On the α-distance spectral radius

Bo Zhou

South China Normal University

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In geometry, we consider n points in a plane and the distances between two points is the Euclidean distance. We may form a distance matrix with (i, j) entry to be the Euclidean distance between the i-th and the j-th points for $1 \leq i, j \leq n$.

A. Cayley, A theorem in the geometry of position, Cambridge Math. J. 2 (1841) 267–271.

I. Schoenberg, Remarks to Maurice Fréchet's article "Sur la définition axiomatique d'une classe d'espace distanciés vectoriellement applicable sur l'espace de Hilbert", Ann. Math. 36 (1935) 724–732.

G. Young, A. Householder, Discussion of a set of points in terms of their mutual distances, Psy-chometrika 3 (1938) 19–22.

Hakimi and Yau considerd a graph G on n vertices with weights w_{uv} for each edge uv. The distance matrix $D = (d_{uv})$ is an $n \times n$ matrix whose entry d_{uv} is the shortest weighted distance between vertices u and v.

For a given real symmetric $n \times n$ matrix $D = (d_{ij})$ such that $d_{ii} = 0$ and $0 \leq d_{ij} \leq d_{ik} + d_{kj}$ for any $1 \leq i, j, k \leq n$, they consider the problem whether there is there a graph G for which D is its distance matrix.

Particularly, they also considered the case $w_{uv} = 1$ for $uv \in E(G)$.

S.L. Hakimi, S.S. Yau, Distance matrix of a graph and its realizability, Quart. Appl. Math. 22 (1965) 305–317.

A. Dress, Trees, tight extensions of metric spaces, and the cohomological dimension of certain groups: a note on combinatorial properties of metric spaces, Adv. Math. 53 (1984) 321–402.

We consider graph-theoretical distance and facts on spectral properties distance matrix. Let G be a connected graph with vertex set $V(G)$. The distance between vertices u, v is defined as the number of edges of a shortest path between them in G, denoted by $d_G(u, v)$ or d_{uv}.

Let $V(G) = \{v_1, \ldots, v_n\}$. The distance matrix of G is the $n \times n$ matrix $D(G) = (d_{v_i v_j})$.

The eigenvalues of $D(G)$ are known as the distance eigenvalues of G. Label them as $\rho_1(G) \geq \cdots \geq \rho_n(G)$.

$\rho(G) = \rho_1(G)$: The distance spectral radius of G, i.e., the largest distance eigenvalue of G.

Graham and Pollack established a relationship between the number of negative distance eigenvalues and the addressing problem in data communication systems, and they showed that the determinant of the distance matrix of a tree is a function of its order only.

Graham and Lovász computed the inverse of the distance matrix of a tree.

R.L. Graham, H.O. Pollack, On the addressing problem for loop switching, Bell System Tech. J. 50 (1971) 2495–2519.

R.L. Graham, L. Lovász, Distance matrix polynomials of trees, Adv. Math. 29 (1978) 60–88.

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L.H. Brandenburg, B. Gopinath, R.P. Kurshan, On the addressing problem of loop switching, Bell System Tech. J. 51 (1972) 1445–1469.

A. C.-C. Yao, On the loop switching addressing problem, Siam J. Comput. 7 (1978) 515–523.

Generalizations on determinant and inverse of distance matrices of various classes of (di)graphs:

R.L. Graham, A.J. Hoffman, H. Hosoya, On the distance matrix of a directed graph, J. Graph Theory 1 (1977) 85–88.

K.L. Collins, Distances matrices of trees, PhD thesis, Massachusetts Institute of Technology, 1986.

R.B. Bapat, Determinant of the distance matrix of a tree with matrix weights, Linear Algebra Appl. 416 (2006) 2–7.

R.B. Bapat, Distance matrix and Laplacian of a tree with attached graphs, Linear Algebra Appl. 411 (2005) 295–308.

R.B. Bapat, S.J. Kirkland, M. Neumann, On distance matrices and Laplacians, Linear Algebra Appl. 401 (2005) 193–209.

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Recall that the inertia of the distance matrix of a tree is determined.

R.L. Graham, L. Lovász, Distance matrix polynomials of trees, Adv. Math. 29 (1978) 60–88.

The inertia of the distance matrix of a unicyclic graph with an odd cycle is determined.

