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Abstract

The distance energy of a graph G is defined as $E_D(G) = \sum |\mu_i|$, where μ_i is the i^{th} eigenvalue of the distance matrix of G. In this paper, we express the distance spectra and distance energy of complete split graphs and graphs composed of two cliques joined by a matching. We also give some spectral properties of complete multipartite graphs. Finally, we identify structural and numerical conjectures on E_D for graphs with number of vertices n and number of edges m are fixed.

Key Words: Distance energy, Eigenvalues, Distance matrices of graphs

Résumé

L'énergie de distance d'un graphe G est définie par $E_D(G) = \sum |\mu_i|$, où μ_i représente la $i^{\text{ième}}$ valeur propre de la matrice des distances de G. Dans cet article, nous exprimons le spectre des distances et l'énergie de distance de graphes fendus complets, et de graphes composés de deux cliques reliées par un couplage. Nous donnons aussi des propriétés spectrales de graphes multiparti complets. Finalement, nous identifions des conjectures structurelles et numériques sur E_D pour des graphes avec le nombre de sommets n et d'arêtes m fixés.

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1 Introduction

Topological descriptors play significant role in the theoretical chemistry, especially in QSPR/QSAR researches. Nowadays, there are hundreds topological indices that found some applications in chemistry [1]. Among them topological indices based on spectrum of graphs play significant role. Maybe, the most used and investigated is so–called graph energy (E) [2]. It is defined as follows:

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

where λ_i is the i^{th} eigenvalue of adjacency matrix A.

This invariant had been introduced in 1978. but only recently it attracted attention of researches and now there are more than 200 papers dealing with this quantity [3]. Some recent results about graph energy can be found in [4, 5, 6, 7, 8, 9, 10].

Nowadays, there are a number of energy–like invariants such as laplacian energy [12], laplacian–energy–like invariant [13], incidence energy [14], distance energy [17], etc. The general formulation of energy–like quantities was given by Connsoni and Todeschini [11]. They defined energy–like quantity for any $n \times n$ matrix as follows:

$$E_{general}(\mathbf{M}, w) = \sum_{i=1}^{n} \left| \xi_i - \overline{\xi} \right| \qquad (1)$$

where $\mathbf{M}$ is the some $n \times n$ matrix, calculated with the weighting scheme w, ξ_i is the set of corresponding eigenvalues. The $\overline{\xi}$ is the arithmetic mean of all eigenvalues.

When $\overline{\xi}$ is equal to 0, as it is case for eigenvalues of adjacency and distance matrix the equation (1) is reduced to:

$$E_{general} = \sum_{i=1}^{n} |\xi_i| \quad \text{when} \quad \overline{\xi} = 0$$

Distance energy is a recently introduced energy–like invariant and it is defined in following manner [17]:

$$E_D(G) = \sum_{i=1}^{n} |\mu_i| \qquad (2)$$

where μ_i are the eigenvalues of distance matrix of a graph G.

Even though this quantity is a new one there are a number of papers (especially mathematical) dealing with this index [16, 17, 18, 19, 20, 21, 22, 23, 24, 11].

In the remaining of this paper, we denote by n the order, or number of vertices of the graph G, by m its size or the number of its edges and $D(G)$ denotes the distance matrix of the graph G. All the graphs considered in this paper are simple graphs, i.e., without loops or multiple edges, indeed, these graphs are connected.

Some properties of distance energy and distance spectra for some families of graphs are discussed in Section 2 and conjectures obtained with AutoGraphiX on E_D when n and m are fixed will be given in Section 3.

2 Distance spectrum and distance energy of special families of graphs

A complete multipartite graph CMG is a graph such that if it is properly colored (with the minimum required colors such that two adjacent vertices do not share the same color) any pair of vertices of different colors corresponds to an edge. The special nature of the distance matrix of complete multipartite graphs has a direct impact on their corresponding D-spectrum. The family of complete multipartite graphs includes the complete graphs, the stars, the complete bipartite graphs and the complete split graphs. Note that complete multipartite graphs have diameter 2 (2 vertices of the same color are adjacent to all vertices of other colors), so that $D(CMG)$ only has entries of value 1 or 2.

After giving some useful lemmas, we describe the D-spectra of complete split graphs and complete bipartite graphs.

