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Upper Bounds on Distance Energy

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Abstract

New upper bounds on the distance energy of a graph are presented, in terms of several graph invariants used as topological indices in chemical graph theory.

1 Introduction

Since 2008, when the concept of distance energy $\mathcal{D}E$ was introduced [16], numerous lower and upper bounds on $\mathcal{D}E$ were obtained and communicated in quite a few publications [4, 5, 9, 10, 13, 15, 16, 20–22, 25]. In this paper we report a few more such bounds.

Let $G = (V, E)$ be a graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G)$, and let $|V(G)| = n$ and $|E(G)| = m$. If the vertices v_i and v_j are adjacent, we write $v_iv_j \in E(G)$. For $i = 1, 2, \ldots, n$, let $d_G(v_i)$ be the degree (= number of first neighbors) of the vertex v_i. The distance between vertices v_i and v_j, denoted by $d_G(v_i, v_j)$, is the length of a shortest path between v_i and v_j. The diameter of the graph G, is $d = \max\limits_{1\leq i<j\leq n} d_G(v_i, v_j)$.

As usual, by K_n and P_n, we denote the complete graph and the path on n vertices.

A clique of the graph G is a subset of its vertex set in which all vertices are mutually adjacent. The clique number $\omega(G)$ is the size of the largest clique of G.

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By $\mathcal{W}_{n,k}$ we denote the set of connected n-vertex graphs with clique number k. A kite graph $Ki_{n,\omega}$ is a graph obtained from a clique K_ω and a path $P_{n-\omega}$ by adding an edge between a vertex from the clique and an endpoint from the path.

For other undefined notations and terminology from graph theory, the readers are referred to [3].

The distance matrix of a connected graph G, denoted by $\mathbf{DI}(G)$, is the real symmetric matrix of order n whose (i,j)-entry is $d_G(v_i, v_j)$. Its eigenvalues are $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$, forming the distance spectrum of G. The *distance energy* of G is defined as [16]

$$\mathcal{D}E = \mathcal{D}E(G) = \sum_{i=1}^{n} |\rho_i| \, .$$

For the basic spectral properties of the distance matrix see the survey [2]. For details of the theory of distance energy see [16, 17, 19].

In the next few lines we repeat the definitions of certain degree– and distance–based topological indices, which later will be related with the distance energy. For details on this matter and additional references see [23, 24].

The *zeroth–order general Randić index* is

$$^0R_\alpha(G) = \sum_{v_i \in V(G)} d_G(v_i)^\alpha$$

where α is a real number. The same quantity is sometimes referred to as the "*general first Zagreb index*". Recall that this index found many useful applications in information theory and network reliability, and received considerable attentions also in "pure" graph theory (see [6–8, 12]). In what follows, we shall need the special case of this index for $\alpha = -2$, that is,

$$^0R_{-2}(G) = \sum_{v_i \in V(G)} \frac{1}{d_G(v_i)^2} \, .$$

For $\alpha = -1$, we have

$$ID(G) = \sum_{i=1}^{n} \frac{1}{d_G(v_i)}$$

which is called the *inverse degree* of the graph G.

The oldest and most popular topological index, the Wiener index, is defined as

$$W(G) = \sum_{\{v_i, v_j\} \subseteq V(G)} d_G(v_i, v_j) \, .$$

The *degree distance* of G is

$$DD(G) = \sum_{\{v_i,v_j\}\subseteq V(G)} \Big[d_G(v_i) + d_G(v_j)\Big]\, d_G(v_i,v_j)\,.$$

In this paper we present upper bounds on the distance energy of graph G in terms of the above defined graph invariants. In order to achieve this goal, we first need some preparations.

2 Auxiliary results

We first state here two previously known results that are needed to prove our main results.

Let $\mathcal{M}_{p\times q}(C)$ be the set of all $p\times q$ dimensional matrices with complex elements. For $p \le q$, the singular values of a matrix $B \in \mathcal{M}_{p\times q}(C)$, denoted as $s_1(B) \ge s_2(B) \ge \cdots \ge s_p(B) \ge 0$, are the square roots of the eigenvalues of $B\,B^{\dagger}$.

Lemma 1. [1,18] *Let $B \in \mathcal{M}_{n\times n}(C)$, and let $\mathcal{E}(B)$ be the sum of the absolute values of the eigenvalues of B. Then,*

$$\mathcal{E}(B) \le \sum_{i=1}^{n} s_i(B)\,.$$

The equality holds if and only if B is a normal matrix.

