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ORIGINAL RESEARCH

On the sum of distance signless Laplacian eigenvalues of graphs

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Abstract For a connected graph Γ with order n, size m and diameter d, the distance signless Laplacian matrix $\mathcal{D}^{\mathcal{Q}}(\Gamma)$ is defined as $\mathcal{D}^{\mathcal{Q}}(\Gamma) = Tr(\Gamma) + \mathcal{D}(\Gamma)$, where $Tr(\Gamma)$ is the diagonal matrix of vertex transmissions and $\mathcal{D}(\Gamma)$ is the distance matrix of Γ. The eigenvalues of $\mathcal{D}^{\mathcal{Q}}(\Gamma)$ are the distance signless Laplacian eigenvalues of Γ and are denoted by $\partial_1 \geq \partial_2 \geq \cdots \geq \partial_n$. The largest eigenvalue ∂_1 is called the distance signless Laplacian spectral radius. Let $M_k(\Gamma) = \sum_{i=1}^{k} \partial_i$ and $N_k(\Gamma) = \sum_{i=0}^{k-1} \partial_{n-i}$ be the sum of k-largest and the sum of k-smallest distance signless Laplacian eigenvalues of Γ, respectively. In this paper, we obtain the upper bounds for $M_k(\Gamma) = \sum_{i=1}^{k} \partial_i$ and determine the extremal cases. Also, we obtain the upper bounds for ∂_1 and determine the extremal graphs. As a consequence, we obtain the lower bounds for $N_k(\Gamma) = \sum_{i=0}^{k-1} \partial_{n-i}$ and for smallest eigenvalue ∂_n and determine the extremal graphs. Moreover, we obtain the upper bounds for the sum of the squares of the vertex transmissions and sum of the squares of the distances of the vertices and show that the bounds are best possible in each case. As an application, we obtain the upper bounds for the distance signless Laplacian energy of graphs and determine the extremal cases.

Keywords Distance matrix · Distance signless Laplacian matrix · Distance signless Laplacian eigenvalues · Diameter · Wiener index

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1 Introduction

A simple connected graph $\Gamma = (V, E)$ consists of the vertex set $V(\Gamma) = \{v_1, v_2, \ldots, v_n\}$ and the edge set $E(\Gamma)$ with $|V(\Gamma)| = n$ and $|E(\Gamma)| = m$ as the *order* and *size* of Γ. The number of edges incident on a vertex v is the *degree* of v and is denoted by $d_\Gamma(v)$ (we simply write d_v). A complete graph on n vertices is denoted by K_n. Also, $K_{r,n-r}$, $1 \leq r \leq n-1$, denotes a complete bipartite graph with two partite sets V_1 and V_2 of cardinalities r and $n-r$, respectively. More on definitions and notations, we refer the reader to [10,27].

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Let $A(\Gamma)$ and $\mathrm{Deg}(\Gamma)$ be respectively the adjacency and degree matrix of Γ. The Laplacian matrix is $L(\Gamma) = \mathrm{Deg}(\Gamma) - A(\Gamma)$ and the signless Laplacian matrix is $Q(\Gamma) = \mathrm{Deg}(\Gamma) + A(\Gamma)$. Both $L(\Gamma)$ and $Q(\Gamma)$ are real symmetric and positive semi-definite matrices. We take $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$ to be the eigenvalues of $L(\Gamma)$ and $Q(\Gamma)$, respectively.

The *distance* between the two vertices $v_i, v_j \in V(\Gamma)$ in Γ, denoted by $d_\Gamma(v_i, v_j)$ (or simply d_{ij}), is defined to be the length of a shortest path between vertices v_i and v_j. The maximum distance between any two vertices of Γ is called the *diameter* of Γ and is denoted by $d(\Gamma)$ (or shortly d when the graph Γ is clear from the context). The matrix $\mathcal{D}(\Gamma) = (d_{ij})_{v_i, v_j \in V(\Gamma)}$ is called the *distance matrix* of Γ . For any vertex $v_i \in V(\Gamma)$, the sum of the distances from v_i to all the other vertices in Γ is called the *vertex transmission* of v_i and is denoted by $Tr_\Gamma(v_i)$, that is, $Tr_\Gamma(v_i) = \sum\limits_{v_j \in V(\Gamma)} d_{ij}$. A *k-transmission regular* graph Γ is one in which $Tr_\Gamma(v_i) = k$, for all $v_i \in V(\Gamma)$. The sum of distances between all unordered pairs of vertices in Γ is called the *transmission* of Γ and is denoted by $\sigma(\Gamma)$, that is, $\sigma(\Gamma) = \frac{1}{2}\sum_{v_i \in V(\Gamma)} Tr_\Gamma(v_i)$. For any vertex $v_i \in V(\Gamma)$, the vertex transmission $Tr_\Gamma(v_i)$ is also called the *transmission degree* of v_i.

Let $Tr(\Gamma) = diag(Tr(1), Tr(2), \ldots, Tr(n))$ be the diagonal matrix of vertex transmissions of Γ. Aouchiche and Hansen [7] defined the *distance Laplacian matrix* and *distance signless Laplacian matrix* for a connected graph Γ as $\mathcal{D}^{\mathcal{L}}(\Gamma) = Tr(\Gamma) - D(\Gamma)$ and $\mathcal{D}^{\mathcal{Q}}(\Gamma) = Tr(\Gamma) + D(\Gamma)$, respectively. The matrix $\mathcal{D}^{\mathcal{Q}}(\Gamma)$ is real symmetric and positive semi-definite. We take $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n$ and $\partial_1 \geq \partial_2 \geq \cdots \geq \partial_n$ to be the eigenvalues of matrices $\mathcal{D}^{\mathcal{L}}(\Gamma)$ and $\mathcal{D}^{\mathcal{Q}}(\Gamma)$, respectively. The largest eigenvalue ∂_1 is called the distance signless Laplacian spectral radius of Γ. Some recent work on the matrix $\mathcal{D}^{\mathcal{L}}(\Gamma)$ can be found in [22,28,29] and on the matrix $\mathcal{D}^{\mathcal{Q}}(\Gamma)$ can be seen in [1,4,6,8,12,13,21,23,26,31].