Lemma 1 *Let CMG be a complete multipartite graph. Let n_k be the number of colors that have k vertices. Then the D-spectrum of CMG has the eigenvalue $k-2$ with multiplicity at least $n_k - 1$.*

Proof. It is possible to label the vertices of CMG in such a way that vertices with the same color are consecutive. It is also possible that colors are ordered in decreasing values of k.

After reordering the vertices, $D(CMG)$ will have all its 2's as blocks around the main diagonal. Consider now two blocks corresponding to the same value k and concentrate on the corresponding rectangular submatrix $D'(2k \times n)$.

Each column of D' is either composed of 1's only, or of k times 1, $k-1$ times 2 and a 0. The sum on each column is either $2k$ or $k + 2k - 2 = 3k - 2$.

Replacing the entry 0 by $-\mu = -(k-2)$, all the columns will sum up to $2k$, then $Det(D(CMG) - \mu I) = 0$, which indicates that one of these lines is a linear combination of the others and hence $\mu = k-2$ is an eigenvalue of $D(CMG)$.

If there are more than two colors with the same cardinality, the corresponding eigenvalue will have an algebraic multiplicity of $n_k - 1$. □

Note that if $k = 1$, each block only has one line and the value $\mu = -1$ is an eigenvalue of $D(CMG)$ with multiplicity at least $n_k - 1$.

Lemma 2 *Let CMG be a complete multipartite graph and n_k be the number of colors that have $k \geq 2$ vertices. Then the D-spectrum of CMG has the eigenvalue -2 with multiplicity at least $\sum_{k\geq 2} n_k(k-1)$.*

Proof. After ordering the vertices in the same way as for the proof of Lemma 1, consider the one block of lines of $D(CMG)$ corresponding to vertices of a given color. Replacing the entries 0 by $-\mu = 2$ will yield k similar lines, which indicates that the value -2 is an eigenvalue of $D(CMG)$ with multiplicity $k-1$. Repeating this operation for each color will lead to the result. □

Corollary 1 *If G is a complete multipartite graph with only two values k, then all eigenvalues of $D(G)$ are known except at most 2.*

Proof. For each value of k, $k-1$ eigenvalues are identified for each color according to Lemma 2 and $n_k - 1$ additional values are found according to Lemma 1. Overall, considering all the kn_k vertices involved, $(k-1)n_k + n_k - 1 = kn_k - 1$ eigenvalues are identified. □

From Corollary 1, in the case of complete split graphs as well as complete bipartite graphs, all the D-eigenvalues are known except at most 2.

Theorem 1 *Let G be either a complete split graph or a complete bipartite graph. Note μ_i $(i = 3 \dots n)$ the known D-eigenvalues of G according to Lemma 1 and Lemma 2. The remaining two D-eigenvalues of G are the following :*

$$\mu_1 = \frac{-\sum_{i=3}^{n}\mu_i + \sqrt{2\left(\sum_{1\leq i,j\leq n} d_{ij}^2 - \sum_{i=3}^{n}\mu_i^2\right) - \left(\sum_{i=3}^{n}\mu_i\right)^2}}{2} \tag{3}$$

$$\mu_2 = \frac{-\sum_{i=3}^{n}\mu_i - \sqrt{2\left(\sum_{1\leq i,j\leq n} d_{ij}^2 - \sum_{i=3}^{n}\mu_i^2\right) - \left(\sum_{i=3}^{n}\mu_i\right)^2}}{2} \tag{4}$$

Note that μ_2 is not necessarily the second largest D-eigenvalue of CMG.

Proof. Let

$$\begin{aligned} R &= \sum_{1\leq i,j\leq n} d_{ij}^2 \\ S &= -\sum_{i=3}^{n}\mu_i \\ \text{and } T &= \sum_{i=3}^{n}\mu_i^2. \end{aligned}$$

As $Tr(D) = 0 = \sum_{i=1}^{n}\mu_i$, we have

$$S = \mu_1 + \mu_2. \tag{5}$$

After some simple substitutions, we obtain

$$2\mu_1\mu_2 = S^2 - R + T. \tag{6}$$

From equations (5) and (6), μ_1 and μ_2 are the roots of the following second degree equation:

$$\mu^2 - S\mu + \frac{S^2 - R + T}{2} = 0. \tag{7}$$

Solving (7) gives the solutions:

$$\mu_1 = \frac{S + \sqrt{2(R-T) - S^2}}{2} \tag{8}$$

$$\mu_2 = \frac{S - \sqrt{2(R-T) - S^2}}{2}. \tag{9}$$

Replacing R, S and T by their expressions completes the proof. □

Corollary 2 *Let CSG be a complete split graph of order $n \geq 7$ and stability number $3 \leq s \leq n-3$, then the distance energy of CSG is $E_D(CSG) = 2(n+s-3)$.*

