On the sum of k-th largest distance eigenvalues of graphs

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Abstract

For a connected graph G with order n and an integer $k \geq 1$, we denote by

$$S_k(D(G)) = \lambda_1(D(G)) + \cdots + \lambda_k(D(G))$$

the sum of k largest distance eigenvalues of G. In this paper, we consider the sharp upper bound and lower bound of $S_k(D(G))$. We determine the sharp lower bounds of $S_k(D(G))$ when G is connected graph and is a tree, respectively, and characterize both the extremal graphs. Moreover, we conjecture that the upper bound is attained when G is a path of order n and prove some partial result supporting the conjecture. To prove our result, we obtain a sharp upper bound of $\lambda_2(D(G))$ in terms of the order and the diameter of G, where $\lambda_2(D(G))$ is the second largest distance eigenvalue of G. As applications, we prove a general inequality involving $\lambda_2(D(G))$, the independence number of G, and the number of triangles in G. An immediate corollary is a conjecture of Fajtlowicz, which was confirmed in [10] by a different argument. We conclude this paper with some open problems for further study.

Keywords: Distance matrix, distance eigenvalue, eigenvalue sum, the second largest distance eigenvalue

Mathematics Subject Classification (2010): 05C50

1 Introduction

Throughout this paper, we consider simple, undirected and connected graphs. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let $N(v)$ denote the neighbor set of v in G. Let $S \subset V(G)$. We use $G[S]$ to denote the subgraph of G induced by S. The *distance* between vertices v_i and v_j, denoted by $d_G(v_i, v_j)$, is the length of a shortest path from v_i to v_j in G. The *diameter* of a graph is the maximum distance between any two vertices of G.

*Supported by the National Natural Science Foundation of China (Nos. 11401211 and 11471121) and Fundamental Research Funds for the Central Universities (No. 222201714049).
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Throughout this note, we use $M(G)$ to denote a real symmetric matrix respect to a connected graph G. We use $\lambda_1(M(G)) \geq \lambda_2(M(G)) \geq \cdots \geq \lambda_n(M(G))$ to denote all eigenvalues of $M(G)$ and denote by

$$S_k(M(G)) = \lambda_1(M(G)) + \cdots + \lambda_k(M(G)),$$

where $k \geq 1$ is an integer. The *distance matrix* of G, denoted by $D(G)$ (or simply by D), is the real symmetric matrix with (i, j)-entry being $d_G(v_i, v_j)$ (or d_{ij}). The *distance eigenvalues* (resp., *distance spectrum*) of G, are denoted by

$$\lambda_1(D(G)) \geq \lambda_2(D(G)) \geq \cdots \geq \lambda_n(D(G)).$$

Recently, the distance matrix of a graph has received increasing attention. Aouchiche and Hansen [2] and Lin, Das and Wu [12] proved some results on the relations between the distance eigenvalues and some graphic parameters. Lin [11] proved an upper bound on the least distance eigenvalue of a graph in terms of it order and diameter. By using some graph operations, Pokorný, Híc, Stevanović and Milošević [16] obtained many infinite families of distance integral graphs. Very recently, Lu, Huang and Huang [13] characterized all graphs with exactly two distance eigenvalues different from -1 and -3. Huang, Huang and Lu [9] characterized all graphs with exactly three distance eigenvalues different from -1 and -2. For more results on the distance matrix of graphs, we refer the reader to the survey [3].

Our main motivations of this note come from two aspects. The first one is a paper of Mohar [15], in which he proved that $S_k(A(G)) \leq \frac{1}{2}(\sqrt{k} + 1)n$ for any graph of order n and an integer $k \geq 1$. His theorem is originally motivated by a result of Gernert which states that $S_2(A(G)) \leq n$ for any regular graphs G and the upper bound is best possible. Another motivations are the Grone-Merris conjecture [7, 8] and Brouwer's conjecture [5]. For any graph G on n vertices with degree sequence $d_1 \geq \cdots \geq d_n$, its conjugate degree sequence is defined as the sequence $d'_1 \geq d'_2 \geq \cdots \geq d'_n$ where $d'_k := |\{v_i : d_i \geq k\}|$. The Grone-Merris conjecture, which is proved by Bai [4], states that and for any $k \in \{1, \ldots, n\}$, $S_k(L(G)) \leq \sum_{i=1}^{k} d'_i$. Brouwer's conjecture says that $S_k(L(G)) \leq m + \binom{k}{2}$ holds for any simple graph G of order n and size m and any $1 \leq k \leq n$. These topics have received much attentions and Brouwer's conjecture is widely open now. However, till to now, it seems to have no study on upper and lower bounds of $S_k(D(G))$.