Let $S_k(\Gamma) = \sum_{i=1}^{k} \mu_i$ and $S_k^+(\Gamma) = \sum_{i=1}^{k} \lambda_i$, for $1 \leq k \leq n$, be the sum of the k-largest Laplacian and the signless Laplacian eigenvalues of a graph Γ, respectively. We refer to [9,15–19,24,25,32,34] for the work done involving the invariants $S_k(\Gamma)$ and $S_k^+(\Gamma)$. Analogous to $S_k(\Gamma)$, the authors in [30] introduced the invariants $U_k = \sum_{i=1}^{k} \delta_i$ and $L_k = \sum_{i=1}^{k} \delta_{n-i}$, $1 \leq k \leq n-1$, for the sum of k-largest distance Laplacian eigenvalues and the sum of the k-smallest positive distance Laplacian eigenvalues of the graph Γ, respectively.

Motivated by the definitions of the graph invariants $S_k(\Gamma)$ and $S_k^+(\Gamma)$, Alhevaz et al. [2] put forward the graph invariants $M_k(\Gamma) = \sum_{i=1}^{k} \partial_i$ and $N_k(\Gamma) = \sum_{i=0}^{k-1} \partial_{n-i}$, respectively, for the sum of k-largest distance signless Laplacian eigenvalues and the sum of k-smallest distance signless Laplacian eigenvalues of the graph Γ. In the same paper, they proposed the following Brouwer-type conjecture for the sum of k-largest distance signless Laplacian eigenvalues:

Conjecture If Γ is a connected graph and order n, then for $k = 1, 2, \ldots, n$,

$$M_k(\Gamma) \leq \sigma(\Gamma) + \binom{k+1}{2}\left(n - \frac{2k+1}{3}\right).$$

This conjecture is still open. For more work on the graph invariants $M_k(\Gamma)$ and $N_k(\Gamma)$, we refer to [5].

The *Distance signless Laplacian energy* of a graph Γ is defined as

$$DSLE(\Gamma) = \sum_{i=1}^{n} |\xi_i| = \sum_{i=1}^{n} \left| \partial_i - \frac{2\sigma(\Gamma)}{n} \right|$$

where $\xi_i = \partial_i - \frac{2\sigma(\Gamma)}{n}$ are called the *auxillary eigenvalues*. Let Ω_1 be the class of connected graphs Γ of order n with m edges, diameter d and transmission $\sigma(\Gamma)$. Let Ω_2 be the class of connected graphs Γ of order n with diameter d and transmission $\sigma(\Gamma)$.

This paper is organized as follows. In Sect. 2, we obtain upper bounds for $M_k(\Gamma) = \sum_{i=1}^{k} \partial_i$ and ∂_1 and we determine the extremal graphs. As a consequence, we obtain lower bounds for $N_k(\Gamma) = \sum_{i=0}^{k-1} \partial_{n-i}$ and ∂_n and characterize the extremal cases. We also give upper bounds for the sum of the squares of vertex transmissions and the sum of the squares of the distances of vertices and show that the bounds are best possible in each case. As an application, in Sect. 3, we obtain upper bounds for the distance signless Laplacian energy and determine the extremal cases.

2 On the sum of the distance signless Laplacian eigenvalues of graphs

We recall the following lemmas which will be useful in the sequel.

Lemma 2.1 [30] *Let $\Gamma \in \Omega_2$. Then*

$$\sum_i Tr^2(i) \leq \frac{2\sigma^2(\Gamma)}{n-1} + \frac{n(n-1)(n-2)d^2}{2}$$

with equality iff $\Gamma \cong K_n$.

Lemma 2.2 [30] *Let Γ be a connected graph with order $n \geq 2$, size m and diameter d. Then*

$$\sum_{1\leq i<j\leq n} d_{ij}^2 \leq \frac{2m(1-d^2) + d^2 n(n-1)}{2}$$

with equality iff $d \leq 2$.

Lemma 2.3 [6] *Let $(Tr(1), Tr(2), \ldots, Tr(n))$ be the sequence of transmission degrees of the vertices of the graph Γ with n vertices. Then*

$$\sum_{i=i}^{n} \partial_i = 2\sigma(\Gamma), \quad \sum_{i=i}^{n} \partial_i^2 = 2\sum_{1\leq i<j\leq n} (d_{ij})^2 + \sum_{i=i}^{n} Tr^2(i).$$

Now, we obtain an upper bound for the invariant $M_k(\Gamma)$ in terms of the order n, size m, diameter d and the transmission $\sigma(\Gamma)$ of Γ.

Theorem 2.4 *Let $\Gamma \in \Omega_1$. For $1 \leq k \leq n-1$,*

$$M_k(\Gamma) \leq \frac{2\sigma(\Gamma)k}{n} + \frac{\sqrt{k(n-k)\Big(4mn(n-1)(1-d^2) + n(dn(n-1))^2 - 4\sigma^2(\Gamma)(n-2)\Big)}}{n\sqrt{2(n-1)}} \tag{2.1}$$

with equality iff $k = 1$ and $\Gamma \cong K_n$. Equality always holds for $k = n$.

