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Sharp bounds on the distance spectral radius and the distance energy of graphs

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Abstract

The D-eigenvalues $\{\mu_1, \mu_2, \ldots, \mu_p\}$ of a graph G are the eigenvalues of its distance matrix D and form the D-spectrum of G denoted by $spec_D(G)$. The greatest D-eigenvalue is called the D-spectral radius of G denoted by μ_1. The D-energy $E_D(G)$ of the graph G is the sum of the absolute values of its D-eigenvalues. In this paper we obtain some lower bounds for μ_1 and characterize those graphs for which these bounds are best possible. We also obtain an upperbound for $E_D(G)$ and determine those maximal D-energy graphs.

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Keywords: Distance spectral radius; Distance energy

1. Introduction

Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_p\}$. The distance matrix $D = D(G)$ of G is defined so that its (i, j)-entry, d_{ij}, is equal to $d_G(v_i, v_j)$, the distance (= length of the shortest path [1]) between the vertices v_i and v_j of G. The eigenvalues of $D(G)$ are said to be the D-eigenvalues of G and form the D-spectrum of G, denoted by $spec_D(G)$. Since the distance matrix is symmetric, all its eigenvalues μ_i, $i = 1, 2, \ldots, p$, are real and can be labelled so that $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_p$. If $\mu_{i_1} > \mu_{i_2} > \cdots > \mu_{i_g}$ are the distinct D-eigenvalues, then the D-spectrum can be written as

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$$spec_D(G) = \begin{pmatrix} \mu_{i_1} & \mu_{i_2} & \dots & \mu_{i_g} \\ m_1 & m_2 & \dots & m_g \end{pmatrix},$$

where m_j indicates the algebraic multiplicity of the eigenvalue μ_{i_j}. Of course, $m_1 + m_2 + \cdots + m_g = p$.

The ordinary spectrum of G, which is the spectrum of the adjacency matrix of G is well studied and many properties of graphs in connection with the spectrum are revealed during the past years. For details see the book [2] and the references cited therein. The greatest eigenvalue of the distance matrix of a graph G, μ_1 is called the distance spectral radius. The spectral radii of the adjacency matrix and the laplacian matrix of G are studied in detail in past years. For some recent works see [13] and also the papers cited therein.

The D-energy, $E_D(G)$, of G is defined as

$$E_D(G) = \sum_{i=1}^{p} |\mu_i|. \tag{1}$$

The concept of D-energy, Eq. (1), was recently introduced [8]. This definition was motivated by the much older [4] and nowadays extensively studied [5–7,10–12,14,15] graph energy, defined in a manner fully analogous to Eq. (1), but in terms of the ordinary graph eigenvalues (eigenvalues of the adjacency matrix, see [2]). For some recent works on distance spectrum and D-energy of graphs, see [8,9].

This paper is organized as follows. In the first section we obtain some bounds for the distance spectral radius of graphs. In the second section we obtain an upperbound for the distance energy and characterize those graphs for which the bounds are best possible. The considerations in the subsequent sections are based on the applications of the following definitions and lemmas:

Definition 1. Let G be a graph with $V(G) = \{v_1, v_2, \dots, v_p\}$ and a distance matrix D. Then the distance degree of v_i, denoted by D_i is given by $D_i = \sum_{j=1}^{p} d_{ij}$.

Definition 2. Let G be a graph with $V(G) = \{v_1, v_2, \dots, v_p\}$ and a distance matrix D. Let the distance degree sequence be $\{D_1, D_2, \dots, D_p\}$. Then the second distance degree of v_i, denoted by T_i is given by $T_i = \sum_{j=1}^{p} d_{ij} D_j$.

Definition 3. Let G be a graph with distance degree sequence $\{D_1, D_2, \dots, D_p\}$. Then G is k-distance regular if $D_i = k$ for all i.

Definition 4. Let G be a graph with distance degree sequence $\{D_1, D_2, \dots, D_p\}$ and second distance degree sequence $\{T_1, T_2, \dots, T_p\}$. Then G is pseudo k-distance regular if $\frac{T_i}{D_i} = k$ for all i.