Lemma 2. [11] *Let $X,Y,Z \in \mathcal{M}_{n\times n}(C)$, such that $X+Y=Z$. Then*

$$\sum_{i=1}^{n} s_i(Z) \le \sum_{i=1}^{n} s_i(X) + \sum_{i=1}^{n} s_i(Y)\,.$$

Equality holds if and only if there exists an orthogonal matrix P, such that PX and PY are both positive semi-definite.

Let $Q(G) = \sum\limits_{1\le i<j\le n} d_G(v_i,v_j)^2$. Then

$$\begin{aligned}
Q(Ki_{n,k}) &= \frac{1}{2}\,k(k-1) + (k-1)\left[4+9+16+\cdots+(n-k+1)^2\right] \\
&+ \left[1+4+9+\cdots+(n-k)^2\right] + Q(P_{n-k}) \\
&= \frac{1}{2}\Big[(k-1)(k-2)\Big] + \frac{1}{6}\Big[k\,(n-k)(n-k+1)(2n-2k+1)\Big] \\
&+ (k-1)(n-k+1)^2 + \frac{1}{12}\Big[(n-k)^2\,(n-k-1)(n-k+1)\Big] \\
&= \frac{1}{12}\Big[n^4 - n^2(6k^2-18k+13) + 4n(2k^3-9k^2+13k-6) \\
&- 3k(k^3-6k^2+11k-6)\Big]. \qquad (1)
\end{aligned}$$

Theorem 1. *Let $G \in \mathcal{W}_{n,k}$. Then*

$$Q(G) \leq Q(Ki_{n,k}) \tag{2}$$

with equality holding if and only if $G \cong Ki_{n,k}$.

Proof. Since k is the clique number in G, we have $n \geq k$. For $n = k$, we have $G \cong K_n$ and hence the equality holds in (2). For $n = k+1$, G is isomorphic to a graph, K_{n-1} with one vertex adjacent to some vertices in $V(K_{n-1})$, but not all. Suppose $v_r \in V(G) \backslash V(K_{n-1})$ and the vertex v_r is adjacent to $d_G(v_r)$ vertices in $V(K_{n-1})$, such that $1 \leq d_G(v_r) < n-1$. Then

$$\begin{aligned} Q(G) &= \frac{1}{2}(n-1)(n-2) + d_G(v_r) + 4(n-1-d_G(v_r)) \\ &= \frac{1}{2}(n-1)(n+6) - 3d_G(v_r) \leq \frac{1}{2}(n^2+5n-12) = Q(Ki_{n,n-1}), \end{aligned}$$

by (1). Hence the inequality holds in (2). Moreover, the above equality holds if and only if $d_G(v_r) = 1$, that is, $G \cong Ki_{n,n-1}$. Otherwise, $n \geq k+2$. We have to prove that the inequality holds in (2). We prove this by mathematical induction on n.

Assume that the inequality in (2) holds for n and prove it for $n+1$. For this we consider a graph H of order $n+1$ such that $G \cong H \backslash \{v_{n+1}\}$ (that is, the graph G is obtained from H by deleting the vertex v_{n+1}). Then $k \leq \omega(H) \leq k+1$. Let d be the diameter of H. Then $d \leq n-k+2$ as H is of order $n+1$.

Let $q = \max\limits_{1 \leq i \leq n} d_H(v_{n+1}, v_i)$. Then $q \leq d \leq n-k+2$. Let a_i $(1 \leq i \leq q)$ be the number of vertices at distance i from vertex v_{n+1} of H. Then $\sum\limits_{i=1}^{q} a_i = n$, where $a_i \geq 1$. Combining this with $q \leq n-k+2$, we obtain

$$\begin{aligned} \sum_{i=1}^{n} d_H(v_i, v_{n+1})^2 &= a_1 + 4\,a_2 + 9\,a_3 + \cdots + (q-1)^2\,a_{q-1} + q^2\,a_q \\ &\leq 1 + 4 + 9 + \cdots + (q-1)^2 + (n-q+1)\,q^2 \\ &\leq 1 + 4 + 9 + \cdots + (n-k+1)^2 + (k-1)\,(n-k+2)^2 \\ &= \frac{1}{6}(n-k+2)(n-k+3)(2n-2k+5) + (k-2)(n-k+2)^2. \end{aligned} \tag{3}$$