Proof For $1 \leq k \leq n-1$, by using Cauchy–Schwarz inequality and Lemma 2.3, we obtain

$$\begin{aligned}
&(2\sigma(\Gamma) - M_k(\Gamma))^2\\
&\quad = (\partial_{k+1} + \partial_{k+2} + \cdots + \partial_n)^2 \leq (n-k)(\partial_{k+1}^2 + \partial_{k+2}^2 + \cdots + \partial_n^2)\\
&\quad = (n-k)\left(\sum_i Tr^2(i) + 2\sum_{1\leq i<j\leq n} (d_{ij})^2 - (\partial_1^2 + \partial_2^2 + \cdots + \partial_k^2)\right)\\
&\quad \leq (n-k)\left(\sum_i Tr^2(i) + 2\sum_{1\leq i<j\leq n} (d_{ij})^2 - \frac{M_k^2(\Gamma)}{k}\right),
\end{aligned}$$

which implies that

$$M_k^2(\Gamma) - \frac{4k\sigma(\Gamma)M_k(\Gamma)}{n} + \frac{4k\sigma^2(\Gamma)}{n} - \frac{k(n-k)}{n}\left(\sum_i Tr^2(i) + 2\sum_{1\leq i<j\leq n} (d_{ij})^2\right) \leq 0.$$

Thus,

$$M_k(\Gamma) \leq \frac{2\sigma(\Gamma)k}{n} + \frac{\sqrt{k(n-k)\left(n\left(\sum_i Tr^2(i) + 2\sum_{1\leq i<j\leq n} d_{ij}^2\right) - 4\sigma^2(\Gamma)\right)}}{n}. \tag{2.2}$$

Using Lemmas 2.1 and 2.2 with (2.2), we get

$$M_k(\Gamma) \leq \frac{2\sigma(\Gamma)k}{n} + \frac{\sqrt{k(n-k)\left(n\left(\frac{2\sigma^2(\Gamma)}{n-1} + \frac{n(n-1)(n-2)d^2}{2} + 2m(1-d^2) + d^2n(n-1)\right) - 4\sigma^2(\Gamma)\right)}}{n}.$$

Further simplification gives

$$M_k(\Gamma) \leq \frac{2\sigma(\Gamma)k}{n} + \frac{\sqrt{k(n-k)\Big(4mn(n-1)(1-d^2) + n(dn(n-1))^2 - 4\sigma^2(\Gamma)(n-2)\Big)}}{n\sqrt{2(n-1)}}$$

The first part of the proof is done.

Suppose that equality holds in (2.1). Then the equality must hold in all the above inequalities, that is, the equality must hold in the Cauchy–Schwarz inequality, Lemmas 2.1 and 2.2. From the equality in Lemmas 2.1 and 2.2, we have $\Gamma \cong K_n$. From the equality in the Cauchy–Schwarz inequality, we have $\partial_1 = \partial_2 = \cdots = \partial_k$ and $\partial_{k+1} = \partial_{k+2} = \cdots = \partial_n$. Since the distance signless Laplacian spectrum of K_n is $\{2n-2, n-2^{[n-1]}\}$, from the above results, we must have $k = 1$. Hence $k = 1$ and $\Gamma \cong K_n$.

Conversely, let $k = 1$ and $\Gamma \cong K_n$. Then, $M_k(\Gamma) = M_1(\Gamma) = \partial_1(K_n) = 2n-2$, $d = 1$, $m = \frac{n(n-1)}{2}$ and $\sigma(\Gamma) = \frac{n(n-1)}{2}$. Substituting all these values in (2.1), we observe that the equality holds.

When $k = n$, the left-hand side of (2.1) is equal to $M_n(\Gamma) = \sum_{i=1}^n \partial_i$ and the right-hand side is equal to $2\sigma(\Gamma) = \sum_{i=1}^n Tr(i) =$ trace of $\mathcal{D}^{\mathcal{Q}}(\Gamma) = \sum_{i=1}^n \partial_i$. Thus, the equality holds when $k = n$. This completes the proof. □

Remark 2.5 We note that Inequality (2.2) can also be seen in both [2,5].

Taking $k = 1$ in Theorem 2.4, we get the following upper bound for ∂_1.

Theorem 2.6 *Let $\Gamma \in \Omega_1$. Then*

$$\partial_1 \leq \frac{2\sigma(\Gamma)}{n} + \frac{\sqrt{(n-1)\Big(4mn(n-1)(1-d^2) + n(dn(n-1))^2 - 4\sigma^2(\Gamma)(n-2)\Big)}}{n\sqrt{2(n-1)}}$$

with equality iff $\Gamma \cong K_n$.

Now, proceeding exactly as in Theorem 2.4 and knowing that the distance signless Laplacian spectrum of K_n is given by $\{2n-2, n-2^{[n-1]}\}$, we get the following lower bound for $N_k(\Gamma)$.

Theorem 2.7 *Let $\Gamma \in \Omega_1$. For $1 \leq k \leq n-1$, we have*

$$N_k(\Gamma) \geq \frac{2\sigma(\Gamma)k}{n} - \frac{\sqrt{k(n-k)\Big(4mn(n-1)(1-d^2) + n(dn(n-1))^2 - 4\sigma^2(\Gamma)(n-2)\Big)}}{n\sqrt{2(n-1)}}$$

with equality iff $k = n-1$ and $\Gamma \cong K_n$. Equality always holds for $k = n$.

Taking $k = 1$ in Theorem 2.7, we get the following lower bound for ∂_n.

