Distance Spectra and Energy of Graphs

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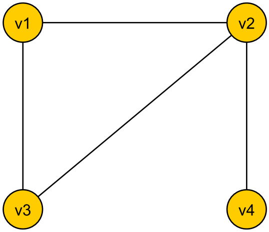
Distance Matrix

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



$$\begin{array}{c c} & \begin{array}{cccc} v_1 & v_2 & v_3 & v_4 \end{array} \\ \begin{array}{c} v_1 \\ v_2 \\ v_3 \\ v_4 \end{array} & \begin{pmatrix} 0 & 1 & 1 & 2 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 2 \\ 2 & 1 & 2 & 0 \end{pmatrix} \end{array}$$

Distance Matrix

- Distance matrix of a graph is a **real symmetric matrix** with diagonal entries 0's.
- All the **distance eigenvalues are real**.
- The **distance spectrum** of G is $\{\lambda_1, \ldots, \lambda_n\}$, where $\lambda_i's$ are the eigenvalues of $D(G)$.
- The largest eigenvalue of the distance matrix D of G is called the **distance spectral radius** $\rho_D(G)$.

Integral Distance Spectrum

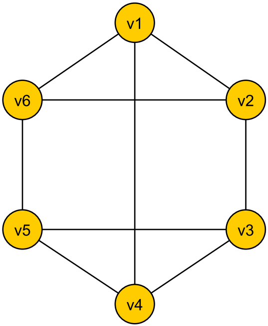


Figure: A graph with integral distance spectrum $\{7, 0, 0, -2, -2, -3\}$

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Transmission Regular Graph

- The transmission $Tr(v)$ of a vertex v in G is the sum of the distances from v to all other vertices in G, i.e., $\mathrm{Tr(v)} = \sum\limits_{\mathrm{u \in V}} \mathrm{d(u,v)}$.
- We say that G is a $k-$transmission regular graph if $Tr(v) = k$ for every $v \in V$.
- A $k-$transmission regular graph has distance spectral radius k.

Transmission Regular Graph

- K_n is $(n-1)$ transmission regular.
- C_n and $K_{m,m}$ are both regular and transmission regular.
- There exists regular and non-regular transmission regular graphs.

Transmission Regular Graph

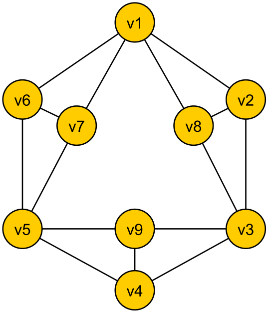

Figure: A transmission regular graph which is not degree regular

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Strongly Regular Graph

- A $k-$regular graph G on n vertices is said to be strongly regular if there exist two integers p and q such that any two adjacent vertices in G have p common neighbors and any non-adjacent vertices have q common neighbors. In this case n, k, p and q are the called the parameters of G, and G is called $(n, k, p, q)-$ strongly regular graph.
- Strongly regular graphs have exactly three distinct distance eigenvalues [3].
- Strongly regular graphs are transmission regular [17].

$SRG(10, 3, 0, 1)$:

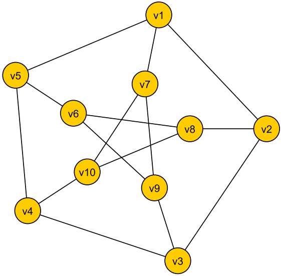

Figure: Petersen graph has distance spectrum $\begin{pmatrix} -3 & 0 & 15 \\ 5 & 4 & 1 \end{pmatrix}$

.

Shrikhande graph - $SRG(16, 6, 2, 2)$

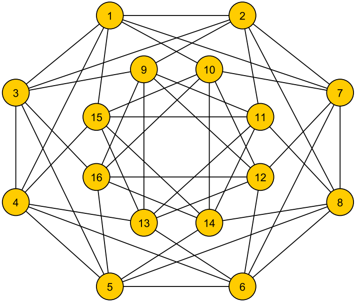

Figure: Shrikhande graph has distance spectrum $\begin{pmatrix} -4 & 0 & 24 \\ 6 & 9 & 1 \end{pmatrix}$

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Perron Frobenius theorem [16]

Let A be an irreducible non-negative *nxn* matrix with spectral radius $\rho(A)$. Then the following statements hold:

- The number $\rho(A)$ is a positive real number and is an eigenvalue of the matrix A, called the Perron Frobenius eigenvalue.
- The Perron Frobenius eigenvalue $\rho(A)$ is simple.
- A has an eigenvector corresponding to eigenvalue $\rho(A)$ whose components are all positive.
- The only eigenvectors whose components are all positive are those associated with the eigenvalue $\rho(A)$.