Proof. According to Lemma 1 and Lemma 2 we have:

$$\mu_3 \dots \mu_{n-s+1} = -1 \tag{10}$$

$$\mu_{n-s+2} \dots \mu_n = -2 \tag{11}$$

Using these values and the special structure of the distance matrix of a complete split graph we have:

$$\begin{aligned} R &= n(n-1) + 3s(s-1) \\ S &= 2(s-1) + n - s - 1 = n + s - 3 \\ T &= 4(s-1) + n - s - 1 = n + 3s - 5. \end{aligned}$$

Replacing R, S and T in (8) and (9) gives

$$\mu_1 = \frac{n+s-3+\sqrt{n(n-2s+2)+s(5s-6)+1}}{2} \quad (12)$$

$$\mu_2 = \frac{n+s-3-\sqrt{n(n-2s+2)+s(5s-6)+1}}{2} \quad (13)$$

Since $\mu_i < 0\ \forall i = 3 \ldots n$, we have $S = \sum_{i=3}^{n} |\mu_i|$. As $\sum_{i=1}^{n} \mu_i = 0$, μ_1 which is the largest D-eigenvalue of CSG is greater than 0, there remains to prove that $\mu_2 \geq 0$ or, equivalently, that $\mu_1\mu_2 = n(s-2)+2-s^2 \geq 0$. Clearly, it is not the case when $s \leq 2$. If $s \geq 3$, the relation may be expressed as

$$\begin{aligned} n &\geq \frac{s^2-2}{s-2} \\ \Leftrightarrow n &\geq s + 2 + \frac{2}{s-2} \end{aligned}$$

For $s = 3$ and $s = 4$, we have $n \geq 7$. When $s \geq 5$, $2/(s-2) < 1$ and, since s and n are integers, the relation becomes

$$n \geq s + 3.$$

□

Corollary 3 *Let CBG be a complete bipartite graph of order $n \geq 4$ and note $2 \leq a \leq n-2$ the number of vertices in one of its parts. The distance energy of CBG is $4(n-2)$.*

This result was proved by Stevanović and Indulal [19], but may also be found proved in a similar way as Corollary 2 using

$$\begin{aligned} R &= n(n-1) + 3a(a-1) + 3(n-a)(n-a-1) \\ S &= 2(n-2) \\ T &= 4(n-2). \end{aligned}$$

Some of the D-eigenvalues of complete multipartite graphs are known by Lemma 1 and Lemma 2. Unfortunately, when we have more than 2 values of k, more than 2 D-eigenvalues are then unknown. A study of complete multipartite graphs achieved with AutoGraphiX led to the following conjecture:

Conjecture 1 *Let CMG be a complete multipartite graph with γ as chromatic number and at least 2 vertices of each color, then the distance energy of CMG is $E_D(CMG) = 4(n-\gamma)$.*

Theorem 2 *Let G be a graph made of two k-cliques connected in such a way that each vertex of a clique is connected to exactly one vertex of the other, then the distance spectrum of G is the followings:*

$$spec_D(G) = \begin{pmatrix} 3k-2 & -k & 0 & -2 \\ 1 & 1 & k-1 & k-1 \end{pmatrix},$$

the eigenvalues being on the first line and their associated algebraic multiplicity on the second one.

Proof. The proof of this theorem is based upon the following lemma from [15].

Lemma 3 *[15] Let*

$$D = \begin{bmatrix} D_0 & D_1 \\ D_1 & D_0 \end{bmatrix}$$

be a symmetric 2×2 *block matrix. Then the spectrum of* D *is the union of the spectra of* $D_0 - D_1$ *and* $D_0 + D_1$.