Corollary 2.8 *Let $\Gamma \in \Omega_1$. Then*

$$\partial_n \geq \frac{2\sigma(\Gamma)}{n} - \frac{\sqrt{(n-1)\Big(4mn(n-1)(1-d^2) + n(dn(n-1))^2 - 4\sigma^2(\Gamma)(n-2)\Big)}}{n\sqrt{2(n-1)}}$$

with equality iff $\Gamma \cong K_2$.

To proceed further, we note the following lemma [20].

Lemma 2.9 [20] *Let* $a = (a_1, a_2 \ldots, a_n)$ *and* $b = (b_1, b_2 \ldots, b_n)$ *be* n*-tuples of real numbers satisfying* $0 \le m_1 \le a_i \le M_1$, $0 \le m_2 \le b_i \le M_2$ *with* $i = 1, 2, \ldots, n$ *and* $M_1 M_2 \ne 0$. *Let* $\alpha = \frac{m_1}{M_1}$ *and* $\beta = \frac{m_2}{M_2}$. *If* $(1+\alpha)(1+\beta) \ge 2$, *then*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \le \frac{n^2}{4}(M_1 M_2 - m_1 m_2)^2. \tag{2.3}$$

Let $Tr_{max} = \max\{Tr(i) : i = 1, 2, \ldots, n\}$, $Tr_{min} = \min\{Tr(i) : i = 1, 2, \ldots, n\}$ and $\overline{Tr}$ be the maximum transmission, the minimum transmission and the average transmission of the graph Γ, respectively. Using Lemma 2.9, we have the following upper bounds for the graph invariants $\sum_{i=1}^{n} Tr^2(i)$ and $\sum_{1 \le i < j \le n} (d_{ij})^2$.

Theorem 2.10 *Let* Γ *be a connected graph with order* n. *Then,*

$$\sum_{i=1}^{n} Tr^2(i) \le \frac{4\sigma^2(\Gamma)}{n} + \frac{n}{4}(Tr_{max} - Tr_{min})^2 \tag{2.4}$$

and

$$\sum_{1 \le i < j \le n} (d_{ij})^2 \le \frac{4\sigma^2(\Gamma) + n^2(d-1)^2}{2n(n-1)}. \tag{2.5}$$

Moreover, both the inequalities are sharp for the transmission regular graphs and the complete graph K_n, *respectively.*

Proof In Lemma 2.9, take $a = (Tr(1), Tr(2), \ldots, Tr(n))$, $b = (1, 1, \ldots, 1)$, $M_1 = Tr_{max}$, $m_1 = Tr_{min}$ and $M_2 = m_2 = 1$. Since $(1+\alpha)(1+\beta) = \left(1 + \frac{m_1}{M_1}\right)\left(1 + \frac{m_2}{M_2}\right) \ge 2$ in Lemma 2.9 gets satisfied, from the Inequality (2.3), we get

$$\sum_{i=1}^{n} Tr^2(i) \sum_{i=1}^{n} 1 - \left(\sum_{i=1}^{n} Tr(i)\right)^2 \le \frac{n^2}{4}(Tr_{max} - Tr_{min})^2,$$

$$\text{that is,}\quad n\sum_{i=1}^{n} Tr^2(i) - 4\sigma^2(\Gamma) \le \frac{n^2}{4}(Tr_{max} - Tr_{min})^2,$$

$$\text{that is,}\quad \sum_{i=1}^{n} Tr^2(i) \le \frac{4\sigma^2(\Gamma)}{n} + \frac{n}{4}(Tr_{max} - Tr_{min})^2.$$

Assume that Γ is k- transmission regular. Then

$$\sum_{i=1}^{n} Tr^2(i) = nk^2 = \frac{k^2 n^2}{n} = \frac{4\sigma^2(\Gamma)}{n} = \frac{4\sigma^2(\Gamma)}{n} + \frac{n}{4}(Tr_{max} - Tr_{min})^2,$$

which shows that the equality always holds when Γ is a transmission regular graph.

For the second inequality, taking $a = (d_{ij})_{1 \le i < j \le n}$, $b = (1, 1, \ldots, 1)$, $M_1 = d$ and $M_2 = m_2 = m_1 = 1$, from Lemma 2.9, we get

$$\sum_{1 \le i < j \le n} (d_{ij})^2 \sum_{1 \le i < j \le n} 1 - \left(\sum_{1 \le i < j \le n} d_{ij}\right)^2 \le \frac{n^2}{4}(d-1)^2,$$

$$\text{that is,}\quad \frac{n(n-1)}{2} \sum_{1 \le i < j \le n} (d_{ij})^2 - \sigma^2(\Gamma) \le \frac{n^2}{4}(d-1)^2,$$

$$\text{that is,}\quad \sum_{1 \le i < j \le n} (d_{ij})^2 \le \frac{2\sigma^2(\Gamma)}{n(n-1)} + \frac{n(d-1)^2}{2(n-1)},$$

$$\text{that is,}\quad \sum_{1 \le i < j \le n} (d_{ij})^2 \le \frac{4\sigma^2(\Gamma) + n^2(d-1)^2}{2n(n-1)}$$

proving the required inequality.

If $\Gamma \cong K_n$, then $d_{ij} = 1$ for all $1 \leq i < j \leq n$, $d = 1$ and $\sigma(K_n) = \frac{n(n-1)}{2}$. Thus we have

$$\sum_{1 \leq i < j \leq n} (d_{ij})^2 = \frac{n(n-1)}{2} = \frac{4\sigma^2(\Gamma) + n^2(d-1)^2}{2n(n-1)}.$$

Hence the equality holds in (2.5). □

Proposition 2.11 *Let Γ be a connected graph with order n and m edges and diameter d. Then*

$$\sum_{1 \leq i < j \leq n} (d_{ij})^2 \leq \binom{n}{2} d^2 - (d^2 - 1)\, m$$

with equality if and only if $d \leq 2$.