In this paper, we try to bound it in terms of some parameters of graphs. We will study the following general problem which seems interesting and non-trivial.

Problem 1. For a connected graph G and an integer $k \geq 2$, to give tight upper and lower bounds on $S_k(G)$ and to characterize the extremal graphs corresponding to them, respectively.

We first give a lower bound of $S_k(D(G))$.

Theorem 1. *Let $k \geq 2$ be an integer and n be sufficiently large with respect to k. Let G be a connected graph of order n.*
(i) Then $S_k(D(G)) \geq n - k$ where the equality holds if and only if $G \cong K_n$.
(ii) If G is a tree, then $S_k(D(G)) \geq 2n - 2k$ where the equality holds if and only if $G \cong K_{1,n-1}$.

We then consider the upper bound of $S_k(D(G))$. The following problem is our original motivation.

Problem 2. Let $G \ncong P_n$ be a connected graph with order n. For an integer $k \geq 2$ and sufficiently large n with respect to k, does there hold $S_k(D(G)) < S_k(D(P_n))$?

Very interesting for us, in order to prove some results supporting this problem, we need to obtain a sharp upper bound on $\lambda_2(D)$, which may be of its own interest.

Theorem 2. *Let G be a connected graph of order n with diameter d. Then $\lambda_2(D(G)) \leq \frac{n(d-1)}{2} - d$, where the equality holds if and only if $G \cong K_n$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$.*

As an application of Theorem 2, we can prove the following result. In particular, we can reprove a conjecture by Fajtlowicz [6], which was confirmed in [10].

Theorem 3. *Let G be a connected graph of order $n > s^3 + s^2 - 2s + 1$, where $s \geq 2$. Suppose that the independence number $\alpha(G) \leq s$. Then there hold:*
(i) $\lambda_2(D(G)) < 3s^3 \cdot \frac{t(G)}{m}$.
(ii) (Lin [10, Theorem 1.2]) If $t = 2$, then $\lambda_2(D(G)) < t(G)$, where $t(G)$ denotes the number of triangles in G.

If there is some information on the diameter of a connected graph, we can prove the following result supporting Problem 2 affirmatively.

Proposition 1. *Let G be a connected graph with order n and diameter d. For an integer $k \geq 2$ and sufficiently large n with respect to k, if $d < \frac{2n}{3(k+2)}$ then $S_k(D(G)) < S_k(D(P_n))$.*

2 Preliminaries

In this section, we will list some preliminaries and prove some lemmas. Our one main tool is Cauchy Interlacing Theorem.

Theorem 4 (Cauchy Interlacing Theorem)**.** *Let A be a Hermitian matrix with order n and let B be a principal submatrix of A with order m. If $\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_n(A)$ are the eigenvalues of A and $\mu_1(B) \geq \mu_2(B) \geq \cdots \geq \mu_m(B)$ are the eigenvalues of B, then $\lambda_{n-m+i}(A) \leq \mu_i(B) \leq \lambda_i(A)$ for $i = 1, \ldots, m$.*

Another tool is the famous Ramsey Theorem, which has already turned out to be powerful for problems in spectral graph theory. For example, see [19] due to Zhang and Cao.

Theorem 5 (Ramsey [17])**.** *Given any positive integers k and l, there exists a smallest integer $R(k,l)$ such that every graph on $R(k,l)$ vertices contains either a clique of k vertices or an independent set of l vertices.*

The third one is a theorem due to Merris, which helps us to obtain bounds of distance eigenvalues.

