On the eccentricity matrices of graphs

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Outline

- Motivation
- Some Basic Concepts
- Main Results
- Some Open Problems
- References

Matrices associated with graphs:

Adjacency Matrix

Incidence Matrix

Laplacian Matrix

Distance Matrix, and many more.

We are dealing with a new class of matrix :

Eccentricity matrix.

Originally, the eccentricity matrix is introduced by M. Randic in 'D_{MAX}-matrix of dominant distances in a graph',2013,[5] as the D_{MAX}-matrix, which is renamed as eccentricity matrix by Wang, Lu, Belardo and Randic in 'The anti-adjacency matrix of a graph:Eccentricity matrix',2018,[9].

Some applications of eccentricity matrix

On the branching pattern of molecular graphs. [6]

In terms of molecular descriptors. [9]

On the boiling point of hydrocarbons. [7]

Some recent works on the eccentricity matrix

- Jianfeng Wang, Mei Lu, Francesco Belardo, and Milan Randic, The anti-adjacency matrix of a graph:Eccentricity matrix, Discrete Appl. Math. 251(2018), 299-309.
- Jianfeng Wang, Lu Lu, Milan Randic, and Guozheng Li, Graph energy based on the eccentricity matrix,Discrete Math. 342(2019), no. 9, 2636-2646.
- Jianfeng Wang, Mei Lu, Lu Lu, and Francesco Belardo,Spectral properties of the eccentricity matrix of graphs, Discrete Applied Mathematics,279(2020), 168â177.
- Iswar Mahato, R Gurusamy, M Rajesh Kannan, and S Arockiaraj, Spectra of eccentricity matrices of graphs, Discrete Applied Mathematics,285(2020), 252â260.
- Wei Wei, Xiaocong He, and Shuchao Li. Solutions for two conjectures on the eigenvalues of the eccentricity matrix, and beyond. Discrete Mathematics, 343(8):111925, 2020.
- Jianfeng Wang, Xingyu Lei, Shuchao Li, Wei Wei, and Xiaobing Luo.On the eccentricity matrix of graphs and its applications to the boiling point of hydrocarbons. Chemometrics and Intelligent Laboratory Systems, page 104-173, 2020.

1. Let G be a simple connected graph with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$.
2. The cardinality of the vertex set $V(G)$ is called the **order** of the graph G.
3. The **distance** $d(v_i, v_j)$ between the vertices $v_i, v_j \in V(G)$ is the length of the shortest path between the vertices v_i and v_j.
4. The **eccentricity** $e(u)$ of the vertex u is defined as $e(u) = max\{d(u, v) : v \in V(G)\}$.
5. A vertex v is said to be an **eccentric vertex** of the vertex u if $d(u, v) = e(u)$.
6. The **diameter** $diam(G)$, and the **radius** $rad(G)$ of a graph G is the maximum and the minimum eccentricity of all vertices of G, respectively.
7. A vertex $u \in V(G)$ is said to be **diametrical vertex** of G if $e(u) = diam(G)$.
8. If each vertex of G has a unique diametrical vertex, then G is called a **diametrical graph**.

Definitions

Adjacency matrix

The adjacency matrix $A(G)$ of a connected graph G with $V(G) = \{v_1, v_2, \ldots, v_n\}$, is an $n \times n$ matrix, whose rows and columns are indexed by the vertex set of G and the entries are defined by

$$A(G)_{ij} = \begin{cases} 1 & \text{if } v_i \sim v_j, \\ 0 & \text{otherwise.} \end{cases}$$

Distance matrix

The distance matrix of a connected graph G is $D(G) = [d_{ij}]_{n \times n}$, where d_{ij} be the distance between the vertices v_i and v_j in G.