One can easily see that

$$\sum_{1 \leq i < j \leq n+1} d_H(v_i, v_j)^2 - \sum_{i=1}^{n} d_H(v_i, v_{n+1})^2 \leq \sum_{1 \leq i < j \leq n} d_G(v_i, v_j)^2\,,$$

that is,

$$\begin{aligned}Q(H)-Q(G) &\leq \sum_{i=1}^{n} d_H(v_i,v_{n+1})^2\\ &\leq \frac{1}{6}(n-k+2)(n-k+3)(2n-2k+5)+(k-2)(n-k+2)^2\end{aligned}$$

by (3). Therefore, by the induction hypothesis with the above result, we obtain

$$\begin{aligned}Q(H) &\leq Q(G)+\frac{1}{6}(n-k+2)(n-k+3)(2n-2k+5)+(k-2)(n-k+2)^2\\ &\leq Q(Ki_{n,k})+\frac{1}{6}(n-k+2)(n-k+3)(2n-2k+5)+(k-2)(n-k+2)^2\\ &= Q(Ki_{n+1,k})\end{aligned}$$

by (1). The inequality in (2) holds by induction. Moreover, the equality holds if and only if $G \cong Ki_{n,k}$, and

$$\sum_{i=1}^{n} d_H(v_i,v_{n+1})^2=\frac{1}{6}(n-k+2)(n-k+3)(2n-2k+5)+(k-2)(n-k+2)^2\,,$$

that is, if and only if $H \cong Ki_{n+1,k}$. This completes the proof of the theorem. ■

Corollary 3. [14] *Let G be a connected graph of order n. Then*

$$Q(G)=\sum_{1\leq i<j\leq n} d_G(v_i,v_j)^2 \leq \frac{n^2(n^2-1)}{12}$$

with equality holding if and only if $G \cong P_n$.

Proof. Bearing in mind Eq. (1), one can easily check that

$$Q(Ki_{n,k}) \leq \frac{n^2(n^2-1)}{12}=Q(P_n)$$

with equality holding if and only if $Ki_{n,k} \cong P_n$. By Theorem 1, we get the required result. ■

Corollary 4. *Let G be a connected graph of order n. Then*

$$\sum_{i=1}^{n} \rho_i^2(G) \leq \frac{n^2(n^2-1)}{6} \tag{4}$$

with equality holding if and only if $G \cong P_n$.

Proof. The left–hand side of inequality (4) is equal to the trace of $\mathbf{DI}(G)^2$. Bearing this in mind, one can easily verify that

$$\sum_{i=1}^{n} \rho_i^2(G)=2\sum_{1\leq i<j\leq n} d_G(v_i,v_j)^2\,.$$

Corollary 4 follows by combining the above result with Corollary 3. ■

3 Main results

Theorem 2. *Let G be a connected graph of order n with diameter d. Then*

$$\mathcal{DE}(G) \le \sqrt{2n}\left[(2-\sqrt{2})\,d + (\sqrt{2}-1)\,W(G)\right], \tag{5}$$

where $W(G)$ is a Wiener index. Equality holds if and only if $G \cong K_2$.

Proof. For $n = 2$, we have $G \cong K_2$. It is easy to check that both sides of (5) are equal to 2. Assume therefore that $n > 2$.

Let $\mathbf{\Omega} = diag(w_1, w_2, \dots, w_n)$ be the diagonal matrix of order n, in which w_i , $1 \le i \le n$, are real numbers. The (i,j)-th entry of $\mathbf{\Omega}^{-1}\mathbf{DI}(G)\mathbf{\Omega}$ is

$$\begin{cases} 0 & \text{if } i = j, \\ \dfrac{w_j}{w_i}\, d_G(v_i, v_j) & \text{otherwise.} \end{cases}$$

We can write

$$\mathbf{\Omega}^{-1}\mathbf{DI}(G)\mathbf{\Omega} = \mathbf{B}_1(G) + \mathbf{B}_2(G) + \cdots + \mathbf{B}_n(G)\,,$$

where $\mathbf{B}_i(G)$ is the $n \times n$ matrix whose i-th row is same as the i-th row of $\mathbf{\Omega}^{-1}\mathbf{DI}(G)\mathbf{\Omega}$ whereas the other rows are zero. Since for any matrix $\mathbf{M}$, the non-zero eigenvalues of $\mathbf{M}^T\mathbf{M}$ and $\mathbf{M}\mathbf{M}^T$ are same, we obtain

$$\begin{aligned} \sum_{k=1}^{n} s_k(\mathbf{B}_i(G)) &= \sum_{k=1}^{n} \sqrt{\mu_k(\mathbf{B}_i(G)^T\mathbf{B}_i(G))} = \sum_{k=1}^{n} \sqrt{\mu_k(\mathbf{B}_i(G)\mathbf{B}_i(G)^T)} \\ &= \sqrt{\mu_1(\mathbf{B}_i(G)\mathbf{B}_i(G)^T)} = \sqrt{\sum_{j=1, j\neq i}^{n} \frac{w_j^2}{w_i^2}\, d_G(v_i, v_j)^2}\,, \end{aligned}$$