Review of Literature

- The remarkable theorem proved by Graham and Pollack [8] gives a formula for the determinant of the distance matrix of a tree depending only on the order n. If T is a tree on $n \geq 2$ vertices with distance matrix D, then

$$det(D) = (-1)^{(n-1)}(n-1)^{(2n-2)}.$$

- Graham and Lovasz [7] proved that it is possible to compute the inverse of the distance matrix of a tree in terms of the degrees and the entries of the adjacency matrix.

Review of Literature

- Graphs having a unique positive distance eigenvalue have been intensively studied in literature.
- In 1971 Graham and Pollack [8] showed that trees have a unique positive distance eigenvalue.
- In 1994 Koolen and Schpectorov characterised the distance-regular graphs with unique positive distance eigenvalue [18].
- In 2005 Bapat, Kirkland and Neumann [2] proved that unicyclic graphs have a unique positive distance eigenvalue.

Review of Literature

- Non-isomorphic graphs with the same distance spectrum are called **distance cospectral graphs**.
- In 2016 Koolen etal. [23] proved that the hyper $d-$cube is determined by the spectrum of its distance matrix.

Review of Literature

- Note that the $d-$cube is not determined by its adjacency spectrum as the Hoffman graph has the same adjacency spectrum as the $4-$cube.

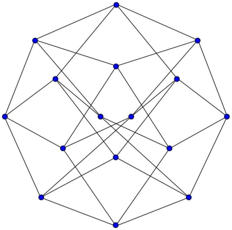

Figure: Hoffman Graph

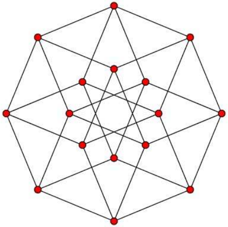

Figure: $4-$cube

Distance Energy

Definition [16]

The **distance energy** of G is defined by $E_D(G) = \sum_{i=1}^{n} |\lambda_i|$.

Motivation

- chemistry$\leftrightarrow$mathematics
- conjugated hydrocarbons$\leftrightarrow$graph G
- (atoms and bonds) $\leftrightarrow$ (vertices and edges)
- molecular orbital energy levels$\leftrightarrow$graph eigenvalues
- total energy of $\pi-$electrons$\leftrightarrow$graph energy $E(G)$

Distance Energy

- [1] Distance matrix has its applications in the design of communication networks, network flow algorithms, graph embedding theory as well as molecular stability.
- Balaban, Ciubotariu and Medeleanu [24] proposed the use of $\rho_D(G)$ as a molecular descriptor, later [26] it is used in QSPR (Quantitative Structure-Property Relationship) modelling and in [25] it was successfully used to infer the extent of branching and model boiling points of alkanes.

Preliminaries

- The distance matrix has zero diagonal entries, so that $\lambda_1 + \cdots + \lambda_n = tr(D(G)) = 0$. Hence

$$E_D(G) = 2\sum_{\lambda_i>0} \lambda_i = -2\sum_{\lambda_i<0} \lambda_i.$$

- Let $\rho_D(G)$ denote the spectral radius of $D(G)$, then by Perron-Frobenius theory [9], $E_D(G) \geq 2\rho_D(G)$, and equality holds if and only if G has a unique positive distance eigenvalue.

Review of Literature

- Distance energy of path P_n [19] is approximately $0.6948n^2 - 0.7964$.
- Distance energy of a cycle C_n is $\begin{cases} \frac{n^2-1}{2}, if\, n\, is\, odd \\ \frac{n^2}{2}, if\, n\, is\, even \end{cases}$
- Distance energy of star S_n [22] is $2\,(n-2) + 2\sqrt{(n-2)^2 + (n-1)}$.
- Distance energy of complete bipartite graph $K_{m,n}$ [21] is $4(m+n-2)$.
- Distance energy of a complete split graph $CS_{m,n}$ is given by $2(2m+n-3)$.

Possible types of Problems

- Derive energy bounds using graph parameters:
  order, size, degrees,...
- Characterize graphs with extremal energy in a specific family:
  bipartite, trees, unicyclic,...
- Characterize how energy changes due to a specific operation:
  vertex deletion, edge deletion, subdivision,...

How to Solve?