Theorem 6 (Merris [14])**.** *Let G be a tree of order n. Let $\lambda_1(D(G)) \geq \cdots \geq \lambda_n(D(G))$ be the eigenvalues of $D(G)$ and let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq 0$ be the eigenvalues of $L(G)$. Then*

$$0 > \frac{-2}{\mu_1} > \lambda_2(D(G)) \geq \frac{-2}{\mu_2} \geq \cdots \geq \lambda_{n-1}(D(G)) \geq \frac{-2}{\mu_{n-1}} \geq \lambda_n(D(G)).$$

Lemma 1. *Let G be a graph of order n. If $\Delta(G) \leq l$ and $diam(G) \leq d$, then*

$$n \leq 1 + l + l(l-1) + l(l-1)^2 + \cdots + l(l-1)^{d-1}.$$

Now we shall give the proof of Lemma 2, whose proof relies on Theorems 4, 5 and 6. Part of technique is inspired by Zhang and Cao [19].

Lemma 2. *Let G be a connected graph of order n. For any integer $k \geq 2$, if n is sufficiently large with respect to k then $\lambda_k(D(G)) \geq -2$.*

Proof. We divide the proof into two cases.

Case 1. $\Delta(G) \geq R(k-1, k-1)$

Let $v \in V(G)$ with $d_G(v) = \Delta(G)$. By Theorem 5, $G' := G[N(v)]$ either contains a clique A of size $k-1$ or an independent set B of size $k-1$.

If the first case occurs, then $H = G[A \cup \{v\}] \cong K_k$. By Theorem 4 and the inequality $k \geq 2$, $\lambda_k(D(G)) \geq \lambda_k(D(H)) = -1$.

If the second case occurs, then $H = G[B \cup \{v\}] \cong K_{1,k-1}$. By Theorem 4 and the inequality $k \geq 2$, $\lambda_k(D(G)) \geq \lambda_k(D(H)) = -2$.

Case 2. $\Delta(G) < R(k-1, k-1)$

Take $l = R(k-1, k-1) - 1$ and $d \geq 2k$. By Lemma 1, if $n \geq 1 + l + l(l-1) + l(l-1)^2 + \cdots + l(l-1)^{d-1}$, then $diam(G) \geq d+1$. Thus, the distance matrix D' of P_d is a principle submatrix of D. Note that $\mu_i(P_d) = 2 + 2\cos\frac{i\pi}{d}$ for $i = 1, \cdots, d$. Thus, by Theorems 4 and 6, we have $\lambda_k(D(G)) \geq \lambda_k(D(P_d)) \geq \frac{-2}{\mu_k(P_d)} \geq -1$ for $2k \leq d$. The proof is complete. $\square$

The following three theorems are used in the proof of Proposition 1.

Theorem 7 (Merris [14]). *Let T be a tree with diameter d. Then $\lambda_{\lfloor \frac{d}{2} \rfloor}(D(T)) > -1$.*

Theorem 8 (Zhou and Ilić [20]). *Let G be a connected graph on n vertices with diameter d, minimum degree δ_1 and the second minimum degree δ_2. Then*

$$\lambda_1(D(G)) \leq \sqrt{[dn - \frac{d(d-1)}{2} - 1 - \delta_1(d-1)][dn - \frac{d(d-1)}{2} - 1 - \delta_2(d-1)]},$$

where the equality holds if and only if G is a regular graph with $d \leq 2$.

Theorem 9 (Ruzieh and Powers [18, Corollary 2.2]). *The distance spectral radius of the path P_n is $\lambda_1(D(P_n)) = \frac{n^2}{2a^2} - \frac{2+a^2}{6a^2} + O(\frac{1}{n^2})$, where a is the root of $a\tanh a = 1$. ($a \doteq 1.199679$.)*

Finally, we prove an easy but useful fact to conclude this section.

Lemma 3. *Let $G = G[V_1, V_2]$ be a connected bipartite graph with $|V_1| = r$ and $|V_2| = n - r$ and $e(G) = m$. Then*

$$\lambda_1(D(G)) \geq \frac{2(n^2 + (r-1)n - r^2 - 2m)}{n}.$$

Proof. Note that

$$\begin{aligned} W(G) &\geq m + 2\left(\binom{r}{2} + \binom{n-r}{2}\right) + 3(r(n-r) - m) \\ &= r(r-1) + (n-r)(n-r-1) + 3r(n-r) - 2m \\ &= n^2 + (r-1)n - r^2 - 2m. \end{aligned}$$