Definition

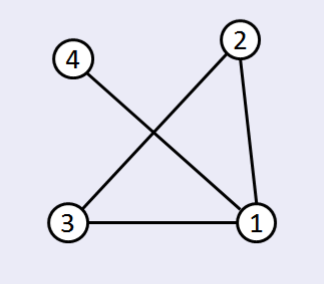
Eccentricity matrix [J Wang, M Lu, F Belardo, and M Randic [9], 2018]

The eccentricity matrix of a connected graph G is obtained from the distance matrix of G by retaining the largest distances in each row and each column, and setting the remaining entries as 0. In other words, the *eccentricity matrix* $\varepsilon(G) = (\epsilon_{uv})_{n \times n}$ of a connected graph G is defined as

$$\epsilon_{uv} = \begin{cases} d(u,v) & \text{if } d(u,v) = min\{e(u), e(v)\}, \\ 0 & \text{otherwise.} \end{cases}$$

Example

Consider a **simple connected graph** G :



Let $D(G)$-Distance matrix, $\varepsilon(G)$-Eccentricity matrix. Then

$$D(G) = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 2 \\ 1 & 1 & 0 & 2 \\ 1 & 2 & 2 & 0 \end{bmatrix} \qquad \varepsilon(G) = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 2 \\ 1 & 0 & 0 & 2 \\ 1 & 2 & 2 & 0 \end{bmatrix}$$

Notations

1. The eigenvalues of $\varepsilon(G)$ is called the ε**-eigenvalues** of G and they form the ε**-spectrum** of G.
2. The largest eigenvalue of $\varepsilon(G)$ is called the ε**-spectral radius** and is denoted by $\rho(\varepsilon(G))$.
3. The ε**-degree** of a vertex $v_i \in V(G)$ is defined as $\varepsilon(i) = \sum_{j=1}^{n} \epsilon_{ij}$.
4. Let $\{\varepsilon(1), \varepsilon(2), \ldots, \varepsilon(n)\}$ be the ε-degree sequence of the graph G. Then G is said to be ε**-regular** if $\varepsilon(i) = k$, for all i.
5. Two graphs are said to be ε**-cospectral** if they have the same ε-spectrum.

Interlacing theorem

Suppose $A \in \mathbb{R}^{n\times n}$ is symmetric. Let $B \in \mathbb{R}^{m\times m}$ with $m < n$ be a principal submatrix of A (submatrix whose rows and columns are indexed by the same index set $\{i_1, \dots, i_m\}$, for some m). Suppose A has eigenvalues $\lambda_1 \leq \dots \leq \lambda_n$, and B has eigenvalues $\beta_1 \leq \dots \leq \beta_m$. Then,
$\lambda_k \leq \beta_k \leq \lambda_{k+n-m}$ for $k = 1, \dots, m$, and if $m = n-1$, then
$\lambda_1 \leq \beta_1 \leq \lambda_2 \leq \beta_2 \leq \dots \leq \beta_{n-1} \leq \lambda_n$.

Lemma (Huiqiu Lin, Yuan Hong, Jianfeng Wang, and Jinlong Shu,[2])

The graph $K_{1,n-1}$ is the unique graph, which have maximum distance spectral radius among all graphs with diameter 2.

Definitions

Energy of a graph

The energy (or A-energy) of a graph is defined as

$$E_A(G) = \sum_{i=1}^{n} |\lambda_i|,$$

where λ_i, $i = 1, 2, \ldots, n$ are the eigenvalues of the adjacency matrix of G.

ε-energy of a graph

In a similar way, the eccentricity energy (or ε-energy) of a graph G is defined [8] as

$$E_\varepsilon(G) = \sum_{i=1}^{n} |\xi_i|,$$

where $\xi_1, \xi_2, \ldots, \xi_n$ are the ε-eigenvalues of G.

ε-equienergetic graphs

Two graphs are said to be ε-**equienergetic** if they have the same ε-energy.

Wiener index

The Wiener index of a graph is defined as

$$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u, v).$$

ε-Wiener index [I Mahato, R Gurusamy, M R Kannan, and S Arockiaraj [3]]

Similar to the Wiener index of a graph, we define the *eccentric Wiener index* (or ε-Wiener index) of a connected graph G as

$$W_\varepsilon(G) = \frac{1}{2} \sum_{u,v \in V(G)} \epsilon_{uv}.$$

Main results

Conjecture for the least eigenvalue of a tree

In 2018, J Wang, M Lu, F Belardo, and M Randic [9] made the following conjecture for the least eigenvalue of a tree.

Conjecture (J Wang, M Lu, F Belardo, and M Randic [9], 2018)

Let T be a tree on n vertices, with $n \geq 3$, and let $\varepsilon_n(T)$ be the least eigenvalue of $\varepsilon(T)$. Then, $\varepsilon_n(T) \leq -2$, and equality holds if and only if T is the star.