R.B. Bapat, S.J. Kirkland, M. Neumann, On distance matrices and Laplacians, Linear Algebra Appl. 401 (2005) 193–209.

The characteristic polynomial of the distance matrix (called distance polynomial) of a graph was also investigated, and certain, and in some cases all, the coefficients of the distance characteristic polynomial are calculated.

H. Hosoya, M. Murakami, M. Gotoh, Distance polynomial and characterization of a graph, Natur. Sci. Rep. Ochanomizu Univ. 24 (1973) 27–34.

M. Edelberg, M. R. Garey, R. L. Graham, On the distance matrix of a tree, Discrete Math. 14 (1976) 23–39.

R.L. Graham, L. Lovász, Distance matrix polynomials of trees, Adv. Math. 29 (1978) 60–88.

A. Graovac, G. Jashari, M. Strunje, On the distance spectrum of a cycle, Appl. Math. 30 (1985) 286–290.

H. Hosoya, On some counting polynomials in chemistry. Applications of graphs in chemistry and physics, Discrete Appl. Math. 19 (1988) 239–257.

K. Balasubramanian, computer generation of distance polynomials of graphs, J. Comput. Chem. 11 (1990) 829–836.

Z. Mihalić, D. Veljan, D. Amić, S. Nikolić, D. Plavšić, N. Trinajstić, The distance matrix in chemistry, J. Math. Chem. 11 (1992) 223–258.

K.L. Collins, Factoring distance matrix polynomials, Discrete Math. 122 (1993) 103–112.

K. Balasubramanian, A topological analysis of the C_{60} buckminsterfullerene and C_{70} based on distance matrices, Chem. Phys. Lett. 239 (1995) 117–123.

Merris provided the first estimation of the distance spectrum of a tree using its Laplacian spectrum.

R. Merris, The distance spectrum of a tree, J. Graph Theory 14 (1990) 365–369.

Ruzieh and Powers showed that the complete graph achieves the minimum and the path achieves the maximum distance spectral radius among connected graphs.

S.N. Ruzieh, D.L. Powers, The distance spectrum of the path P_n and the first distance eigenvector of connected graphs, Linear Multilinear Algebra 28 (1990) 75–81.

Koolen and Shpectorov proved that if the distance matrix of a distance-regular graph G has exactly one positive eigenvalue then either G is of diameter 2, or G is an isometric subgraph of a halved cube.

J.H., Koolen, S.V. Shpectorov, Distance-regular graphs the distance matrix of which has only one positive eigenvalue, European J. Combin. 15 (1994) 269–275.

Conjectures

S. Fajtlowicz, Written on the wall, University of Houston, 1998.

Balaban, Ciubotariu and Medeleanu proposed the use of the distance spectral radius as a molecular descriptor. Gutman and Medeleanu used the distance spectral radius to infer the extent of branching and model boiling points of an alkane.

A. T. Balaban, D. Ciubotariu, M. Medeleanu, Topological indices and real number vertex invariants based on graph eigenvalues or eigenvectors, J. Chem. Inf. Comput. Sci. 31 (1991) 517–523.

I. Gutman, M. Medeleanu, On the structure–dependence of the largest eigenvalue of the distance matrix of an alkane, Indian J. Chem. A 37 (1998) 569–573.

Lower and upper bounds for the distance spectral radius are found.

I. Gutman, M. Medeleanu, On the structure–dependence of the largest eigenvalue of the distance matrix of an alkane, Indian J. Chem. A 37 (1998) 569–573.

B. Zhou, On the largest eigenvalue of the distance matrix of a tree, MATCH Commun. Math. Comput. Chem. 58 (2007) 657–662.

B. Zhou, N. Trinajstić, On the largest eigenvalue of the distance matrix of a connected graph, Chem. Phys. Lett. 447 (2007) 384–387.

B. Zhou, N. Trinajstić, Further results on the largest eigenvalues of the distance matrix and some distance-based matrices of connected (molecular) graphs, Internet Electron.J. Mol. Des. 6 (2007) 375–384.

B. Zhou, A. Ilić, On distance spectral radius and distance energy of graphs, MATCH Commun. Math. Comput. Chem. 64 (2010) 261–280.

B. Zhou, N. Trinajstić, Mathematical properties of molecular descriptors based on distances, Croat. Chem. Acta 83 (2010) 227–242.