Definition 5 [3]. Let G be a graph with distance matrix D. Then the Wiener index of G denoted by $W(G)$ is given by $W(G) = \frac{1}{2} \sum_{i=1}^{p} D_i$.

In the following discussions G is always a connected graph with D as a distance matrix. All graphs considered in this paper are simple and we follow [2] for spectral graph theoretic terminology.

We begin with the following lemma.

Lemma 1

$$T_1 + T_2 + \cdots + T_p = D_1^2 + D_2^2 + D_3^2 + \cdots + D_p^2.$$

Proof. We have

$$D_i = \sum_{j=1}^{p} d_{ij} \quad \text{and} \quad T_i = \sum_{j=1}^{p} d_{ij} D_j.$$

Now

$$\begin{aligned} T_1 + T_2 + \cdots + T_p &= [1, 1, 1, \ldots, 1](D[D_1, D_2, D_3, \ldots, D_p]^{\mathrm{T}}) \\ &= ([1, 1, 1, \ldots, 1]D)[D_1, D_2, D_3, \ldots, D_p]^{\mathrm{T}}, \\ &\quad \text{by associativity of matrix multiplication} \\ &= D_1^2 + D_2^2 + D_3^2 + \cdots + D_p^2 \qquad \square \end{aligned}$$

2. Bounds on the distance spectral radius

Theorem 1. *Let G be a graph with Wiener index W. Then* $\mu_1 \geqslant \frac{2W}{p}$ *and the equality holds if and only if G is distance regular.*

Proof. Let $x = \frac{1}{\sqrt{p}}(1, 1, 1, \ldots, 1)$ be a unit P-vector. Then by Raleigh principle, applied to the distance matrix D of G, we get

$$\begin{aligned} \mu_1 &\geqslant \frac{xDx^{\mathrm{T}}}{xx^{\mathrm{T}}} \\ &= \frac{\frac{1}{\sqrt{p}}[D_1, D_2, D_3, \ldots, D_p]\frac{1}{\sqrt{p}}[1, 1, 1, \ldots, 1]^{\mathrm{T}}}{1} \\ &= \frac{1}{p}\sum_{i=1}^{p} D_i \\ &= \frac{2W}{p} \end{aligned}$$

Now suppose G is distance regular. Then each row of D sums to a constant, say k and $2W = pk$. Then by the Theorem of Frobenius [2], k is the simple and greatest eigenvalue of D. Thus $\mu_1 = k = \frac{pk}{p} = \frac{2W}{p}$ and hence equality holds.

Conversely if equality holds, then x is the eigenvector corresponding to μ_1 and hence $xD = \mu_1 x$. This then gives $D_i = \mu_1$ for all i. Since D_i is an integer it follows that G is distance regular. Hence the theorem. $\square$

Theorem 2. *Let G be a graph with distance degree sequence* $\{D_1, D_2, \ldots, D_p\}$. *Then*

$$\mu_1 \geqslant \sqrt{\frac{D_1^2 + D_2^2 + D_3^2 + \cdots + D_p^2}{p}}$$

The equality holds if and only if G is distance regular.

Proof. Let D be the distance matrix of G and $X = (x_1, x_2, \ldots, x_p)$ be the unit positive Perron eigenvector of D corresponding to μ_1.

Take $C = \frac{1}{\sqrt{p}}(1, 1, 1, \ldots, 1)$. Then C is a unit positive vector.

So we have $\mu_1 = \mu_1(D) = \sqrt{\mu_1(D^2)} = \sqrt{XD^2X^{\mathrm{T}}} \geqslant \sqrt{CD^2C^{\mathrm{T}}}$

Now

$$\begin{aligned} CD &= \frac{1}{\sqrt{p}}(1, 1, 1, \ldots, 1)D \\ &= \frac{1}{\sqrt{p}}[D_1, D_2, D_3, \ldots, D_p] \end{aligned}$$

Hence $CD^2C^{\mathrm{T}} = CDDC^{\mathrm{T}} = CD(CD)^{\mathrm{T}} = \frac{\sum_{i=1}^p D_i^2}{p}$

Thus $\mu_1 \geqslant \sqrt{CD^2C^{\mathrm{T}}} = \sqrt{\frac{\sum_{i=1}^p D_i^2}{p}}$ and hence the inequality.