Proof Since d is the diameter, we have

$$\sum_{1 \leq i < j \leq n} (d_{ij})^2 = m + \sum_{\substack{1 \leq i < j \leq n \\ v_i v_j \notin E(G)}} (d_{ij})^2 \leq m + d^2 \sum_{\substack{1 \leq i < j \leq n \\ v_i v_j \notin E(G)}} 1 = m + d^2 \left(\binom{n}{2} - m \right).$$

Suppose that equality holds. Then $d_{ij} = d$, whenever $1 \leq i < j \leq n$, $v_i v_j \notin E(G)$. Since G is connected, we obtain $d \leq 2$.

Conversely, it is easy to see that the equality holds for $d \leq 2$. □

Now, we obtain an upper bound for $M_k(\Gamma)$ in terms of the order n, the diameter d, the transmission $\sigma(\Gamma)$, Tr_{max} and Tr_{min} of the graph Γ.

Theorem 2.12 *Let $\Gamma \in \Omega_2$. For $1 \leq k \leq n-1$, we have*

$$M_k(\Gamma) \leq \frac{2\sigma(\Gamma)k}{n} + \frac{\sqrt{k(n-k)\Big((Tr_{max} - Tr_{min})^2 + 4(n-1)d^2\Big)}}{2} \tag{2.6}$$

with equality iff $k = 1$ and $\Gamma \cong K_n$. Equality always holds for $k = n$.

Proof We proceed similarly up to Inequality (2.2) of Theorem 2.4. Now, using Lemma 2.10 and Proposition 2.11 in the Inequality (2.2), we get

$$M_k(\Gamma) \leq \frac{2\sigma(\Gamma)k}{n} + \frac{\sqrt{k(n-k)\left(4\sigma^2(\Gamma) + \frac{n^2}{4}(Tr_{max} - Tr_{min})^2 + (n-1)n^2d^2 - 4\sigma^2(\Gamma)\right)}}{n},$$

$$\text{that is,} \quad M_k(\Gamma) \leq \frac{2\sigma(\Gamma)k}{n} + \frac{\sqrt{k(n-k)\Big((Tr_{max} - Tr_{min})^2 + 4(n-1)d^2\Big)}}{2}$$

proving the inequality.

Suppose that equality holds in (2.6). Then the equality must hold in the Cauchy–Schwarz inequality, Theorem 2.10 and Proposition 2.11. The equality in Cauchy–Schwarz inequality gives $\partial_1 = \cdots = \partial_k$ and $\partial_{k+1} = \cdots = \partial_n$. This shows that $k = 1$ as ∂_1 is a simple eigenvalue of Γ, by the Perron–Frobenius theorem. The equality in both Lemma 2.10 and Proposition 2.11 shows that $\Gamma \cong K_n$. Thus, equality holds in the Inequality (2.6) if $k = 1$ and $\Gamma \cong K_n$.

Conversely, we can easily see that the equality holds in the Inequality (2.6) when $k = 1$ and $\Gamma \cong K_n$. It is trivial to check that equality holds when $k = n$. □

Putting $k = 1$ in Theorem 2.12, we get the following upper bound for ∂_1.

Theorem 2.13 *Let* $\Gamma \in \Omega_2$. *Then*

$$\partial_1 \leq \frac{2\sigma(\Gamma)}{n} + \frac{\sqrt{(n-1)\Big((Tr_{max} - Tr_{min})^2 + 4(n-1)d^2\Big)}}{2}$$

with equality iff $\Gamma \cong K_n$.

Using similar arguments as in Theorem 2.12, we obtain the following lower bound for the graph invariant $N_K(\Gamma)$.

Theorem 2.14 *Let* $\Gamma \in \Omega_2$. *For* $1 \leq k \leq n-1$, *we have*

$$N_k(\Gamma) \geq \frac{2\sigma(\Gamma)k}{n} - \frac{\sqrt{k(n-k)\Big((Tr_{max} - Tr_{min})^2 + 4(n-1)d^2\Big)}}{2}$$

with equality iff $k = n-1$ *and* $\Gamma \cong K_n$. *Equality always holds for* $k = n$.

Putting $k = 1$ in Theorem 2.14, we get the following lower bound for ∂_n.

Corollary 2.15 *Let* $\Gamma \in \Omega_2$. *Then*

$$\partial_n \geq \frac{2\sigma(\Gamma)}{n} - \frac{\sqrt{(n-1)\Big((Tr_{max} - Tr_{min})^2 + 4(n-1)d^2\Big)}}{2}$$

with equality iff $\Gamma \cong K_2$.

We will make use of the following lemma [33].

Lemma 2.16 [33] *If* a_i *and* b_i, $1 \leq i \leq n$, *are positive real numbers, then*

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1 M_2}{m_1 m_2}} + \sqrt{\frac{m_1 m_2}{M_1 M_2}}\right)^2 \left(\sum_{i=1}^{n} a_i b_i\right)^2,$$

where $M_1 = max\{a_i : 1 \leq i \leq n\}$, $m_1 = min\{a_i : 1 \leq i \leq n\}$, $M_2 = max\{b_i : 1 \leq i \leq n\}$ *and* $m_2 = min\{b_i : 1 \leq i \leq n\}$.

From Lemma 2.16, we obtain the following upper bound for the graph invariants $\sum_{i=1}^{n} Tr^2(i)$ and $\sum_{1 \leq i < j \leq n} (d_{ij})^2$.