Z. Liu, On spectral radius of the distance matrix. Appl. Anal. Discrete Math. 4 (2010) 269–277.

D. Stevanović, A. Ilić, Distance spectral radius of trees with fixed maximum degree, Electron. J. Linear Algebra 20 (2010) 168–179.

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M. Aouchiche, P. Hansen, Distance spectra of graphs: A survey, Linear Algebra Appl. 458 (2014) 301–386.

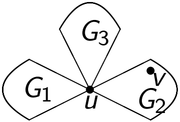
Let G be a non-trivial connected graph with $u \in V(G)$. For positive integers k and ℓ with $k \geq \ell$, let $G_u(k, \ell)$ be the graph obtained from G by attaching two pendant paths of length k and ℓ respectively at u, and $G_u(k, 0)$ the graph obtained from G by attaching a pendant path of length k at u.

Theorem

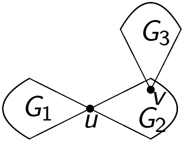
Let H be a non-trivial connected graph with $u \in V(H)$. If $k \geq \ell \geq 1$, then $\rho(H_u(k, \ell)) < \rho(H_u(k+1, \ell-1))$.

Let G be a connected graph with u being a cut vertex. Suppose that G_1, G_2 and G_3 are subgraphs of G such that $|V(G_i)| \geq 2$ for $1 \leq i \leq 3$, $V(G_i) \cap V(G_j) = \{u\}$ for $1 \leq i < j \leq 3$ and $\cup_{i=1}^{3} V(G_i) = V(G)$. For $v \in V(G_2) \setminus \{u\}$, let

$$G' = G - \{uw : w \in N_{G_3}(u)\} + \{vw : w \in N_{G_3}(u)\}.$$



G



G'

For $w \in V(G)$, define

$$f(w) = \sum_{z \in V(G_1)} d_G(w, z) - \sum_{z \in V(G_2) \setminus \{u\}} d_G(w, z).$$

Theorem

If $f(w) \geq 0$ for all $w \in V(G_3) \setminus \{u\}$, and for some nonnegative number k,

$$\min_{w \in V(G_1)} f(w) \geq -k \quad \text{and} \quad \min_{w \in V(G_2) \setminus \{u\}} f(w) \geq k,$$

then $\rho(G') > \rho(G)$.

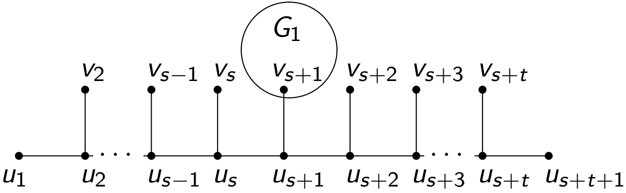
Theorem

If $|V(G_1)| \geq |V(G_2)| - 1$, $f(u) \geq 0$ and

$$\min_{w \in V(G_2) \setminus \{u\}} f(w) \geq \max \left\{ 0, - \min_{w \in V(G_1)} f(w) \right\},$$

then $\rho(G') > \rho(G)$.

Let $G_1(s,t)$ be the graph shown below, where G_1 is a nontrivial connected graph, and $s,t \geq 1$.



Theorem

Let G_1 be a nontrivial connected graph. For $s \geq t \geq 2$,

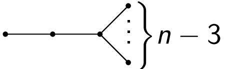
$$\rho(G_1(s+1,t-1)) > \rho(G_1(s,t)).$$

Among connected graphs on n vertices,
the complete graph achieves uniquely minimum distance spectral radius, the path achieves uniquely maximum distance spectral radius.

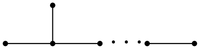
Among trees on n vertices,
the star achieves uniquely minimum distance spectral radius.

S.N. Ruzieh, D.L. Powers, The distance spectrum of the path P_n and the first distance eigenvector of connected graphs, Linear Multilinear Algebra 28 (1990) 75–81.

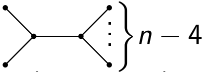
D. Stevanović, A. Ilić, Distance spectral radius of trees with fixed maximum degree, Electron. J. Linear Algebra 20 (2010) 168–179.