Now assume that G is distance regular. Then $D_i = k$ for all i and hence by the Theorem of Frobenius [2], k is the simple and the greatest eigenvalue of D. But then

$$\mu_1 = k = \sqrt{\frac{pk^2}{p}} = \sqrt{\frac{\sum_{i=1}^p D_i^2}{p}}$$

and hence equality holds.

Conversely if equality holds, then C is the eigenvector corresponding to μ_1. Then as in the proof of Theorem 1, we get G is distance regular. □

Theorem 3. *Let G be a graph with distance degree sequence $\{D_1, D_2, \ldots, D_p\}$ and second distance degree sequence $\{T_1, T_2, \ldots, T_p\}$. Then*

$$\mu_1 \geqslant \sqrt{\frac{T_1^2 + T_2^2 + T_3^2 + \cdots + T_p^2}{D_1^2 + D_2^2 + D_3^2 + \cdots + D_p^2}}$$

Equality holds if and only if G is pseudo distance regular.

Proof. Let D be the distance matrix of G and $X = (x_1, x_2, \ldots, x_p)$ be the unit positive Perron eigenvector of D corresponding to μ_1.

Take

$$C = \frac{1}{\sqrt{\sum_{i=1}^p D_i^2}}(D_1, D_2, \ldots, D_p)$$

Then C is a unit positive vector. So we have

$$\mu_1(D) = \sqrt{\mu_1(D^2)} = \sqrt{XD^2X^{\mathrm{T}}} \geqslant \sqrt{CD^2C^{\mathrm{T}}}$$

Now

$$\begin{aligned} CD &= \frac{1}{\sqrt{\sum_{i=1}^p D_i^2}}(D_1, D_2, \ldots\ldots, D_p)[d_{ij}]_{p\times p} \\ &= \frac{1}{\sqrt{\sum_{i=1}^p D_i^2}}(T_1, T_2, \ldots\ldots, T_p) \end{aligned}$$

Thus $CD^2C^{\mathrm{T}} = CD(CD)^{\mathrm{T}} = \frac{T_1^2+T_2^2+T_3^2+\cdots+T_p^2}{D_1^2+D_2^2+D_3^2+\cdots+D_p^2}$

Therefore

$$\mu_1 \geqslant \sqrt{\frac{T_1^2+T_2^2+T_3^2+\cdots+T_p^2}{D_1^2+D_2^2+D_3^2+\cdots+D_p^2}}.$$

Now assume that G is pseudo distance regular. So $\frac{T_i}{D_i} = k$ or $T_i = kD_i$ for all i. Then $CD = kC$, showing that C is an eigenvector corresponding to k and hence $\mu_1 = k$. Thus the equality holds.

Conversely if equality holds then as in the proof Theorem 1, we get C is the eigenvector corresponding to μ_1 and that $CD = \mu_1 C$. This then implies that $\frac{T_i}{D_i} = \mu_1$ or in other words G is pseudo distance regular. $\square$

Theorem 4. *The bound for μ_1 is improving from Theorems 1 to 3.*

Proof. By Lemma 1 we have $\sum_{i=1}^{p} T_i = \sum_{i=1}^{p} D_i^2$. Also by Cauchy–Schwartz inequality $\left(\sum_{i=1}^{p} T_i\right)^2 \leqslant p\sum_{i=1}^{p} T_i^2$ and $\left(\sum_{i=1}^{p} D_i\right)^2 \leqslant p\sum_{i=1}^{p} D_i^2$. Now

$$\mu_1 \geqslant \sqrt{\frac{\sum_{i=1}^{p} T_i^2}{\sum_{i=1}^{p} D_i^2}} \geqslant \sqrt{\frac{\left(\sum_{i=1}^{p} T_i\right)^2}{p\sum_{i=1}^{p} D_i^2}} = \sqrt{\frac{\left(\sum_{i=1}^{p} D_i^2\right)^2}{p\sum_{i=1}^{p} D_i^2}}$$
$$= \sqrt{\frac{\sum_{i=1}^{p} D_i^2}{p}} \geqslant \sqrt{\frac{\left(\sum_{i=1}^{p} D_i\right)^2}{p\times p}} = \frac{2W}{p}. \qquad \square$$

In the following theorem we give another bound for μ_1 which cannot be compared with the bounds so far obtained.