Theorem 2.17 *Let* Γ *be a connected graph with order* n *and diameter* d. *Then,*

$$\sum_{i=1}^{n} Tr^2(i) \leq \frac{(Tr_{max} + Tr_{min})^2 \sigma^2(\Gamma)}{nTr_{max}Tr_{min}}$$

and

$$\sum_{1 \leq i < j \leq n} (d_{ij})^2 \leq \frac{(d+1)^2 \sigma^2(\Gamma)}{2dn(n-1)}. \tag{2.7}$$

Both the inequalities are sharp and are shown by all the transmission regular graphs and the complete graph K_n, *respectively.*

Proof We take $a = (Tr(1), Tr(2), \ldots, Tr(n))$ and $b = (1, 1, \ldots, 1)$ in Lemma 2.16, so that $M_2 = m_2 = 1$, $M_1 = Tr_{max}$ and $m_1 = Tr_{min}$. On substituting these values, we get

$$\sum_{i=1}^{n} Tr^2(i) \sum_{i=1}^{n} 1 \leq \frac{1}{4}\left(\sqrt{\frac{Tr_{max}}{Tr_{min}}} + \sqrt{\frac{Tr_{min}}{Tr_{max}}}\right)^2 \left(\sum_{i=1}^{n} Tr(i)\right)^2,$$

$$\text{that is,} \quad n\sum_{i=1}^{n} Tr^2(i) \leq \frac{1}{4}\left(\frac{Tr_{max} + Tr_{min}}{\sqrt{Tr_{max}Tr_{min}}}\right)^2 4\sigma^2(\Gamma),$$

$$\text{that is,} \quad \sum_{i=1}^{n} Tr^2(i) \leq \frac{(Tr_{max} + Tr_{min})^2 \sigma^2(\Gamma)}{nTr_{max}Tr_{min}}$$

Suppose Γ is k- transmission regular. Then $Tr_{max} = Tr_{min} = k$. The left hand side of Inequality (2.7) becomes nk^2 and the right hand side becomes $\frac{4\sigma^2(\Gamma)}{n} = \frac{k^2n^2}{n} = nk^2$, which shows that the equality always holds when Γ is a transmission regular graph.

For the second inequality, we take $a = (d_{ij})_{1 \leq i < j \leq n}$ and $b = (1, 1, \ldots, 1)$ in Theorem 2.10. Clearly, $M_1 = d$ and $M_2 = m_2 = m_1 = 1$. Substituting these values in Theorem 2.10, we get

$$\sum_{1 \leq i < j \leq n} (d_{ij})^2 \sum_{1 \leq i < j \leq n} 1 \leq \frac{1}{4}\left(\sqrt{d} + \frac{1}{\sqrt{d}}\right)^2 \left(\sum_{1 \leq i < j \leq n} d_{ij}\right)^2,$$

$$\text{that is,} \quad \frac{n(n-1)}{2} \sum_{1 \leq i < j \leq n} (d_{ij})^2 \leq \frac{1}{4}\frac{(d+1)^2}{d}\sigma^2(\Gamma),$$

$$\text{that is,} \quad \sum_{1 \leq i < j \leq n} (d_{ij})^2 \leq \frac{(d+1)^2\sigma^2(\Gamma)}{2dn(n-1)}$$

Finally, we easily see that the equality holds for K_n. □

Corollary 2.18 *Let Γ be a connected graph with order n with diameter d and maximum degree Δ, minimum degree δ. Then*

$$\sum_{i=1}^{n} Tr^2(i) \leq \frac{\left[(n-1)\,d - (d-1)\,\delta + 2n - \Delta - 2\right]^2}{(2n - \Delta - 2)\left[(n-1)\,d - (d-1)\delta\right]} \, \frac{\sigma^2(\Gamma)}{n}$$

with equality if and only if Γ is a regular graph of diameter 2.

Proof For any vertex $v_i \in V(G)$, we have $Tr_i \leq d_i + (n - d_i - 1)\,d = (n-1)\,d - (d-1)\,d_i \leq (n-1)\,d - (d-1)\,\delta$ and $Tr_i \geq d_i + 2\,(n - 1 - d_i) = 2\,(n-1) - d_i \geq 2\,(n-1) - \Delta$. Thus we have $Tr_{max} \leq (n-1)\,d - (d-1)\,\delta$ and $Tr_{min} \geq 2(n-1) - \Delta$. Therefore,

$$\sqrt{\frac{Tr_{max}}{Tr_{min}}} \leq \sqrt{\frac{(n-1)\,d - (d-1)\,\delta}{2(n-1) - \Delta}} \quad \text{and} \quad \sqrt{\frac{Tr_{min}}{Tr_{max}}} \geq \sqrt{\frac{2(n-1) - \Delta}{(n-1)\,d - (d-1)\,\delta}}.$$

From the above, we obtain

$$\sqrt{\frac{Tr_{max}}{Tr_{min}}} - \sqrt{\frac{Tr_{min}}{Tr_{max}}} \leq \sqrt{\frac{(n-1)\,d - (d-1)\,\delta}{2(n-1) - \Delta}} - \sqrt{\frac{2(n-1) - \Delta}{(n-1)\,d - (d-1)\,\delta}}$$
$$= \frac{(n-1)d - (d-1)\delta + \Delta + 2 - 2n}{\sqrt{(2n - \Delta - 2)\left[(n-1)d - (d-1)\,\delta\right]}}.$$

Now,

$$\left(\sqrt{\frac{Tr_{max}}{Tr_{min}}}+\sqrt{\frac{Tr_{min}}{Tr_{max}}}\right)^2=\left(\sqrt{\frac{Tr_{max}}{Tr_{min}}}-\sqrt{\frac{Tr_{min}}{Tr_{max}}}\right)^2+4$$
$$\leq\left(\frac{(n-1)d-(d-1)\delta+\Delta+2-2n}{\sqrt{(2n-\Delta-2)\Big[(n-1)d-(d-1)\,\delta\Big]}}\right)^2+4$$
$$=\frac{\Big[(n-1)\,d-(d-1)\,\delta+2n-\Delta-2\Big]^2}{(2n-\Delta-2)\Big[(n-1)\,d-(d-1)\delta\Big]}.$$

By Theorem 2.17, we get the result.