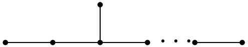
$D(n;1,n-3)$



$S(n;1,1,n-3)$



$D(n;2,n-4)$



$S(n;1,2,n-4)$

Theorem

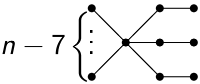
Among trees with $n \geq 6$ vertices,

$D(n;1,n-3)$ achieves uniquely 2nd minimum distance spectral radius,

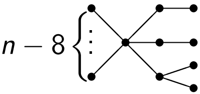
$S(n;1,1,n-3)$ achieves uniquely 2nd maximum distance spectral radius;

$D(n;2,n-4)$ achieves uniquely 3rd minimum distance spectral radius,

$S(n;1,2,n-4)$ achieves uniquely 3rd maximum distance spectral radius.



$B(n; n-7, 1, 1, 1)$



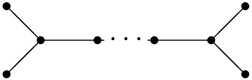
$B(n; n-8, 1, 1, 2)$

Theorem

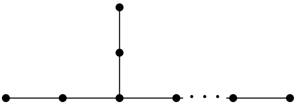
Among non-caterpillar trees on $n \geq 7$ vertices, $B(n; n-7, 1, 1, 1)$ is the unique graph with minimum distance spectral radius.

Theorem

Among non-starlike non-caterpillar trees on $n \geq 8$ vertices, $B(n; n-8, 1, 1, 2)$ is the unique graph with minimum distance spectral radius.



D_n



$S(n; 2, 2, n-5)$

Theorem

Among non-starlike trees on $n \geq 6$ vertices, D_n is the unique graph with maximal distance spectral radius.

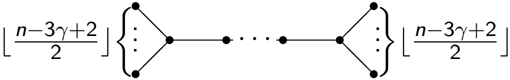
Theorem

Among non-caterpillar trees on $n \geq 7$ vertices, $S(n; 2, 2, n-5)$ is the unique graph with maximum distance spectral radius.

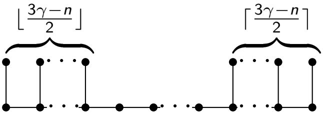
For $n \geq 8$, let $P = v_1 v_2 \cdots v_{n-3}$, let $P(n; 2, n-5)$ be the tree obtained from P by attaching a pendant vertex to v_2 and a path $P_2 = v_n v_{n-1}$ at the terminal vertex to v_{n-5}.

Theorem

Among non-starlike non-caterpillar trees on $n \geq 8$ vertices, $P(n; 2, n-5)$ is the unique graph with maximal distance spectral radius.



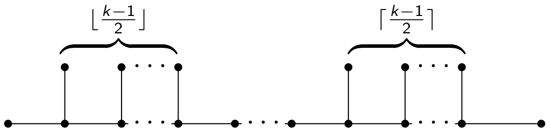
$$D\left(n, \lceil \frac{n-3\gamma+2}{2} \rceil, \lfloor \frac{n-3\gamma+2}{2} \rfloor\right)$$



$$E\left(n, \lfloor \frac{3\gamma-n}{2} \rfloor, \lceil \frac{3\gamma-n}{2} \rceil\right)$$

Theorem

Among connected graphs with n vertices and domination number γ, where $1 \leq \gamma \leq \lfloor \frac{n}{2} \rfloor$, $D\left(n, \left\lceil \frac{n-3\gamma+2}{2} \right\rceil, \left\lfloor \frac{n-3\gamma+2}{2} \right\rfloor\right)$ for $1 \leq \gamma < \lceil \frac{n}{3} \rceil$, $E\left(n, \left\lfloor \frac{3\gamma-n}{2} \right\rfloor, \left\lceil \frac{3\gamma-n}{2} \right\rceil\right)$ for $\lceil \frac{n}{3} \rceil < \gamma \leq \lfloor \frac{n}{2} \rfloor$ are the unique graphs with maximum distance spectral radius.



$C\left(n, \lfloor \frac{k-1}{2} \rfloor, \lceil \frac{k-1}{2} \rceil\right)$

Theorem

Among trees with n vertices and $2k$ odd vertices, where $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$, $C\left(n, \lfloor \frac{k-1}{2} \rfloor, \lceil \frac{k-1}{2} \rceil\right)$ is the unique tree with maximum distance spectral radius.

Watanabe et al. studied some spectral properties of the distance matrix of a uniform hypertree.

S. Watanabe, K. Ishi, M. Sawa, A Q-analogue of the addressing problem of graphs by Graham and Pollak, SIAM J. Discrete Math. 26 (2012) 527–536.