Theorem 5. *Let G be graph with Wiener index W and distance degree sequence $\{D_1, D_2, \ldots, D_p\}$. Then*

$$\mu_1 \geqslant \mathrm{Max}_i \frac{1}{p-1}\left((W-D_i)+\sqrt{(W-D_i)^2+(p-1)D_i^2}\right).$$

Proof. Let v_i be a vertex of G with distance degree D_i. Then this vertex gives rise a partition to the distance matrix with quotient matrix

$$B = \begin{bmatrix} 0 & D_i \\ \frac{D_i}{p-1} & \frac{2(W-D_i)}{p-1} \end{bmatrix}$$

Then B has eigenvalues

$$\eta_1 = \frac{1}{p-1}\left((W-D_i)+\sqrt{(W-D_i)^2+(p-1)D_i^2}\right),$$
$$\eta_2 = \frac{1}{p-1}\left((W-D_i)-\sqrt{(W-D_i)^2+(p-1)D_i^2}\right).$$

By the theorem of interlacing, we have eigenvalues of B interlace those of D. Thus

$$\mu_1 \geqslant \eta_1 = \frac{1}{p-1}\left((W-D_i)+\sqrt{(W-D_i)^2+(p-1)D_i^2}\right).$$

Since this is true for all i, theorem follows. $\square$

Now we prove the following lemma regarding the number of D- eigenvalues of a graph.

Lemma 2. *A connected graph G has two distinct D-eigenvalues if and only if G is a complete graph.*

Proof. Let G be a connected graph with distance matrix D. Suppose that G has exactly two distinct D-eigenvalues. Let them be $\mu_1 > \mu_2$. Since G is connected, D is irreducible and by the theorem of Frobenius, μ_1 is the greatest and simple eigenvalue of D so that the multiplicity of μ_1 is one. Thus all other D-eigenvalues of G are μ_2. Now we prove that diameter of G is one. □

Claim. G does not contain an induced shortest path P_m, $m \geqslant 3$.

Assume that G contains an induced shortest path P_m, $m \geqslant 3$. Let B be the principal submatrix of D indexed by the vertices in P_m. Let $\theta_i(A)$ denote the ith eigenvalue of the matrix A. Then by the interlacing theorem we have

$$\theta_i(D) \geqslant \theta_i(B) \geqslant \theta_{p-m+i}(D), \quad i = 1, 2, \ldots, m,$$
$$\text{i.e.} \quad \mu_2 \geqslant \theta_2(B) \geqslant \theta_3(B) \geqslant \theta_4(B) \geqslant \cdots \geqslant \theta_m(B) \geqslant \theta_p(D) = \mu_2.$$

This then shows that P_m has atmost 2 distinct D-eigenvalues for $m \geqslant 3$, which is impossible. Therefore G do not contain two vertices at distance two or more and hence it is complete.

Conversely assume that G is a complete graph of order p. Then the distance matrix and adjacency matrix of G coincide and from [2] it follows that G has exactly two distinct D- eigenvalues, $p-1$ and -1. Hence the lemma. □

3. An upperbound for the distance energy

In this section we obtain an upperbound for the distance energy of graphs and characterize those graphs for which this bound is best possible.

Theorem 6. *With the notations described above*

$$E_D(G) \leqslant \sqrt{\frac{\sum_{i=1}^p T_i^2}{\sum_{i=1}^p D_i^2}} + (p-1)\sqrt{S - \frac{\sum_{i=1}^p T_i^2}{\sum_{i=1}^p D_i^2}},$$

where S is the sum of the squares of entries in the distance matrix. Equality holds if and only if either G is a complete graph or a pseudo k-distance regular graph with three distinct D-eigenvalues $\left(k, \sqrt{\frac{S-k^2}{p-1}}, -\sqrt{\frac{S-k^2}{p-1}}\right)$.

