thus we have proven:

Theorem 4. Let $1 \le a \le n-3$. Then the following holds.

(a) If n-a is even, then $LEL(\widehat{G}) \geq LEL(G)$ holds for all graphs $G \in \Sigma_a(n)$, where

$$\widehat{G} = K_a \vee \left(\overline{K}_{\frac{n-a}{2}} \vee \overline{K}_{\frac{n-a}{2}}\right) \in \Sigma_a(n)$$
.

Equality holds if and only if $G \cong \widehat{G}$. The expression for $LEL(\widehat{G})$ is given by Eq. (8).

(b) If n-a is an odd, then $LEL(\widehat{G}) \geq LEL(G)$ holds for all graphs $G \in \Sigma_a(n)$, where

$$\widehat{G} = K_a \vee \left(\overline{K}_{\left\lfloor \frac{n-a}{2} \right\rfloor} \vee \overline{K}_{\left\lfloor \frac{n+1-a}{2} \right\rfloor} \right) \in \Sigma_a(n) .$$

Equality holds if and only if $G \cong \widehat{G}$. The expression for $LEL(\widehat{G})$ is given by Eq. (9).

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