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Estimating the distance Estrada index

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Abstract

Suppose G is a simple graph on n vertices. The D-eigenvalues $\mu_1, \mu_2, \cdots, \mu_n$ of G are the eigenvalues of its distance matrix. The distance Estrada index of G is defined as $DEE(G) = \sum_{i=1}^{n} e^{\mu_i}$. In this paper, we establish new lower and upper bounds for $DEE(G)$ in terms of the Wiener index $W(G)$. We also compute the distance Estrada index for some concrete graphs including the buckminsterfullerene C_{60}.

Keywords: Distance degree; distance matrix; Estrada index; Wiener index.

1. Introduction

Let G be a simple n-vertex graph with vertex set $V(G)$. Denote by $D(G) = (d_{ij}) \in \mathbb{R}^{n\times n}$ the distance matrix of G, where d_{ij} signifies the length of shortest path between vertices $v_i \in V(G)$ and $v_j \in V(G)$. Then the adjacency matrix $A(G) = (a_{ij})$ of the graph can be defined by $a_{ij} = 1$ if $d_{ij} = 1$, and $a_{ij} = 0$ otherwise. Since $D(G)$ is a real symmetric matrix, its eigenvalues are real numbers. We order the eigenvalues in a nonincreasing manner as $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ (they are customarily called D-eigenvalues of G (Cvetkovi´c *et al*., 1995)). The distance Estrada index of G is defined as

$$DEE(G) = \sum_{i=1}^{n} e^{\mu_i}. \tag{1}$$

This graph-spectrum-based structural invariant is recently proposed in Güngör & Bozkurt (2009), and some results on its bounds can be found in Shang (2015a), Bozkurt *et al*. (2013), Bozkurt & Bozkurt (2012). If we replace in (1) the D-eigenvalues $\{\mu_i\}_{i=1}^{n}$ by the eigenvalues $\{\lambda_i\}_{i=1}^{n}$ of the adjacency matrix $A(G)$, we recover the well-researched graph descriptor Estrada index (Estrada, 2000). The Estrada index can be used as an efficient measuring tool in a number of areas in chemistry and physics, and its mathematical properties have been intensively studied (Das & Lee (2009), de la Peña *et al*. (2007), Estrada (2002, 2004), Estrada & Rodríguez-Velázquez (2005), Zhou (2008), Gutman *et al*. (2011), Ilić & Stevanović (2010), Shang (2011, 2013), to mention only a few).

Apart from its formal analogy to the Estrada index, we believe the distance Estrada index (1) is potentially of vast importance in physical chemistry. After all, the most natural description of a molecular graph is in terms of the distance, be them geometric or topological, between pairs of vertices. The oldest distance-based invariant, perhaps, is the Wiener index (Wiener, 1947), which has found useful applications in structure—property correlations; see e.g. Nikolić *et al*. (1995), Randić (1993), Dobrynin *et al*. (2001), Walikar *et al*. (2004). In this paper, we aim to establish lower and upper bounds for $DEE(G)$ by using the Wiener index, which allows us to gain insight into the relationship between the distance Estrada index and the Wiener index, and, in particular, gain better understanding of the dependence of the distance Estrada index on the concept of distance degree, whereby the Wiener index is constructed. We mention that various properties of graph distance and $D(G)$ for some interesting graphs can be found in e.g. Bapat & Sivasubramanian (2013), Indulal & Gutman (2008), Jin & Zhang (2014), Alaeiyan *et al*. (2014).

The rest of the paper is organized as follows. In Section 2, we give some notations and lemmas. The bounds for $DEE(G)$ are provided in Section 3. In Section 4, we compute the distance Estrada index of some concrete graphs, including the buckminsterfullerene C_{60}, to demonstrate the availability of our obtained results.

2. Preliminaries

Let G be a simple connected n-vertex graph with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$. Denote by $D(G)$ the distance matrix of the graph G. The distance degree of a vertex v_i is given by $D_i = \sum_{j=1}^{n} d_{ij}$. This concept first appears in Hilano & Nomura (1984) and is reinvented recently in Indulal (2009) under the name of distance degree.