Let A be a real symmetric matrix partitioned as:

$$A = \begin{pmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,r} \\ A_{2,1} & A_{2,2} & \dots & A_{2,r} \\ \vdots & \vdots & & \vdots \\ A_{r,1} & A_{r,2} & \dots & A_{r,r} \end{pmatrix},$$

where $A_{i,j}$ is a block or submatrix of A.

How to Solve?

- If $q_{i,j}$ denote the average row sum of $A_{i,j}$, then $Q = (q_{i,j})$ is called the **quotient matrix** of A.
- If the row sum of each block $A_{i,j}$ is a constant, then the partition is called **equitable**.

How to Solve?

- Let Q be a quotient matrix of a square matrix A, corresponding to a partition of A. Then the eigenvalues of Q interlace the eigenvalues of A.
- Let Q be a quotient matrix of a square matrix C corresponding to an **equitable partition**. Then the spectrum of C contains the spectrum of Q. Moreover, the **spectral radius of A and Q are equal**.

How to Solve?

Cauchy's Interlacing Theorem : Bapat [16]

Let $A \in M_n$ and $B \in M_m$ be symmetric matrices with eigenvalues $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_n$ and $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_m$ respectively. If B is a principal submatrix of A, then:
$\alpha_k \geq \beta_k \geq \alpha_{k+n-m}$ for $k \in \{1, 2, \ldots, m\}$.

Preliminaries

Let H be a connected induced subgraph of G of order m.

- The adjacency matrix of H is a principal submatrix of the adjacency matrix of G.
- By interlacing theorem the adjacency eigenvalues of G interlace the eigenvalues of H, see [16].

Distance Matrix D_G

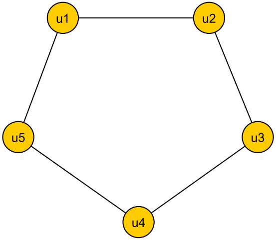

Figure: G

$$
\begin{array}{c c}
 & \begin{array}{ccccc} u_1 & u_2 & u_3 & u_4 & u_5 \end{array} \\
\begin{array}{c} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{array} &
\begin{pmatrix}
0 & 1 & 2 & \mathbf{2} & 1 \\
1 & 0 & 1 & 2 & 2 \\
2 & 1 & 0 & 1 & 2 \\
\mathbf{2} & 2 & 1 & 0 & 1 \\
1 & 2 & 2 & 1 & 0
\end{pmatrix}
\end{array}
$$

Distance Matrix D_H

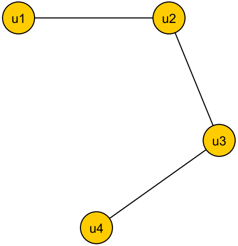

Figure: H

	u_1	u_2	u_3	u_4
u_1	0	1	2	**3**
u_2	1	0	1	2
u_3	2	1	0	1
u_4	**3**	2	1	0

Review of Literature

- The distance matrix, distance eigenvalue, and distance energy of a connected graph have been studied intensively in literature, see [1, 10, 11, 12, 15].
- We discuss a new problem of how the distance energy changes when an edge is deleted.
- Similar problem for adjacency energy of a graph was studied by Day and So in [4, 5].

Review of Literature

- Day and So proved that, if e is a bridge in a simple graph G, then $E(G - e) < E(G)$, hence for a tree the same inequality holds.
- They also proved that, if G' is an induced subgraph of a simple graph G, then $E(G') \leq E(G)$ and equality holds if and only if G' and G has same edge set.
- Also they proved the existence of infinite families of graphs with the property that, deleting a certain edge does not change the energy, deleting any edge will decrease the energy and deleting any edge will increase the energy.

Results

- It turns out that the results for distance energy change and adjacency energy change are quite different.
- From an observation in [15], it follows that, for any connected graph with a unique positive eigenvalue, the deletion of any edge increases the distance energy provided that the resulting graph is still connected.

Results

- For examples, both complete graphs [6] and unicyclic graphs [2] have a unique positive distance eigenvalue. Therefore, for any edge e,

  $$E_D(K_n) < E_D(K_n - e)$$

  and

  $$E_D(C_n) < E_D(C_n - e) = E_D(P_n)$$

  where K_n, C_n and P_n are the complete graph, cycle graph and path graph of order n respectively.

Results

It is interesting to note that:

- $\lim_{n\to\infty} E_D(K_n - e) - E_D(K_n) = 0$, but
- $\lim_{n\to\infty} E_D(P_n) - E_D(C_n) = \infty$.

Results

Two natural questions arise:

1. Is the property of having a unique positive distance eigenvalue a necessary condition for the increase of distance energy by deleting an edge?
2. Does the deletion of an edge always increase the distance energy of any graph?