$T_G(u)$: the transmission of u in G, i.e., $T_G(u) = \sum_{v \in V(G)} d_G(u, v)$.

$T(G)$: the diagonal matrix of transmissions of G.

$\mathcal{Q}(G) = T(G) + D(G)$: the distance signless Laplacian matrix of G.

$\mathcal{L}(G) = T(G) - D(G)$: the distance Laplacian matrix of G.

M. Aouchiche, P. Hansen, Two Laplacians for the distance matrix of a graph, Linear Algebra Appl. 439 (2013) 21–33.

V. Nikiforov, Merging the A- and Q-spectral theories, Appl. Anal. Discrete Math. 11 (2017) 81–107.

$D_\alpha(G)$: the convex combinations of $T(G)$ and $D(G)$, defined as

$$D_\alpha(G) = \alpha T(G) + (1-\alpha)D(G), \alpha \in [0,1).$$

The eigenvalues of $D_\alpha(G)$ are called the distance α-eigenvalues of G, and the largest distance α-eigenvalue of G is called the distance α-spectral radius of G, written as $\mu_\alpha(G)$.

A connected graph G on n vertices is distinguished vertex deleted regular (DVDR) if there is a vertex v of degree $n-1$ such that $G-v$ is regular.

A connected graph G on n vertices is distinguished vertex deleted regular (DVDR) if there is a vertex v of degree $n-1$ such that $G-v$ is regular.

Let G be a connected graph and u and v be vertices such that $T_G(u) = T_{\min}(G)$ and $T_G(v) = T_{\max}(G)$. Let
$m_1 = \max\{T_G(w) - (1-\alpha)d(u,w) : w \in V(G) \setminus \{u\}\}$,
$m_2 = \min\{T_G(w) - (1-\alpha)d(v,w) : w \in V(G) \setminus \{v\}\}$, and
$e(w) = \max\{d(w,z) : z \in V(G)\}$ for $w \in V(G)$.

Then

$$
\begin{aligned}
& \frac{m_2 + \alpha T_{\max}(G) + \sqrt{(m_2 - \alpha T_{\max}(G))^2 + 4(1-\alpha)^2 T_{\max}(G)}}{2} \\
\leq \quad & \mu_\alpha(G) \\
\leq \quad & \frac{m_1 + \alpha T_{\min}(G) + \sqrt{(m_1 - \alpha T_{\min}(G))^2 + 4(1-\alpha)^2 e(u) T_{\min}(G)}}{2}.
\end{aligned}
$$

The first equality holds if and only if G is a complete graph and the second equality holds if and only if G is a DVDR graph.

Let G be a connected graph of order $n \geq 4$, where $G \ncong P_n$. Then $\mu_\alpha(G) \leq \mu_\alpha(B_{n,3}) < \mu_\alpha(P_n)$ with equality if and only if $G \cong B_{n,3}$.

D. Stevanović, A. Ilić, Distance spectral radius of trees with fixed maximum degree, Electron. J. Linear Algebra 20 (2010) 168–179.

Y. Wang, R. Xing, B. Zhou, F. Dong, A note on distance spectral radius of trees, Spec. Matrices 5 (2017) 296–300.

H. Lin, B. Zhou, The distance spectral radius of graphs with given number of odd vertices, Electron. J. Linear Algebra 31 (2016) 286–305.

R. Xing, B. Zhou, F. Dong, The effect of a graft transformation on distance spectral radius, Linear Algebra Appl. 457 (2014) 261–275.

Y. Wang, B. Zhou, On distance spectral radius of graphs, Linear Algebra Appl. 438 (2013) 3490–3503.

R. Xing, B. Zhou, J. Li, On the distance signless Laplacian spectral radius of graphs, Linear Multilinear Algebra 62 (2014) 1377–1387.

G. Yu, H. Jia, H. Zhang, J. Shu, Some graft transformations and its applications on the distance spectral radius of a graph, Appl. Math. Lett. 25 (2012) 315–319.

H. Lin, X. Lu, Bounds on the distance signless Laplacian spectral radius in terms of clique number, Linear Multilinear Algebra 63 (2015) 1750–1759.

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F. Atik, P. Panigrahi, On the distance and distance signless Laplacian eigenvalues of graphs and the smallest Gersgorin disc, Electron. J. Linear Algebra 34 (2018) 191–204.

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