Then the result follows from that $\lambda_1(D(G)) \geq \frac{2W}{n}$. $\square$

3 Proofs

Proof of Theorem 1. (i) By a simple calculation, we have $S_k(D(K_n)) = n - k$ for $k \geq 1$. Let $G \not\cong K_n$ be a connected graph with order n. Then

$$\lambda_1(D(G)) \geq \frac{2W(G)}{n} \geq \frac{2\left[m + 2(\binom{n}{2} - m)\right]}{n} = 2(n-1) - \frac{2m}{n}.$$

If $m \leq \frac{n(n-k)}{2}$, then $\lambda_1(D(G)) \geq n + k - 2$. Note that $\lambda_2(D(G)) \geq -1$. By Lemma 2, if n is sufficiently large with respect to k, then $\lambda_k(D(G)) \geq -2$. So we obtain

$$\begin{aligned} S_k(D(G)) &= \lambda_1(D(G)) + \lambda_2(D(G)) + \cdots + \lambda_k(D(G)) \\ &\geq n + k - 2 - 1 - 2(k-2) \\ &= n - k + 1 \\ &> n - k \\ &= S_k(D(K_n)). \end{aligned}$$

If $m > \frac{n(n-k)}{2}$, then $m > (1 - \frac{1}{k})\frac{n^2}{2}$ when $n \geq k^2$ (recall that n is sufficiently large with respect to k). By Turán's theorem, G contains a K_k. Thus, we have

$$\lambda_i(D(G)) \geq \lambda_i(D(K_k)) = -1 \quad \text{for } i = 2, \ldots, k.$$

Since $G \neq K_n$, we obtain $\lambda_1(D(G)) > n - 1$. It follows that $S_k(D(G)) > n - 1 - (k-1) = n - k = S_k(D(K_n))$. If $G = K_n$, it is easy to find that $S_k(D(G)) = n - k$. This completes the proof. □

(ii) Let $T \not\cong K_{1,n-1}$. Similar to the proof of Lemma 2, we have either $\Delta(T) \geq k-1$ or $diam(T) \geq 2k+1$, where $k \geq 2$. It follows that either $K_{1,k-1} \subset G$ or $P_{2k+2} \subset G$. Then by Theorem 4 and Lemma 2, either $\lambda_k(D(T)) \geq -2$ or $\lambda_k(D(T)) > -1$. Thus, we have $\lambda_3(D(T)) + \cdots + \lambda_k(D(T)) \geq -2(k-2)$. Note that $diam(T) \geq 3$. Then there exists a bipartite partition of $T = T(V_1, V_2)$ such that $|V_1| = r$ and $|V_2| = n - r$ with $2 \leq r \leq \frac{n}{2}$. Then by Lemma 3, we have

$$\begin{aligned} \lambda_1(D(T)) &\geq \frac{2n^2 + 2(r-1)n - 2r^2 - 4m}{n} \\ &= \frac{2n^2 + 2(r-1)n - 2r^2 - 4(n-1)}{n} \\ &\geq \frac{2n^2 + 2(2-1)n - 2 \times 2^2 - 4(n-1)}{n} \\ &= 2n - 2 - \frac{4}{n} \\ &> 2n - 3. \end{aligned}$$

Combing with $\lambda_2(D(T)) \geq -1$, we have

$$S_k(T) > 2n - 3 - 1 - 2(k-2) = 2n - 2k = S_k(K_{1,n-1}).$$

If $T = K_{1,n-1}$, then $S_k(T) = 2n - 2k$. This completes the proof. □

Proof of Theorem 2. If $d = 1$, then $G \cong K_n$ and $\lambda_2(D(G)) = -1$, hence the result holds. In the following, set $\lambda_2(D) = \lambda_2(D(G))$. Assume that $d \geq 2$. Let X

be an eigenvector of $D(G)$ corresponding to $\lambda_2(D)$. We use x_v to denote the entry of X corresponding to the vertex $v \in V(G)$. Define $S^+ = \{v \in V(G) : x_v > 0\}$ and $S^- = \{v \in V(G) : x_v < 0\}$. For $v \in S^+$, we have

$$\lambda_2(D)x_v = \sum_{u\in S^+\setminus\{v\}} d(u,v)x_u + \sum_{w\in S^-} d(w,v)x_w \le d \sum_{u\in S^+\setminus\{v\}} x_u + \sum_{w\in S^-} x_w,$$

that is, $(\lambda_2(D)+d)x_v \le d\sum_{u\in S^+} x_u + \sum_{w\in S^-} x_w$. So

$$(\lambda_2(D)+d)\sum_{v\in S^+} x_v \le |S^+|d\sum_{u\in S^+} x_u + |S^+|\sum_{w\in S^-} x_w,$$

that is,

$$(\lambda_2(D)+d-d|S^+|)\sum_{v\in S^+} x_v \le |S^+|\sum_{w\in S^-} x_w. \tag{1}$$