Theorem (I Mahato, R Gurusamy, M Rajesh Kannan, and S Arockiaraj, [4])

Let T be a tree of order n other than P_2, and let $\varepsilon_n(T)$ be the least eigenvalue of $\varepsilon(T)$. Then $\varepsilon_n(T) \leq -2$ with equality if and only if T is the star.

Proof.

- Let T be a tree on $n \geq 3$ vertices, other than the star. Want to show $\varepsilon_n(T) < -2$.
- WLOG assume that $P(v_1, v_n)$ be a longest path in T. Then, $d(v_1, v_n) = k$ and $3 \leq k \leq n-1$.
- $e(v_1) = e(v_n) = k$.
- $A = \begin{bmatrix} 0 & k \\ k & 0 \end{bmatrix}$ is a 2×2 principal submatrix of $\varepsilon(T)$.
- The eigenvalues of A are are $k, -k$, with $3 \leq k \leq n-1$.
- Therefore, by interlacing theorem, $\varepsilon(T)$ must have an eigenvalue less than or equal to -3.

□

Characterization of the star graph

Theorem (I Mahato, R Gurusamy, M Rajesh Kannan, and S Arockiaraj, [3])

Let T be a tree, other than P_4, then the eccentricity matrix of T is invertible if and only if T is the star.

Proof.

- Let T be the star on n vertices. Since $D(T) = \varepsilon(T)$, $\det(D(T)) = \det(\varepsilon(T) = (-1)^{n-1}(n-1)2^{n-2} \neq 0$.
- For $n = 2, 3$, the proof is trivial. For $n = 4$, P_4 and $K_{1,3}$ are the only trees of order 4, and the eccentricity matrix of both the trees are invertible.
- Consider $n \geq 5$. Let T be a tree on $n \geq 5$ vertices other than the star. We want to show that $det(\varepsilon(T)) = 0$.
- Let $P(v_1, v_m) = v_1 v_2 \dots v_{m-1} v_m$ be a diametrical path of length $m - 1$ in T.
- **Case(I)**: Let either v_2 or v_{m-1} be adjacent to at least one pendant vertex other than v_1 and v_m. WLOG, assume that v_{m-1} is adjacent to p pendant vertices, say, $u_1, u_2, \dots, u_p$. Then the rows corresponding to the vertices $u_1, u_2, \dots, u_p$ and v_m are the same in $\varepsilon(T)$. Thus $det(\varepsilon(T)) = 0$.

□

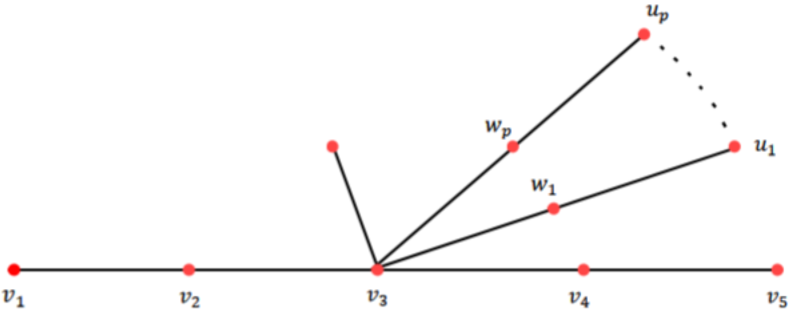
Proof contd.

Case(II)

- Let both the vertices v_2 and v_{m-1} are not adjacent to any of the pendant vertices in G other than v_1 and v_m, respectively.
- If T is a tree on $n \geq 5$ vertices and $diam(T) = 3$, then one of the vertices v_2 or v_{m-1} must be adjacent to at least two pendent vertices, and the proof follows from case(I).
- Let $diam(T) \geq 4$. Let us show that at least two rows of $\varepsilon(T)$ are linearly dependent.
- Let $diam(T) = 4$, and let $P(v_1, v_5) = v_1 v_2 v_3 v_4 v_5$ be a diametrical path in T.
- Let $u_1, u_2, \ldots, u_p$ be the vertices, other than v_1 and v_5, such that each u_i has exactly one common neighbour, say w_i, with v_3.
- The vertices $u_1, u_2, \ldots, u_p$ are pendant.
- The rows corresponding to the vertices $w_1, w_2, \ldots, w_p, v_2, v_4$ and the row corresponding to the vertex v_3, in $\varepsilon(T)$, are linearly dependent .
- Let $diam(T) \geq 5$, and let $P(v_1, v_m) = v_1 v_2 v_3 \ldots v_{m-1} v_m$ be a diametrical path in T. Then the rows corresponding to the vertices v_2 and v_3 are linearly dependent in $\varepsilon(T)$.