It is possible to number the vertices of G in such a way that vertex i ($i \leq k$) is connected to vertex $k+i$. Then, the distance matrix D of G is made of four $k \times k$ blocks: the 2 blocks on the diagonal have all their values being 1's, except 0's on the main diagonal. We shall call D_0 one of those blocks. The 2 other blocks of the distance matrix are made of 2's, except 1's on their main diagonal ; we will call those blocks D_1.

$D_0 - D_1$ being a $k \times k$ block, which values are all -1's, then 0 is an eigenvalue for $D_0 - D_1$, with multiplicity at least $k-1$. And $Det(D_0 - D_1 + kI) = k^k - kk^{k-1} = 0$ implies that $-k$ is also an eigenvalue od D.

$D_0 + D_1$ is a $k \times k$ block, which values are all 3's, except 1's on the diagonal. -2 is therefore an eigenvalue of $D_0 + D_1$ with multiplicity at least $k-1$. Each rows (or column) of $D_0 + D_1$ has $k-1$ 3's and 1, which sums to $3k - 3 + 1 = 3k - 2$, which is also an eigenvalue of D. All the n eigenvalues of D are thus found. □

From this result, we directly deduce that the distance energy of a graph which is composed of two k-cliques connected by a matching is $6k - 4$.

3 Conjectures obtained with AutoGraphiX

The AutoGraphiX (AGX) system aims to help graph theorists in their tasks. One of its most important feature is to find extremal (or close to extremal) graphs by the use of an optimization routine using the variable neighborhood search (VNS) metaheuristic [25, 26]. A complete description of AGX is given in [28] and [27] and it will be omitted here. In the present application, AGX was used to identify graphs minimizing or maximizing distance energy given the number of vertices n and the number of edges m.

The results when attempting to find graphs minimizing of maximizing E_D for all possible values of $12 \leq n \leq 30$ and $n - 1 \leq m \leq n(n-1)/2$ provides a set of about 8000 graphs. All these graphs are not necessarily optimal because the heuristic sometimes fails, but a careful look at them allow us to make some conjectures.

The first remark is that if we only consider the order n of the graphs, the complete graphs seems to minimize E_D while paths seems to maximize E_D. This lower bound was already conjectured by Ramane et al. [20], but the upper bound could be expressed as the following conjecture:

Conjecture 2 *Let* G *be a graph of order* n. *Then, the distance energy of* G, $E_D(G)$ *is less than or equal to* $E_D(Path)$.

We do not know the analytical formula for $E_D(Path)$ but one may easily notice that the distance spectra only has one positive eigenvalue, which indicates that $E_D(Path) = 2\mu_1$.

The numerical values of $E_D(Path)$ indicates a quadratic relation between n and $E_D(Path)$ as follows:

$$E_D(Path) \approx 0.69482n^2 - 0.7964\,.$$

Unfortunately, this relation is not strictly respected but the the relative error is very small ($e_{rel} = |e|/E_D < 10^{-5}$ when $n \geq 10$) and seems to be decreasing when n grows.

Using AGX to find a lower bounds on E_D given n and m, yields the following conjecture:

Conjecture 3 *Let G be a graph of order n and size m. Then, the distance energy of G, $E_D(G)$ is greater than or equal to $4(n-1-m/n)$.*

The upper bounds E_D as a function of n and m involves a more complicated structure. When m is less than or equal to $(n-2)(n-3)/2$, the following structural conjecture describes the graphs for which E_D is maximized.

Conjecture 4 *Let G be a graph on n vertices and $m \leq (n-2)(n-3)/2$ edges, then G is composed of a path appended to a clique with possibly some edges between vertices of the clique and the vertex of the path adjacent to the clique.*

If the number of edges is larger, E_D may be bounded by one of the two following conjectures.

Conjecture 5 *Let G be a graph on n vertices and $(n-2)(n-3)/2 \leq m \leq n(n-3)/2$ edges, then*

$$E_D(G) \leq \frac{4n(n^2-2m-n)}{n^2-2m},$$

and the bound is tight if G is a complete multipartite graph.

Conjecture 6 *Let G be a graph on n vertices and $m \geq n(n-3)/2$ edges, then*

$$E_D(G) \leq 2(n-1) + \left(\frac{n(n-1)}{2} - m\right)\frac{5n+6}{3n}.$$

4 Conclusion

In this paper, we found some results and spectral properties on special families of graphs. We also provide 6 conjectures that are still remains open and could be of interest for some future work on distance energy, a topic that is still in its early phase of study.

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