Applied Mathematics Letters 22 (2009) 1136–1140

Contents lists available at ScienceDirect

Applied Mathematics Letters

journal homepage: www.elsevier.com/locate/aml

The distance spectrum and energy of the compositions of regular graphs ☆

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ARTICLE INFO

Article history:
Received 16 November 2008
Accepted 16 November 2008

Keywords:
Distance spectrum
Distance energy
Join
Regular graphs

ABSTRACT

The distance energy of a graph G is a recently developed energy-type invariant, defined as the absolute deviation of the eigenvalues of the distance matrix of G. It is a useful molecular descriptor in QSPR modelling, as demonstrated by Consonni and Todeschini in [V. Consonni, R. Todeschini, New spectral indices for molecule description, MATCH Commun. Math. Comput. Chem. 60 (2008) 3–14]. We describe here the distance spectrum and energy of the join-based compositions of regular graphs in terms of their adjacency spectrum. These results are used to show that there exist a number of families of sets of noncospectral graphs with equal distance energy, such that for any $n \in \mathbf{N}$, each family contains a set with at least n graphs. The simplest such family consists of sets of complete bipartite graphs.

1. Introduction

Let G be a simple graph on n vertices and let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of its adjacency matrix A. The energy of a graph

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

was defined by Gutman in [1] and it has long known chemical applications; for details see the surveys [2–4]. Following the recent definition of the Laplacian energy in [5], it was observed that other energy-type invariants can be defined as the *absolute deviation of eigenvalues from their average value* for a suitable graph matrix. For example, let D be the distance matrix of G, indexed by the vertices of G, where D_{uv} represents the length of the shortest path between u and v in G. Then:

Definition 1 (*[6,7]*). The *distance energy* $DE(G)$ of a graph G is the sum of absolute values of the eigenvalues of the distance matrix of G.

Several invariants of this type (as well as a few others) were studied by Consonni and Todeschini [6] for possible use in QSPR modelling. Their study showed, among other things, that the distance energy is a useful molecular descriptor, since the values $DE(G)$ or $DE(G)/n$ appear among the best univariate models for the motor octane number of the octane isomers and for the water solubility of polychlorobiphenyls.

☆ This work was supported by the grant 144015G of the Serbian Ministry of Science and the research programme P1-0285 of the Slovenian Agency for Research.
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doi:10.1016/j.aml.2008.11.007

Our motivation for this research came from an initial computer search for the pairs of graphs having equal distance energy. Since the distance energy is calculated from the distance spectrum, graphs with the same distance spectrum trivially have the same distance energy. To avoid trivial cases, we say that the graphs G and H of the same order are *DE-equienergetic* if $DE(G) = DE(H)$, while they have distinct spectra of distance matrices. Some examples of DE-equienergetic graphs are found in the literature [7–9].

The *join* $G\nabla H$ of two vertex-disjoint graphs G and H is the graph obtained from the union $G \cup H$ by adding all edges between a vertex of G and a vertex of H. Our main result (Section 2) is the description of the distance spectrum and the distance energy of the join of regular graphs in terms of their adjacency spectrum. This description is then used to show that there exist a number of families of sets of DE-equienergetic graphs, such that for any $n \in \mathbf{N}$, each family contains a set with at least n graphs. The simplest such family consists of sets of complete bipartite graphs. In Section 3 we further derive the distance spectrum of the join of a regular graph with the union of two regular graphs of distinct vertex degrees, and provide further families of sets of DE-equienergetic graphs.

2. Join of regular graphs

Theorem 2. *For $i = 1, 2$, let G_i be an r_i-regular graph with n_i vertices and eigenvalues of the adjacency matrix A_{G_i}, $\lambda_{i,1} = r_i \geq \lambda_{i,2} \geq \lambda_{i,2} \geq \cdots \geq \lambda_{i,n_i}$. The distance spectrum of $G_1\nabla G_2$ consists of eigenvalues $-\lambda_{i,j} - 2$ for $i = 1, 2$ and $j = 2, 3, \ldots, n_i$ and two more eigenvalues of the form*

$$n_1 + n_2 - 2 - \frac{r_1 + r_2}{2} \pm \sqrt{\left(n_1 - n_2 - \frac{r_1 - r_2}{2}\right)^2 + n_1 n_2}. \tag{1}$$

Proof. The distance matrix D of the join $G_1\nabla G_2$ has the form

$$D = \begin{bmatrix} 2(J - I) - A_{G_1} & J_{n_1\times n_2} \\ J_{n_2\times n_1} & 2(J - I) - A_{G_2} \end{bmatrix}.$$

As a regular graph, G_1 has the all-one vector j as an eigenvector corresponding to eigenvalue r_1, while all other eigenvectors are orthogonal to j. (Note that G_1 need not be connected, and thus, r_1 need not be a simple eigenvalue of G_1.)