The Wiener index (Wiener, 1947) of G, denoted by $W(G)$, is the sum of the distances between all (unordered) pairs of vertices of G, that is

$$W(G)=\sum_{i<j} d_{ij}=\frac{1}{2}\sum_{i=1}^{n} D_i. \tag{2}$$

Let $M(G)=(\prod_{i=1}^{n} D_i)^{1/n}$ be the geometric mean of the distance degrees. Then $2W(G)/n \geq M(G)$ holds, and equality is attained if and only if $D_1=D_2=\cdots=D_n$ (i.e., the graph G is distance degree regular (Hilano & Nomura, 1984)).

Several properties of the spectrum of the distance matrix $D(G)$ follows easily from its definition. For $k \in \mathbb{N}$, let $N_k=\sum_{i=1}^{n}\mu_i^k$ be the kth spectral moment. Since all elements of $D(G)$ are integers, all moments N_k are also integral. In particular, $N_1=0$, i.e., $D(G)$ is traceless; and $N_2=2\sum_{i<j} d_{ij}^2$. The following two lemmas will be needed later.

Lemma 1. (Indulal, 2009) *A connected graph G has two distinct D-eigenvalues if and only if G is a complete graph.*

Lemma 2. (Zhou *et al.*, 2008) *Let $a_1, a_2, \cdots, a_n$ be nonnegative numbers. Then*

$$n\left(\frac{1}{n}\sum_{i=1}^{n} a_i-\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}\right)\leq n\sum_{i=1}^{n} a_i-\left(\sum_{i=1}^{n} a_i^{\frac{1}{2}}\right)^2.$$

3. Bounds for the distance Estrada index

Our main result reads as follows.

Theorem 1. *Let G be a connected graph on n vertices. Denote by $\Delta(G)$ the diameter of G. Then*

$$\begin{aligned} e^{\left(\frac{4W^2(G)-M^2(G)n}{n(n-1)}\right)^{\frac{1}{2}}}+\frac{n-1}{e^{\frac{1}{n-1}\left(\frac{4W^2(G)-M^2(G)n}{n(n-1)}\right)^{\frac{1}{2}}}} &\leq DEE(G) \\ &\leq n-1+e^{\sqrt{2}\Delta^{\frac{1}{2}}(G)W^{\frac{1}{2}}(G)}. \end{aligned} \tag{3}$$

The equality on the left-hand side of (3) holds if and only if G is the complete graph K_n. The equality on the right-hand side of (3) holds if and only if $G=K_1$, i.e., a single vertex.

Remark 1. When $n=1$, we will have $4W^2(G)=M^2(G)n$ and view the leftmost term of (3) as 1.

Proof. *Lower bound*. Using the arithmetic geometric mean inequality, we obtain

$$\begin{aligned} DEE(G) &= \sum_{i=1}^{n} e^{\mu_i} \\ &\geq e^{\mu_1}+(n-1)\left(\prod_{i=2}^{n} e^{\mu_i}\right)^{\frac{1}{n-1}} \\ &= e^{\mu_1}+(n-1)e^{-\frac{\mu_1}{n-1}}, \end{aligned} \tag{4}$$

where we have used the fact that $N_1=\sum_{i=1}^{n}\mu_i=0$.

In Indulal (2009) it was shown that

$$\mu_1 \geq \left(\frac{\sum_{i=1}^{n} D_i^2}{n}\right)^{\frac{1}{2}}. \tag{5}$$

Setting $\sqrt{a_i}=D_i$ in Lemma 2, we get

$$n^2\left(\frac{\sum_{i=1}^{n} D_i^2}{n}-\left(\frac{2W}{n}\right)^2\right) \geq \sum_{i=1}^{n} D_i^2-n\left(\prod_{i=1}^{n} D_i^2\right)^{\frac{1}{n}}.$$

Combining this with (5) yields

$$\mu_1 \geq \left(\frac{4W^2(G)-M^2(G)n}{n(n-1)}\right)^{\frac{1}{2}} \geq 0. \tag{6}$$

Clearly, $4W^2(G)=M^2(G)n$ (namely, the second equality in (6) holds) if and only if $n=1$.

It is elementary to show that for $n \geq 1$ the function

$$f(x)=e^x+\frac{n-1}{e^{\frac{x}{n-1}}} \tag{7}$$

monotonically increases in the interval $[0,+\infty)$ (here we take the limit function $f(x)=e^x$ when $n=1$). Therefore, by means of (4) and (6) we arrive at the first half of Theorem 1.