For $v \in S^-$, we have

$$\lambda_2(D)x_v = \sum_{u\in S^+} d(u,v)x_u + \sum_{w\in S^-\setminus\{v\}} d(w,v)x_w \ge \sum_{u\in S^+} x_u + d\sum_{w\in S^-\setminus\{v\}} x_w.$$

Similarly,

$$(\lambda_2(D)+d-d|S^-|)\sum_{v\in S^-} x_v \ge |S^-|\sum_{w\in S^+} x_w. \tag{2}$$

Combining Eqs. (1) and (2), we obtain

$$(\lambda_2(D)+d-d|S^+|)(\lambda_2(D)+d-d|S^-|)\sum_{v\in S^+} x_v \sum_{u\in S^-} x_u \le |S^+||S^-|\sum_{v\in S^+} x_v \sum_{u\in S^-} x_u,$$

that is,

$$(\lambda_2(D)+d-d|S^+|)(\lambda_2(D)+d-d|S^-|) \ge |S^+||S^-|.$$

Let

$$f(y) = (y+d-d|S^+|)(y+d-d|S^-|) - |S^+||S^-|.$$

Clearly, the roots of $f(y)=0$ are

$$y_1 = \frac{d(|S^+|+|S^-|-2) + \sqrt{d^2(|S^+|+|S^-|)^2 - 4(d^2-1)|S^+||S^-|}}{2}$$

and

$$y_2 = \frac{d(|S^+|+|S^-|-2) - \sqrt{d^2(|S^+|+|S^-|)^2 - 4(d^2-1)|S^+||S^-|}}{2},$$

respectively. From Eqs. (1) and (2), we can see that $\lambda_2(D) \le d|S^+| - d$ and $\lambda_2(D) \le d|S^-| - d$. Hence, $y_1 > \frac{d(|S^+|+|S^-|-2)}{2} \ge \min\{d|S^+|-d, d|S^-|-d\} \ge \lambda_2(D)$. Since $f(\lambda_2(D)) = (\lambda_2(D)-y_1)(\lambda_2(D)-y_2) \ge 0$, we have

$$\begin{aligned}
\lambda_2(D) &\le y_2 \\
&= \frac{d(|S^+|+|S^-|-2) - \sqrt{d^2(|S^+|+|S^-|)^2 - 4(d^2-1)|S^+||S^-|}}{2} \\
&\le \frac{d(|S^+|+|S^-|-2) - (|S^+|+|S^-|)}{2} \\
&\le \frac{d-1}{2}n - d,
\end{aligned}$$

where the second inequality holds since $4|S^+||S^-| \leq (|S^+| + |S^-|)^2$ and the last inequality holds since $|S^+| + |S^-| \leq n$.

If $\lambda_2(D) = \frac{d-1}{2}n - d$, then $|S^+| + |S^-| = n$, $|S^+| = |S^-|$ and the equalities in Eqs. (1) and (2) hold. This implies that for any vertices $v, w \in S^-$, $d(w, v) = d \geq 2$, and hence v, w are nonadjacent; for any vertex $v \in S^-$ and $u \in S^+$, $d(u, v) = 1$, which implies that u and v are adjacent. Thus, $G[S^-]$ and similarly, $G[S^+]$ are independent sets and each vertex in S^+ is adjacent to each vertex in S^-, which implies that $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Conversely, it is routine to check that $\lambda_2(D(K_{\frac{n}{2},\frac{n}{2}})) = \frac{n}{2} - 2$, completing the proof. $\square$

Let G be a graph and $v \in V(G)$. We denote by $t(G, u)$ the number of triangles in G containing the vertex u.