We answer both questions negatively.

Results

- We prove that the distance energy of a complete bipartite graph is always increased when an edge is deleted even though it has two positive distance eigenvalues.
- Also, we give a set of examples of connected graph whose distance energy decreases when a specific edge is deleted.

Results

- We consider the complete bipartite graph $K_{m,n}$ with $m, n > 1$. Since $m, n \geq 2$, both $K_{m,n}$ and $K_{m,n} - e$ are connected for any edge e.
- Moreover, the negative distance eigenvalues of $K_{m,n}$ are exactly -2 of multiplicity $m + n - 2$ [14]. Hence $E_D(K_{m,n}) = 4(m + n - 2)$.
- However, explicit formulae for the distance eigenvalues and the distance energy of $K_{m,n} - e$ are harder to obtain.
- Nonetheless, we are able to compare $E_D(K_{m,n})$ and $E_D(K_{m,n} - e)$.

Results [20] (Anu, So, Vijayakumar)

Theorem

Let $K_{m,n}$ be the complete bipartite graph with $m, n > 1$ and e be any edge. Then the distance eigenvalues of $K_{m,n} - e$ are -2 with multiplicity $m + n - 4$ and the roots $\alpha_4 \leq \alpha_3 \leq \alpha_2 \leq \alpha_1$ of the polynomial

$$\begin{aligned} p(x) &= x^4 + [8 - 2(m+n)]\, x^3 + [3mn - 12(m+n) + 16]\, x^2 \\ &\quad + [12mn - 16(m+n) - 16]\, x + [12(m+n) - 60]\,. \end{aligned}$$

Results [20] (Anu, So, Vijayakumar)

- For $m, n \geq 2$ and any edge e,

$$E_D(K_{m,n}) < E_D(K_{m,n} - e).$$

- The distance energy of a complete multi-partite graph is known in literature, one can see [13] for a short proof: $E_D(K_{n_1,n_2,\ldots,n_r}) = 4(n_1 + \cdots + n_r - r)$. However, $E_D(K_{n_1,n_2,\ldots,n_r} - e)$ is NOT known to have any closed form.