Note that when $G=K_n$, we have $\mu_1=n-1$, $\mu_2=\cdots=\mu_n=-1$, $W(G)=n(n-1)/2$ and $M(G)=n-1$. Hence, $DEE(G)=e^{n-1}+(n-1)e^{-1}$ and the equality on the left-hand side of (3) holds. Conversely, suppose that the equality holds, then from (4) we have $\mu_2=\cdots=\mu_n$. We assume that $n \geq 2$. It follows from (6) that $\mu_1>0$. Then G has exactly two distinct D-eigenvalues, and Lemma 1 indicates that G is the complete graph K_n.

Upper bound. Let n_+ be the number of positive

D-eigenvalues of G, we obtain

$$\begin{aligned}
DEE(G) &\leq n - n_+ + \sum_{i=1}^{n_+} e^{\mu_i} \\
&= n - n_+ + \sum_{i=1}^{n_+} \sum_{k=0}^{\infty} \frac{\mu_i^k}{k!} \\
&= n + \sum_{k=1}^{\infty} \frac{1}{k!} \sum_{i=1}^{n_+} \mu_i^k \\
&\leq n + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\sum_{i=1}^{n_+} \mu_i^2 \right)^{\frac{k}{2}} \\
&= n + \sum_{k=1}^{\infty} \frac{1}{k!} \left(2 \sum_{i<j} d_{ij}^2 \right. \\
&\quad \left. - \sum_{i=n_+ +1}^{n} \mu_i^2 \right)^{\frac{k}{2}} \\
&\leq n - 1 + e^{\sqrt{2 \sum_{i<j} d_{ij}^2}} \\
&\leq n - 1 + e^{\sqrt{2\Delta \sum_{i<j} d_{ij}}},
\end{aligned}$$

which directly leads to the right-hand side inequality in (3).

From the above derivation it is apparent that equality holds if and only if the graph G has all zero D-eigenvalues. Since G is a connected graph, this only happens when $G = K_1$ (and thus $DEE(G) = 1$).

The proof of Theorem 1 is completed. □

Remark 2. In Bozkurt & Bozkurt (2012), it was proved that

$$DEE(G) \geq e^{\frac{2W(G)}{n}} + (n-1)e^{-\frac{2W(G)}{n(n-1)}}. \qquad (8)$$

If we utilize the property $2W(G)/n \geq M(G)$, then we obtain

$$\frac{2W(G)}{n} \leq \left(\frac{4W^2(G) - M^2(G)n}{n(n-1)} \right)^{\frac{1}{2}}.$$

Since the function $f(x)$ defined in (7) is strictly increasing, we see that our lower bound in (3) is better than the bound in (8).

Remark 3. It was shown in Güngör & Bozkurt (2009) that

$$DEE(G) \leq n - 1 + e^{\Delta(G)\sqrt{n(n-1)}}. \qquad (9)$$

Since $d_{ij} \leq \Delta(G)$ for all i and j, $n(n-1)\Delta(G) \geq 2W(G)$. Obviously, our upper bound in (3) is better than the bound in (9).

If the graph G is r-distance regular for some $r \in \mathbb{N}$, we have $D_1 = D_2 = \cdots = D_n = r$ (Indulal, 2009). Consequently, $W(G) = nr/2$ and $M(G) = r$. The following result is immediate.

Corollary 1. *Let G be a connected r-distance regular graph on n vertices. Denote by $\Delta(G)$ the diameter of G. Then*

$$e^r + \frac{n-1}{e^{\frac{r}{n-1}}} \leq DEE(G) \leq n - 1 + e^{\sqrt{\Delta(G)nr}}. \qquad (10)$$

The equality on the left-hand side of (10) holds if and only if G is the complete graph K_n with $n = r+1$. The equality on the righthand side of (10) holds if and only if $G=K_1$, i.e., a single vertex.

4. Some examples

In this section, we provide some concrete examples to demonstrate the calculations of distance Estrada index as well as the feasibility of the above obtained results.

Example 1. In this example, the graph G is the cycle over $n = 6$ vertices, namely, a hexagonal cell. Its distance matrix is shown below

$$D(G) = \begin{pmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{pmatrix}.$$

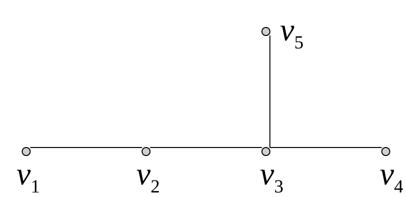

Fig. 1. A chemical tree G on vertex set $V(G) = \{v_1, v_2, \cdots, v_5\}$. Recall that a chemical tree is a tree having no vertex with degree greater than 4.