By Theorem 2.17, the equality holds if and only if Γ is a transmission regular graph. This with $Tr_{max}=(n-1)\,d-(d-1)\,\delta$ and $Tr_{min}=2(n-1)-\Delta$, we conclude that the equality holds if and only if Γ is a regular graph of diameter 2. □

The following result gives an upper bound for the graph invariant $M_k(\Gamma)$ in terms of the diameter d, the order n and the transmission $\sigma(\Gamma)$ of the graph Γ.

Theorem 2.19 *Let $\Gamma\in\Omega_2$. For $1\leq k\leq n-1$, we have*

$$M_k(\Gamma)\leq\frac{2\sigma(\Gamma)k}{n}+\frac{\sqrt{k(n-k)\Big(d(n-2)(dn(n-1))^2+2\sigma^2(\Gamma)(d^2+6d-2nd+1)\Big)}}{n\sqrt{2d(n-1)}}\tag{2.8}$$

with equality if and only if $k=1$ and $\Gamma\cong K_n$. Equality always holds for $k=n$

Proof We argument exactly as in Theorem 2.4 up to Inequality (2.2). Now, using Lemma 2.1 and Theorem 2.17 in Inequality (2.2), we get

$$M_k(\Gamma)\leq\frac{2\sigma(\Gamma)k}{n}+\frac{\sqrt{k(n-k)\left(n\left(\frac{2\sigma^2(\Gamma)}{n-1}+\frac{n(n-1)(n-2)d^2}{2}+\frac{(d+1)^2\sigma^2(\Gamma)}{dn(n-1)}\right)-4\sigma^2(\Gamma)\right)}}{n}.$$

Simplifying further, we get

$$M_k(\Gamma)\leq\frac{2\sigma(\Gamma)k}{n}+\frac{\sqrt{k(n-k)\left(\frac{d(n-2)(dn(n-1))^2+2\sigma^2(\Gamma)(d^2+6d-2nd+1)}{2d(n-1)}\right)}}{n},$$

that is,

$$M_k(\Gamma)\leq\frac{2\sigma(\Gamma)k}{n}+\frac{\sqrt{k(n-k)\Big(d(n-2)(dn(n-1))^2+2\sigma^2(\Gamma)(d^2+6d-2nd+1)\Big)}}{n\sqrt{2d(n-1)}}$$

proving the required inequality.

The rest of the proof follows by the same arguments as in Theorem 2.4. □

By using similar arguments, we have the following lower bound for the graph invariant $N_k(\Gamma)$ in terms of the diameter d, the order n and the transmission $\sigma(\Gamma)$.

Theorem 2.20 *Let $\Gamma\in\Omega_2$. For $1\leq k\leq n-1$, we have*

$$N_k(\Gamma)\geq\frac{2\sigma(\Gamma)k}{n}-\frac{\sqrt{k(n-k)\Big(d(n-2)(dn(n-1))^2+2\sigma^2(\Gamma)(d^2+6d-2nd+1)\Big)}}{n\sqrt{2d(n-1)}}$$

with equality iff $k=n-1$ and $\Gamma\cong K_n$. Equality always holds for $k=n$

Taking $k = 1$, from Theorems 2.19 and 2.20, we have the upper bound for distance signless Laplacian spectral radius and the lower bound for the smallest distance signless Laplacian eigenvalue, respectively.

Corollary 2.21 *Let $\Gamma \in \Omega_2$. Then*

$$\partial_1 \leq \frac{2\sigma(\Gamma)}{n} + \frac{\sqrt{(n-1)\Big(d(n-2)(dn(n-1))^2 + 2\sigma^2(\Gamma)(d^2+6d-2nd+1)\Big)}}{n\sqrt{2d(n-1)}}$$

with equality iff $\Gamma \cong K_n$

Corollary 2.22 *Let $\Gamma \in \Omega_2$. Then*

$$\partial_n \geq \frac{2\sigma(\Gamma)}{n} - \frac{\sqrt{(n-1)\Big(d(n-2)(dn(n-1))^2 + 2\sigma^2(\Gamma)(d^2+6d-2nd+1)\Big)}}{n\sqrt{2d(n-1)}}$$

with equality iff $\Gamma \cong K_2$

3 On distance signless Laplacian energy of graphs

The distance signless Laplacian energy *DSLE* was first introduced in [6]. Alhevaz et al. [3] obtained the *DSLE* of the join of regular graphs in terms of their adjacency spectrum. Das et al. [11] showed that the complete graph gives the smallest *DSLE* among all the graphs of order n and the star graph gives the smallest *DSLE* among all the trees of order n. Ganie et al. [14] obtained the upper bounds for the distance energy, distance Laplacian energy and the distance signless Laplacian energy and determined the extremal graphs. In this section, we present some bounds for $DSLE(\Gamma)$.

The following result can be seen in [8].

Lemma 3.1 [8] *Let Γ be a connected graph with the minimum, the average and the maximum transmissions Tr_{min}, $\overline{Tr}$ and Tr_{max}, respectively. Then*

$$2Tr_{min} \leq 2\overline{Tr} \leq \partial_1 \leq 2Tr_{max}$$

with equalities iff Γ is a transmission regular graph.