Thus $\det(\varepsilon(T)) = 0$ in all the above cases. Therefore, if the eccentricity matrix of T is invertible, then T is the star.

Figure



Maximum ε-spectral radius among graphs with diameter 2

Theorem (I Mahato, R Gurusamy, M Rajesh Kannan, and S Arockiaraj, [3])

Among all connected graphs on n vertices with diameter 2, the star $K_{1,n-1}$ is the unique graph, which has maximum ε-spectral radius.

Proof.

- Note that $\rho(\varepsilon(G)) \leq \rho(D(G))$.
- $D(K_{1,n-1}) = \varepsilon(K_{1,n-1})$.
- $\rho(D(G)) \leq \rho(D(K_{1,n-1})) = (n-2) + \sqrt{n^2 - 3n + 3}$, and the equality holds if and only if G is the star. [2]
- Therefore, $\rho(\varepsilon(G)) \leq \rho(D(G)) \leq \rho(D(K_{1,n-1})) = \rho(\varepsilon(K_{1,n-1}))$, and the equality holds only for the star.

□

Theorem (I Mahato, R Gurusamy, M Rajesh Kannan, and S Arockiaraj, [3])

If G is a connected graph with diameter $d \geq 2$, then $\rho(\varepsilon(G)) \geq d$, and the equality holds if and only if G is the diametrical graph with diameter d.

Sketch of the proof

- Note that $\begin{bmatrix} 0 & d \\ d & 0 \end{bmatrix}$ is a 2×2 principal submatrix of G. So by interlacing theorem, we have $\rho(\varepsilon(G)) \geq d$.
- If G is a diametrical graph with diameter d, then $\varepsilon(G) = \begin{bmatrix} 0 & dI_k \\ dI_k & 0 \end{bmatrix}$. Therefore, $\rho(\varepsilon(G)) = d$.

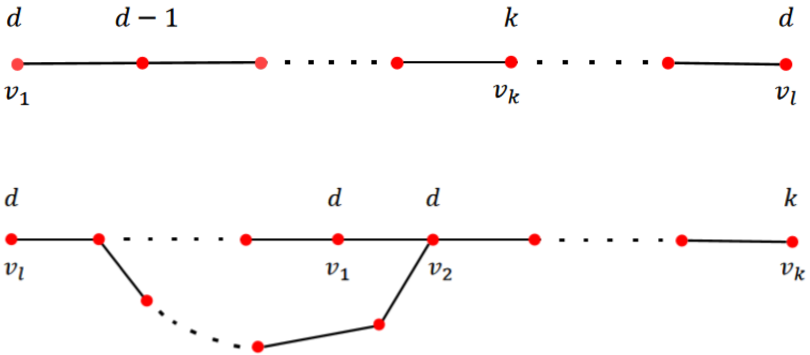
Proof contd.

Conversely, let $\rho(\varepsilon(G)) = d$. Suppose G is not a diametrical graph.

Case 1

- Let G be a graph such that $rad(G) \neq diam(G) = d$.
- Then there exists a $v_k \in V(G)$ with $e(v_k) = k < d$.
- Let $v_1 \in V(G)$ such that $e(v_1) = d$. Since G is a connected graph, there is a path $P(v_1, v_k)$ between the vertices v_1 and v_k.
- The eccentricity of any vertex which is adjacent to v_1 is either d or $d - 1$.
- In $P(v_1, v_k)$, there always exists a pair of adjacent vertices u and v such that $e(u) = d$ and $e(v) = d - 1$.
- Let $d(u, w) = d$, then $d(v, w) = d - 1$.
- Since $e(v) = d - 1$ and w is an eccentric vertex of v, the vw-th entry of $\varepsilon(G)$ is $d - 1$.
- $C = \begin{bmatrix} 0 & 0 & d \\ 0 & 0 & d-1 \\ d & d-1 & 0 \end{bmatrix}$ is a principal submatrix of $\varepsilon(G)$, corresponding to the vertices u, v and w.
- Since $\rho(C) = \sqrt{(d-1)^2 + d^2}$, by interlacing theorem, we have $\rho(\varepsilon(G)) \geq \sqrt{(d-1)^2 + d^2} > d$, a contradiction.