Since $D(G)$ is a circulant matrix, the D-eigenvalues consist of $\{\omega_j + 2\omega_j^2 + 3\omega_j^3 + 2\omega_j^4 + \omega_j^5\}_{j=0}^5$, where $\omega_j = \cos(2\pi j/n) + i\sin(2\pi j/n)$, $i = \sqrt{-1}$, and $j = 0,1, \cdots, 5$. Via some simplifications, we have $\mu_1 = 9$, $\mu_2 = \mu_3 = 0$, $\mu_4 = -1$ and $\mu_5 = \mu_6 = -4$. Thus, we calculate that $DEE(G) = \sum_{k=1}^{6} e^{\mu_k}$

= 8105.5.

It is evident that G is a connected r-distance regular graph with $r = 9$. The diameter is given by $\Delta(G) = 3$. Therefore, from Corollary 1 we have the following bounds

$$8103.9 \leq DEE(G) \leq 337033.2.$$

It turns out that the lower bound is very sharp while the upper bound is conservative in this specific example.

Example 2. In Figure 1 we display a chemical tree of n = 5 vertices. The distance matrix is

$$D(G) = \begin{pmatrix} 0 & 1 & 2 & 3 & 3 \\ 1 & 0 & 1 & 2 & 2 \\ 2 & 1 & 0 & 1 & 1 \\ 3 & 2 & 1 & 0 & 2 \\ 3 & 2 & 1 & 2 & 0 \end{pmatrix}.$$

The D-eigenvalues of the graph are as follows: $\mu_1 = 7.46$, $\mu_2 = -0.51$, $\mu_3 = -1.08$, $\mu_4 = -2$ and $\mu_5 = -3.86$. We obtain $DEE(G) = 1738.2$.

Fig. 2. A projection depiction of the buckminsterfullerene C_{60}.

On the other hand, we can easily obtain $W(G) = 18$, $M(G) = 7.04$ and $\Delta(G) = 3$. Hence, from Theorem 1 we have the following bounds

$$1393.4 \leq DEE(G) \leq 32611.7.$$

Example 3. In this example, we consider the buckminsterfullerene C_{60}, which is a well-known member of the fullerene family (Kroto *et al.*, 1985). As a graph, C_{60} is a truncated icosahedron with n = 60 vertices and 32 faces (including 20 hexagons and 12 pentagons); see Figure 2 for an illustration. The D-eigenvalues of C_{60} were computed in Balasubramanian (1995) by using the Givens-Householder method (see Table 1 in Balasubramanian (1995)). For example, there are exactly 18 positive D-eigenvalues and no zero D-eigenvalue. Based on these D-eigenvalues we calculate by definition (1) that $DEE(C_{60}) = 152.11+e^{278}$.

Since C_{60} contains 60 vertices, a wise approach to capture its distance matrix is to understand the associated distance level diagram, as is done in Figure 1 of Balasubramanian (1995). From that, we conclude that C_{60} is a connected r-distance regular graph with r = 278 and the diameter is $\Delta(C_{60}) = 9$. Hence, $W(C_{60}) = nr/2 = 8340$ and $M(C_{60}) = r = 278$. Corollary 1 leads to the following bounds

$$0.53+e^{278} \leq DEE(C_{60}) \leq 59+e^{387}.$$

Clearly, the upper bound obtained is way above the true value for $DEE(C_{60})$. For future work, it would be desirable to study better behaved estimations. In addition to this obvious direction, we mention that another interesting problem is to investigate the distance Estrada index for evolving networks (Shang, 2015b).

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خلاصة

ليكن G بيان بسيط له n رؤوس. القيم الذاتية D للبيان G هي القيم الذاتية لمصفوفة المسافة. نعرف دليل مسافة استرداد للبيان E على أنه :

$$DEE(G) = \sum_{i=1}^{n} e^{\mu_i} .$$

نقوم في هذا البحث بإيجاد حد أعلى وحد أدني جديدين ل $DEE(G)$ بدلالة دليل واينز $W(G)$. كما نقوم بحساب دليل مسافة استراد لبعض البيانات الفعلية بما فيها بيان باكمنستر فولرنس C_{60} .