where $\mu_k(\mathbf{B}_i(G)\mathbf{B}_i(G)^T)$ is the k-th largest eigenvalue of $\mathbf{B}_i(G)\mathbf{B}_i(G)^T$. Recalling that the spectra of $\mathbf{DI}(G)$ and $\mathbf{\Omega}^{-1}\mathbf{DI}(G)\mathbf{\Omega}$ coincide, combining the above results with Lemmas 1 and 2, we obtain

$$\begin{aligned} \mathcal{DE}(G) &= \mathcal{E}(\mathbf{DI}(G)) = \mathcal{E}(\mathbf{\Omega}^{-1}\mathbf{DI}(G)\mathbf{\Omega}) \le \sum_{i=1}^{n} s_i(\mathbf{\Omega}^{-1}\mathbf{DI}(G)\mathbf{\Omega}) \\ &\le \sum_{i=1}^{n} s_i(\mathbf{B}_1(G)) + \sum_{i=1}^{n} s_i(\mathbf{B}_2(G)) + \cdots + \sum_{i=1}^{n} s_i(\mathbf{B}_n(G)) \\ &= \sum_{i=1}^{n} \sqrt{\sum_{j=1,\, j\neq i}^{n} \frac{w_j^2}{w_i^2}\, d_G(v_i,\, v_j)^2}\,. \end{aligned} \tag{6}$$

Using the Cauchy–Schwarz inequality, from the above, we have

$$\begin{aligned}\mathcal{DE}(G) &\le \sqrt{n\sum_{i=1}^{n}\sum_{j=1,j\neq i}^{n}\frac{w_j^2}{w_i^2}\,d_G(v_i,v_j)^2}\\ &= \sqrt{n\sum_{1\le i<j\le n}\left(\frac{w_j^2}{w_i^2}+\frac{w_i^2}{w_j^2}\right)d_G(v_i,v_j)^2}.\end{aligned} \tag{7}$$

Since d is the diameter of G, without loss of generality, we can assume that $d = d_G(v_1, v_{d+1})$, where $P_{d+1} : v_1v_2 \ldots v_dv_{d+1}$ is a diametral path of G. Then for $n \ge 3$, we obtain

$$\begin{aligned}\left(d+(\sqrt{2}-1)\sum_{\substack{1\le i<j\le n\\(i,j)\neq(1,d+1)}}d_G(v_i,v_j)\right)^2 &= d^2+(3-2\sqrt{2})\left(\sum_{\substack{1\le i<j\le n\\(i,j)\neq(1,d+1)}}d_G(v_i,v_j)\right)^2\\ + \; 2(\sqrt{2}-1)d\sum_{\substack{1\le i<j\le n\\(i,j)\neq(1,d+1)}}d_G(v_i,v_j) &> d^2+(3-2\sqrt{2})\sum_{\substack{1\le i<j\le n\\(i,j)\neq(1,d+1)}}d_G(v_i,v_j)^2\\ + \; (2\sqrt{2}-2)\sum_{\substack{1\le i<j\le n\\(i,j)\neq(1,d+1)}}d_G(v_i,v_j)^2 &= d^2+\sum_{\substack{1\le i<j\le n\\(i,j)\neq(1,d+1)}}d_G(v_i,v_j)^2=\sum_{1\le i<j\le n}d_G(v_i,v_j)^2\end{aligned}$$

as $d \ge d_G(v_i, v_j)$ for any v_i, v_j, and $d = d_G(v_1, v_{d+1})$, that is,

$$\begin{aligned}\sqrt{\sum_{1\le i<j\le n}d_G(v_i,v_j)^2} &< d+(\sqrt{2}-1)\sum_{\substack{1\le i<j\le n\\(i,j)\neq(1,d+1)}}d_G(v_i,v_j)\\ &= (2-\sqrt{2})\,d+(\sqrt{2}-1)\sum_{1\le i<j\le n}d_G(v_i,v_j)\\ &= (2-\sqrt{2})\,d+(\sqrt{2}-1)W(G)\,.\end{aligned} \tag{8}$$

From now on we set $w_i = 1$, $1 \le i \le n$. Then from (7) and (8) we obtain

$$\mathcal{DE}(G)\le\sqrt{2n\sum_{1\le i<j\le n}d_G(v_i,v_j)^2}<\sqrt{2n}\left[(2-\sqrt{2})\,d+(\sqrt{2}-1)\,W(G)\right]. \tag{9}$$

This completes the proof of the theorem. ■

Corollary 5. *Let G be a graph of order n with clique number k. Then*

$$\mathcal{DE}(G)\le\sqrt{2n\,Q(Ki_{n,k})}\,,$$

where $Q(Ki_{n,k})$ is given by Eq. (1).