Proof of Theorem 3. (i) Since $\alpha(G) \leq s$, we have $diam(G) \leq 2s-1$. By Theorem 2,

$$\lambda_2(D) \leq (s-1)n - (2s-1). \tag{3}$$

Recall that a corollary of Turán's inequality says that for any graph of order n and size m, $\alpha(G) \geq \frac{n}{1+\overline{d}}$, where $\overline{d} = \frac{2m}{n}$ (see Alon and Spencer [1, pp.95]). Thus, we obtain $s \geq \alpha(G) \geq \frac{n^2}{n+2m}$, that is,

$$m \geq \frac{n^2 - sn}{2s}. \tag{4}$$

For each vertex $u \in V(G)$, $t(G, u) = e(G[N(u)])$. Note that $\alpha(G[N(u)]) \leq s$. Then (4) becomes

$$t(G; u) \geq \frac{d^2(u) - sd(u)}{2s}. \tag{5}$$

Summing over all vertices for (5), we have

$$3t(G) = \sum_{v \in V(G)} t(G; u) \geq \sum_{u \in V(G)} \frac{d^2(u) - sd(u)}{2s} = \frac{\sum_{v \in V(G)} d^2(u)}{2s} - m. \tag{6}$$

By AG-mean inequality,

$$\frac{\sum_{v \in V(G)} d^2(u)}{2s} - m \geq \frac{(\sum_{v \in V(G)} d(u))^2}{2sn} - m = m(\frac{2m}{sn} - 1) \geq m(\frac{n-s}{s^2} - 1). \tag{7}$$

By (6) and (7), we obtain

$$3s^3 \cdot \frac{t(G)}{m} \geq s(n-s) - s^3 > (s-1)n - (2s-1). \tag{8}$$

By (3) and (8), the proof is completed.

(ii) Setting $s = 2$ in Theorem 3(i), we have $\lambda_2(D(G)) < \frac{24}{m} \cdot t(G)$ for $n > 9$. By Turán's theorem, when $\alpha(G) \leq 2$ and $n \geq 11$, we get

$$m \geq \frac{n^2 - 2n}{4} = \frac{n}{2}(\frac{n}{2} - 1) \geq \frac{11}{2} \cdot \frac{9}{2} = 24.75 > 24.$$

The proof is completed. $\square$

Proof of Proposition 1. By Theorem 9 and Lemma 2, we have $S_k(P_n) \geq \frac{n^2}{3} - 2(k-1)$. From Theorem 8, we have $\lambda_1(D) < dn - \frac{d(d-1)}{2} - 1$. By Theorems 2 and 8, we have

$$\begin{aligned} S_k(G) &\leq dn - \frac{d(d-1)}{2} - 1 + k(\frac{n(d-1)}{2} - d) \\ &= (k\frac{d-1}{2} + d)n - \frac{d(d-1)}{2} - 1 - dk \\ &< \frac{n^2}{3} - 2(k-1) \quad (\text{since } d < \tfrac{2n}{3(k+2)}) \\ &\leq S_k(P_n). \end{aligned}$$

This completes the proof. $\square$

4 Concluding remarks

It is known that $S_k(K_{r,n-r}) = 2n - 2k$ for $k \geq 2$. Theorem 1 (ii) shows that $S_k(D) \geq 2n - 2k = S_k(K_{1,n-1})$ if G is a tree, so we may have the following more general problem.

Problem 3. Let G be a connected bipartite graph of order n. For an integer $k \geq 2$ and sufficiently large n with respect to k, does there always hold $S_k(G) \geq 2n - 2k$, where the equality holds if and only if $G \cong K_{r,n-r}$ for $1 \leq r \leq n-1$?

By Theorem 2, we have $\lambda_2(D) \leq \frac{n(d-1)}{2} - d$. If $d = 2$, then $\lambda_2(D) \leq \frac{n}{2} - 2$. It seems that the upper bound holds for every connected graph of order n, so we have the following problem.

Problem 4. Let G be a connected graph with second largest distance eigenvalue $\lambda_2(D)$. Then $\lambda_2(D) \leq \frac{n}{2} - 2$ and the equality holds if and only if $G \cong K_{\frac{n}{2},\frac{n}{2}}$.

Acknowledgement

The author would like to thank Bo Ning for sharing the proof of theorem 3.

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