Family of Graphs - Distance Energy decreases

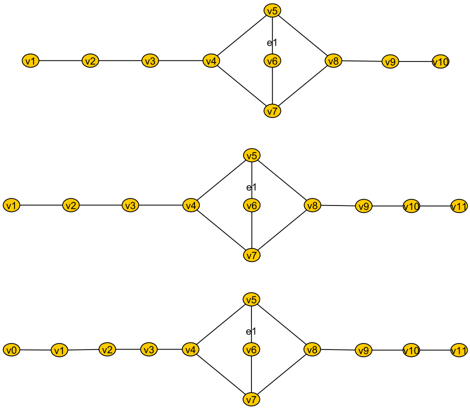

Figure: Graphs in which edge deletion decreases distance energy

Books

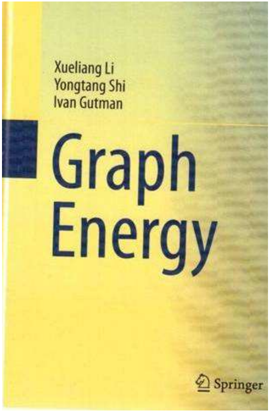

Figure: Book 1

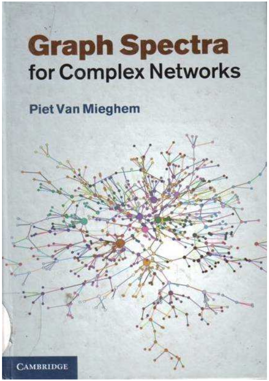

Figure: Book 2

Books

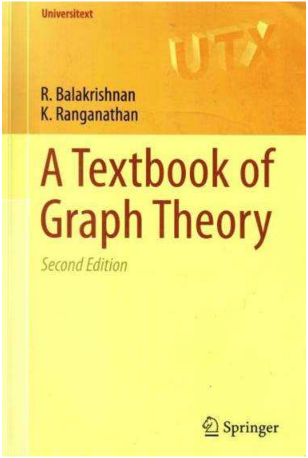

Figure: Book 3

Books

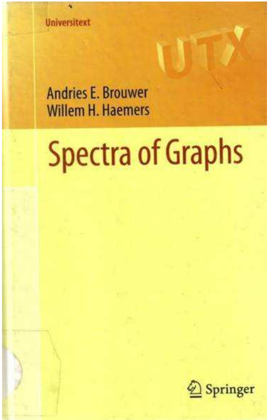

Figure: Book 4

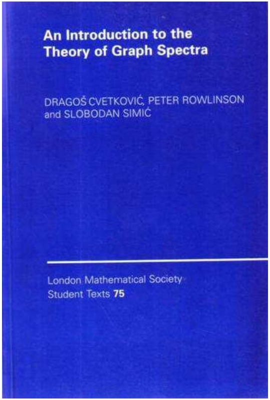

Figure: Book 5

References

1. M. Aouchiche and P. Hansen, Distance spectra of graphs: a survey, *Linear Algebra and its Applications* 458 (2014) 301-386.
2. R. Bapat, S. Kirkland and M. Neumann, On distance matrices and Laplacians, *Linear Algebra and its Applications* 401 (2005) 193-209.
3. J. Azarija, A short note on a short remark of Graham and Lovasz, *arXiv:1303.4517v2 [math.CO]* 30 Sep 2013.
4. J. Day and W. So, Singular value inequality and graph energy change, *Electron. J. Linear Algebra* 16 (2007) 291-299.

References

5. J. Day and W. So, Graph energy change due to edge deletion, *Linear Algebra and its Applications* 428 (2008) 2070-2078.
6. B. Durgi, P. Hampiholi, S. Mekkalike, Distance spectra and distance energy of some cluster graphs, *Mathematica Aeterna* 4 (2014) 817 - 825.
7. R.L. Graham, L. Lovsz, Distance matrix polynomials of trees, *Adv. Math.* 29 (1978) 6088.
8. R.L. Graham, H.O. Pollack, On the addressing problem for loop switching, *Bell Syst. Tech. J.* 50 (1971) 24952519.

References

9. R. Horn and C. Johnson, *Matrix Analysis*, Cambridge University press, 1985.
10. A. Ilic, Distance spectra and distance energy of integral circulant graphs, *Linear Algebra and its Applications* 433 (2010) 1005–1014.
11. G. Indulal, Distance spectrum of graph compositions, *Ars Mathematica Contemporanea* 2 (2009) 93–100.
12. G. Indulal, I. Gutman and A. Vijayakumar, On distance energy of graphs, *MATCH Commun. Math. Comput. Chem.* 60 (2008) 461–472.

References

13. W. So, A shorter proof of the distance energy of complete multipartite graphs, *Special Matrices* 5 (2017) 61–63.
14. D. Stevanovic and G. Indulal, The distance spectrum and energy of the composition of regular graphs, *Appl. Math. Lett.* 22 (2009) 1136–1140.
15. B. Zhou and A. Ilic, On distance spectral radius and distance energy of graphs, *MATCH Commun. Math. Comput. Chem.* 64 (2010) 261–280.
16. R. B. Bapat, *Graphs and Matrices*, Second Edition, Hindustan Book Agency, Springer, 2014.

References

17. F. Atik, P. Panigrahi *On the distance spectrum of distance regular graphs*, Linear Algebra and its Applications 478 (2015) 256273.

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

19. G. Caporossi, E. Chasset, B. Furtula, *Some conjectures and properties on distance energy*, Les Cahiers GERAD G-2009-64 (2009) V+17.

References

20. A. Varghese, W. So, A. Vijayakumar, Distance energy change of Complete-bipartite graph due to edge deletion, Communicated to Linear Algebra and Applications.

21. X. Zhang, *The inertia and energy of distance matrices of complete k-partite graphs*, Linear Algebra and its Applications 450, 108120 (2014) .

22. Dragan Stevanovic, Aleksandar Ilic: *Distance spectral radius of trees with fixed maximum degree*, Electronic Journal of Linear Algebra, Volume 20, pp. 168-179 (2010).

23. J. Koolen, S. Hayat, Q. Iqbal: *Hypercubes are determined by their distance spectra*, arXiv:1512.04160 [math.CO] 28 Apr 2016.

References

24. A. T. Balaban, D. Ciubotariu and M. Medeleanu, Topological indices and real number vertex invariants based on graph eigenvalues or eigenvectors, *J. Chem. Inf. Comput. Sci.* **31** (1991) 517–523.
25. I. Gutman, M. Medeleanu, On the structure dependence of the largest eigenvalue of the distance matrix of an alkane, *Indian J. Chem.* **A37** (1998)569–573.
26. V. Consonni and R. Todeschini, New spectral indices for molecule description, *MATCH Commun. Math. Comput. Chem.*, **60** (2008) 3–14.

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