Proof. Let $\{\mu_1, \mu_2, \ldots, \mu_p\}$ be the D-eigenvalues of G. Then

$$\sum_{i=1}^{p} \mu_i = 0, \sum_{i=1}^{p} |\mu_i| = E_D(G)$$

Also $\sum_{i=1}^p \mu_i^2 = S = \sum_{i,j=1}^p (d_{ij})^2$, being the trace of D^2.

Now applying the Cauchy–Schwartz inequality to the two $p-1$ vectors $(1, 1, \ldots, 1)$ and $(|\mu_2|, |\mu_3|, \ldots, |\mu_p|)$ we get,

$$(E_D - \mu_1)^2 \leqslant (p-1)(S - \mu_1^2) \tag{2}$$

Thus

$$E_D \leqslant \mu_1 + \sqrt{(p-1)(S-\mu_1^2)}$$

Define a function $f(x) = x + \sqrt{(p-1)(S-x^2)}$ for $\frac{2W}{p} \leqslant x \leqslant \sqrt{S}$.

Then by applying the max–min techniques of calculus we can see that $f(x)$ is monotonically decreasing in $x \geqslant \sqrt{\frac{S}{P}}$. Now by Cauchy–Schwartz inequality we have

$$D_i^2 = \left(\sum_{j=1}^{p} d_{ij}\right)^2 \leqslant p\sum_{j=1}^{p} d_{ij}^2.$$

Then

$$\sum_{i=1}^{p} D_i^2 \leqslant \sum_{i=1}^{p} p\sum_{j=1}^{p} d_{ij}^2 = p\sum_{i=1}^{p}\sum_{j=1}^{p} d_{ij}^2 = pS.$$

Also

$$T_i = \sum_{j=1}^{p} d_{ij}D_j \geqslant \sum_{j=1}^{p} d_{ij}^2 \text{ and } \sum_{i=1}^{p} T_i^2 \geqslant \sum_{i=1}^{p}\left(\sum_{j=1}^{p}(d_{ij})^2\right)^2 \geqslant S^2.$$

Hence $\mu_1 \geqslant \sqrt{\frac{\sum_{i=1}^{p} T_i^2}{\sum_{i=1}^{p} D_i^2}} \geqslant \sqrt{\frac{S^2}{pS}} = \sqrt{\frac{S}{p}}$.

Therefore $E_D(G) \leqslant f(\mu_1) \leqslant f\left(\sqrt{\frac{\sum_{i=1}^{p} T_i^2}{\sum_{i=1}^{p} D_i^2}}\right)$ and thus the theorem follows.

Now suppose equality holds. Then

$$\mu_1 = \sqrt{\frac{\sum_{i=1}^{p} T_i^2}{\sum_{i=1}^{p} D_i^2}}$$

and by Theorem 3 we have G is pseudo k-distance regular. Also equality holds in the Cauchy–Schwartz inequality (2). Hence

$$\begin{aligned}
&|\mu_2| = |\mu_3| = \cdots = |\mu_p| \\
&\qquad \Rightarrow \left(\sum_{i=2}^{p} |\mu_i|\right)^2 = (p-1)(S-\mu_1^2) \\
&\qquad \Rightarrow |\mu_i| = \sqrt{\frac{S-\mu_1^2}{p-1}}, i = 2, \ldots, p.
\end{aligned}$$

Since $|\mu_i| = \sqrt{\frac{S-\mu_1^2}{p-1}}$, μ_i can have atmost two distinct values and we arrive at the following.

- G has exactly one distinct D-eigenvalue. Then all D-eigenvalues are zero as the sum of D-eigenvalues is the trace of D and as G is connected, $G = K_1$.
- G has exactly two distinct D-eigenvalues. Then by Lemma 2, G is complete.
- G has exactly three distinct D-eigenvalues.

Then $\mu_1 = \sqrt{\frac{\sum_{i=1}^{p} T_i^2}{\sum_{i=1}^{p} D_i^2}}$ and $|\mu_i| = \sqrt{\frac{S-\mu_1^2}{p-1}}$, $i = 2, \ldots, p$. Also $\frac{T_i}{D_i} = k$ for all i. Then we get G as a graph with three distinct D-eigenvalues $\left(k, \sqrt{\frac{S-k^2}{p-1}}, -\sqrt{\frac{S-k^2}{p-1}}\right)$. Hence the theorem. $\square$

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