Now, we obtain an upper bound for the distance signless Laplacian energy in terms of the order n, the diameter d and the transmission $\sigma(\Gamma)$.

Theorem 3.2 *Let $\Gamma \in \Omega_2$. Then*

$$DSLE(\Gamma) \leq 2Tr_{max} - \frac{2\sigma(\Gamma)}{n} + \frac{\sqrt{\Big(d(n-1)n^2\Big)^2 + 4\sigma^2(\Gamma)(2-n^2)}}{n\sqrt{2}}$$

with equality iff $\Gamma \cong K_n$.

Proof By the Cauchy–Schwarz inequality, we obtain

$$\sum_{i=1}^{n} |\xi_i| = \xi_1 + \sum_{i=2}^{n} |\xi_i| \leq \xi_1 + \sqrt{(n-1)\sum_{i=2}^{n} \xi_i^2}, \quad \text{as} \quad \partial_1 > \overline{Tr}. \tag{3.9}$$

One can easily see that

$$\sum_{i=1}^{n} \xi_i^2 = 2\sum_{1 \leq i < j \leq n} (d_{ij})^2 + \sum_{i=i}^{n} Tr^2(i) - \frac{4\sigma^2(\Gamma)}{n}.$$

Using this in Inequality (3.9), we get

$$DSLE(\Gamma) \le \xi_1 + \sqrt{(n-1)\left(2\sum_{1\le i<j\le n}(d_{ij})^2 + \sum_{i=i}^{n} Tr^2(i) - \frac{4\sigma^2(\Gamma)}{n} - \xi_1^2\right)}. \tag{3.10}$$

Using Lemma 2.1 and Proposition 2.11 in Inequality (3.10), we get

$$DSLE(\Gamma) \le \xi_1 + \sqrt{(n-1)\left(n(n-1)d^2 + \frac{2\sigma^2(\Gamma)}{n-1} + \frac{n(n-1)(n-2)d^2}{2} - \frac{4\sigma^2(\Gamma)}{n} - \xi_1^2\right)}. \tag{3.11}$$

Using Lemma 3.1, we have $\xi_1 = \partial_1 - \overline{Tr} \ge \overline{Tr}$, so that

$$-\xi_1^2 \le -\overline{Tr}^2 = -\frac{4\sigma^2(\Gamma)}{n^2}.$$

Substituting the above inequality in Inequality (3.11) and using Lemma 3.1 again, we get

$$DSLE(\Gamma) \le 2Tr_{max} - \frac{2\sigma(\Gamma)}{n} + \sqrt{(n-1)\left(\frac{(n-1)n^2d^2}{2} + \frac{2\sigma^2(\Gamma)}{n-1} - \frac{4\sigma^2(\Gamma)}{n} - \frac{4\sigma^2(\Gamma)}{n^2}\right)},$$

that is,

$$DSLE(\Gamma) \le 2Tr_{max} - \frac{2\sigma(\Gamma)}{n} + \frac{\sqrt{\left(d(n-1)n^2\right)^2 + 4\sigma^2(\Gamma)(2-n^2)}}{n\sqrt{2}},$$

as required.

Suppose that equality holds. Then the equality must hold in Cauchy–Schwarz inequality, Lemma 2.1 and Proposition 2.11. Now, the equality holds in Lemma 2.1 and Proposition 2.11 only if $\Gamma \cong K_n$ and equality holds in the Cauchy–Schwarz inequality if $|\xi_2| = |\xi_3| = \cdots = |\xi_n|$. Observing the distance signless Laplacian spectrum of K_n, we see that $|\xi_2| = |\xi_3| = \cdots = |\xi_n|$ is satisfied for K_n. Hence $\Gamma \cong K_n$.

Conversely, if $\Gamma \cong K_n$, then we observe that the equality holds in main inequality. □

Proceeding similarly as in Theorem 3.2 and using Theorem 2.10 in Inequality (3.10) in place of Lemma 2.1, we get the following upper bound for $DSLS(\Gamma)$.

Theorem 3.3 *Let* $\Gamma \in \Omega_2$. *Then*

$$DSLE(\Gamma) \le 2Tr_{max} - \frac{2\sigma(\Gamma)}{n} + \frac{\sqrt{(n-1)\left(4n(n-1)n^2d^2 + n(nTr_{max} - nTr_{min})^2 - 16\sigma^2(\Gamma)\right)}}{2n}$$

with equality iff $\Gamma \cong K_n$.

4 Concluding remarks and future work

The mathematical study of the $\sum_{i=1}^{k} \partial_i$ and ∂_1 was accompolished by finding the sharp upper bounds in terms of the graph order n, size m, diameter d, and transmission σ. Extremal graphs that attain the upper bounds were also identified. Moreover, we gave the lower bounds for $\sum_{i=0}^{k-1} \partial_{n-i}$ and for smallest distance signless Laplacian eigenvalue ∂_n and determine the extremal graphs. Further, we obtained upper bounds for the sum of the squares of the vertex transmissions and sum of the squares of the distances of the vertices and prove that the bounds are best possible in each case. A considerable number of graph energy variants have appeared in the literature. However, only some have been studied from an application point of view. In this paper, we gave an upper bound for the distance signless Laplacian energy of graphs and determine the extremal graphs. The following problems will be interesting to investigate:

Problem 1 Characterize the maximal graphs with respect to $\sum_{i=1}^{k} \partial_i$ (or $DSLE(\Gamma)$) among all connected graphs of order n and k.

Problem 2 Characterize the maximal graphs with respect to $\sum_{i=1}^{k}\partial_i$ (or $DSLE(\Gamma)$) among all connected graphs of order n, k and clique number ω.

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Declarations

Conflict of interest The authors declare that they have no conflict of interest.

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