Figures



Proof contd.

Case 2

Let G be a graph such that $rad(G) = diam(G) = d$. Then

$$B = \begin{bmatrix} 0 & d & d \\ d & 0 & 0 \\ d & 0 & 0 \end{bmatrix}$$

is a principal submatrix of $\varepsilon(G)$, and $\rho(B) = d\sqrt{2}$. Therefore, by interlacing theorem, we have $\rho(\varepsilon(G)) \geq d\sqrt{2} > d$, which is not possible.

Therefore, G is a diametrical graph.

Corollary (I Mahato, R Gurusamy, M Rajesh Kannan, and S Arockiaraj, [3])

Among the connected bipartite graphs on $2n$ ($n \geq 3$) vertices, the graph $W_{n,n}$ has the minimum ε-spectral radius, where $W_{n,n}$ is the graph obtained by deleting n independent edges from the complete bipartite graph $K_{n,n}$.

Proof.

- $W_{n,n}$ is a diametrical graph with diameter 3. So $\rho(\varepsilon(W_{n,n})) = 3$.
- Among the bipartite graphs on $2n$ vertices, $K_{1,2n-1}$ and $K_{n,n}$ are the only graphs of diameter 2.
- $\rho(\varepsilon(K_{1,2n-1})) = 2(n-1) + \sqrt{4n^2 - 6n + 3} \geq 3$, and $\rho(\varepsilon(K_{n,n})) = 2(n-1) \geq 3$.

□

Bounds for ε-spectral radius

Theorem (I Mahato, R Gurusamy, M Rajesh Kannan, and S Arockiaraj, [3])

Let G be a connected graph on n vertices with eccentric Wiener index W_ε.

- *Then $\rho(\varepsilon(G)) \geq \frac{2W_\varepsilon}{n}$ and the equality holds if and only if G is ε-regular graph.*
- *If $\{\varepsilon(1), \varepsilon(2), \ldots, \varepsilon(n)\}$ is the ε-degree sequence of G, then*

$$\rho(\varepsilon(G)) \geq \max_i \left\{ \frac{1}{n-1} \left((W_\varepsilon - \varepsilon(i)) + \sqrt{(W_\varepsilon - \varepsilon(i))^2 + (n-1)\varepsilon^2(i)} \right) \right\}.$$

Proof.

The similar types of bounds for distance matrix of a connected graph G is known in the article 'Sharp bounds on the distance spectral radius and the distance energy of graphs' by G Indulal [1], and the idea of the proof is quite same. □

Construction of non ε-cospectral ε-equienergetic graphs

Theorem (I Mahato, R Gurusamy, M Rajesh Kannan, and S Arockiaraj [3])

For $n \geq 6$ and $p, q \geq 2$, the graphs $K_{p,n-p}$ and $K_{q,n-q}$ are ε-equienergetic, but not ε-cospectral .

Proof.

- $\varepsilon(K_{p,q}) = \begin{bmatrix} 2(J_p - I_p) & 0 \\ 0 & 2(J_q - I_q) \end{bmatrix}.$
- $spec_\varepsilon(K_{p,q}) = \left\{ \begin{array}{ccc} 2(p-1) & 2(q-1) & -2 \\ 1 & 1 & p+q-2 \end{array} \right\}$
- $E_\varepsilon(K_{p,q}) = 4(p+q-2).$
- $E_\varepsilon(K_{p,n-p}) = 4(p+n-p-2) = 4(n-2) = 4(q+n-q-2) = E_\varepsilon(K_{q,n-q}).$

□

Some open problems

Problem (Jianfeng Wang, Lu Lu, Milan Randic, and Guozheng Li, [8])

For each pair of integers (n, d) with n even, $d \geq 2$ and $n \geq 4d - 4$, can one give a construction for the diametrical graphs with order n and diameter d ?

Problem (Jianfeng Wang, Mei Lu, Lu Lu, and Francesco Belardo, [10])

Which trees have the maximum ε-spectral radius ?

Problem (Jianfeng Wang, Mei Lu, Lu Lu, and Francesco Belardo, [10])

Determine the graphs with the least ε-eigenvalue $\xi_n = -d$, where $d \geq 3$ is the diameter of the graph.

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Thank You