Proof. By Theorem 1, from (9), we obtain

$$\mathcal{DE}(G) \leq \sqrt{2n \sum_{1\leq i<j\leq n} d_G(v_i,v_j)^2} \leq \sqrt{2n\, Q(Ki_{n,k})}\,.$$

■

Using Corollary 3, from (9), we have

Corollary 6. [21] *Let G be a connected graph of order $n > 2$. Then*

$$\mathcal{DE}(G) < n^2 \sqrt{\frac{1}{6}\left(n - \frac{1}{n}\right)}.$$

Corollary 7. *Let G be a graph of diameter d. Then*

$$\mathcal{DE}(G) \leq \sqrt{d\, ID(G)\, DD(G)}\,,$$

where $ID(G)$ and $DD(G)$ are the inverse degree and the degree distance of G. Moreover, equality holds if and only if $G \cong K_2$.

Proof. If $d = 1$, then $G \cong K_n$ and thus

$$\mathcal{DE}(G) = 2(n-1) \leq n\sqrt{n-1} = \sqrt{d\, ID(G)\, DD(G)}$$

with equality holding if and only if $G \cong K_2$. Therefore, in what follows we assume that $d \geq 2$.

Using the Cauchy–Schwarz inequality, from (6), we get

$$\begin{aligned} \mathcal{DE}(G) &\leq \sum_{i=1}^{n} \frac{1}{w_i} \sqrt{\sum_{j=1, j\neq i}^{n} w_j^2\, d_G(v_i,v_j)^2} \\ &\leq \sqrt{\sum_{i=1}^{n} \frac{1}{w_i^2} \sum_{i=1}^{n} \sum_{j=1, j\neq i}^{n} w_j^2\, d_G(v_i,v_j)^2}\,. \end{aligned} \tag{10}$$

Setting $w_i = \sqrt{d_G(v_i)}$ in (10), we obtain

$$\begin{aligned} \mathcal{DE}(G) &\leq \sqrt{\sum_{i=1}^{n} \frac{1}{d_G(v_i)} \sum_{i=1}^{n} \sum_{j=1, j\neq i}^{n} d_G(v_j)\, d_G(v_i,v_j)^2} \\ &= \sqrt{ID(G) \sum_{1\leq i<j\leq n} \big[d_G(v_i) + d_G(v_j)\big] d_G(v_i,v_j)^2} < \sqrt{d\, ID(G)\, DD(G)} \end{aligned}$$

as $d_G(v_i,v_j) \leq d$ and $d_G(v_i,v_j) < d$ for at least one vertex pair v_i, v_j. ■

Corollary 8. *Let G be a graph of maximum degree Δ with diameter d. Then*

$$\mathcal{DE}(G) \leq \sqrt{d\,\Delta\,{}^0R_{-2}(G)\,DD(G)}\,,$$

where ${}^0R_{-2}(G)$ and $DD(G)$ are the zeroth-order general Randić index and the degree distance. Moreover, equality holds if and only if $G \cong K_2$.

Proof. If $d = 1$, then $G \cong K_n$ and thus

$$\mathcal{DE}(G) = 2(n-1) \leq n\sqrt{n-1} = \sqrt{d\,\Delta\,{}^0R_{-2}(G)\,DD(G)}$$

with equality holding if and only if $G \cong K_2$. Therefore, in what follows we assume that $d \geq 2$.

Setting $w_i = d_G(v_i)$ in (10), we obtain

$$\begin{aligned}\mathcal{DE}(G) &\leq \sqrt{\sum_{i=1}^{n} \frac{1}{d_G(v_i)^2} \sum_{i=1}^{n} \sum_{j=1, j\neq i}^{n} d_G(v_j)^2\, d_G(v_i, v_j)^2} \\ &= \sqrt{{}^0R_{-2}(G) \sum_{1\leq i<j\leq n} \left[d_G(v_i)^2 + d_G(v_j)^2\right] d_G(v_i, v_j)^2} < \sqrt{d\,\Delta\,{}^0R_{-2}(G)\,DD(G)}\end{aligned}$$

as $d_G(v_i, v_j) \leq d$ and $d_G(v_i, v_j) < d$ for at least one vertex pair v_i, v_j, as well as $d_G(v_i) \leq \Delta$.

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