Let λ be an arbitrary eigenvalue of the adjacency matrix of G_1 with corresponding eigenvector x, such that $j^{\mathsf{T}}x = 0$. Then $\left(x\ 0_{n_2\times 1}\right)^\top$ is the eigenvector of D corresponding to eigenvalue $-\lambda-2$. A similar argument holds for an arbitrary eigenvalue μ of A_{G_2}, with the corresponding eigenvector y such that $j^{\mathsf{T}}y = 0$. In this way, forming the eigenvectors of the forms $(x\ 0)^\top$ and $(0\ y)^\top$, we can construct a total of $n_1 + n_2 - 2$ mutually orthogonal eigenvectors of D. All of these eigenvectors are orthogonal to the vectors $(j\ 0)^\top$ and $(0\ j)^\top$, which means that they are spanned by the remaining two eigenvectors of D. This implies that the two remaining eigenvectors of D have the form $(\alpha j\ \beta j)^\top$ for a suitable choice of α and β.

Suppose now that ν is an eigenvalue of D with an eigenvector of the form $(\alpha j\ \beta j)^\top$. Then, from $D\,(\alpha j\ \beta j)^\top = \nu\,(\alpha j\ \beta j)^\top$, using $A_{G_1}j = r_1 j$ and $A_{G_2}j = r_2 j$, we get the system

$$(2n_1 - r_1 - 2)\alpha + n_2\beta = \nu\alpha,$$
$$n_1\alpha + (2n_2 - r_2 - 2)\beta = \nu\beta.$$

Eliminating α and β we get the quadratic equation in ν

$$\nu^2 - \nu\left((2n_1 - r_1 - 2) + (2n_2 - r_2 - 2)\right) + (2n_1 - r_1 - 2)(2n_2 - r_2 - 2) - n_1 n_2 = 0,$$

whose solutions are given by (1). One easily checks that these two solutions are indeed the remaining two eigenvalues of D. □

Note that the complete bipartite graph $K_{m,n}$ is isomorphic to a join $\bar{K}_m\nabla\bar{K}_n$ of the empty graphs $\bar{K}_m$ and $\bar{K}_n$. Hence,

Corollary 3. *The distance spectrum of the complete bipartite graph $K_{m,n}$ consists of simple eigenvalues $m + n - 2 \pm \sqrt{m^2 - mn + n^2}$ and an eigenvalue -2 with multiplicity $m + n - 2$.*

If $m, n \geq 2$, then $m + n - 2 \geq \sqrt{m^2 - mn + n^2}$ and we get

Corollary 4. *$DE(K_{m,n}) = 4(m + n - 2)$ for $m, n \geq 2$.*

So, any two complete bipartite graphs with the same number of vertices, apart from stars, have the same distance energy. Since the distance eigenvalues different from -2 uniquely determine parameters m and n, different complete bipartite graphs have different distance spectra. Thus, our simplest family of sets of DE-equienergetic graphs is given by

$$\{\{K_{2,n-2}, K_{3,n-3}, \ldots, K_{\lfloor n/2\rfloor,\lceil n/2\rceil}\}: n \geq 4\}.$$

The key to the successful application of Theorem 2 lies in regular graphs for which most (if not all) adjacency eigenvalues are at least -2, and so the corresponding eigenvalue $-\lambda - 2$ of the distance matrix is always negative. Such graphs are, for example, the empty graph $\bar{K}_m$, the complete graph K_m, the complete bipartite graph $K_{m/2,m/2}$ for even m, the cycle C_m, as well as regular line graphs [10] (which are themselves line graphs of regular or semiregular graphs). For such graphs, we can use the well-known fact that the sum of all adjacency eigenvalues is zero (see, e.g., [10]) in order to determine the distance energy of their join.

Theorem 5. *For $i = 1, 2$, let G_i be an r_i-regular graph with n_i vertices, whose smallest eigenvalue of the adjacency matrix is at least -2 and such that $G_i \ncong K_n$. Then*

$$DE(G_1\nabla G_2) = 4(n_1 + n_2) - 2(r_1 + r_2) - 8.$$

Proof. For $i = 1, 2$, denote the eigenvalues of the adjacency matrix A_{G_i} by $\lambda_{i,1} = r_i \geq \lambda_{i,2} \geq \cdots \geq \lambda_{i,n_i}$. According to Theorem 2, the distance eigenvalues of $G_1\nabla G_2$ are

$$n_1 + n_2 - 2 - \frac{r_1 + r_2}{2} \pm \sqrt{\left(n_1 - n_2 - \frac{r_1 - r_2}{2}\right)^2 + n_1 n_2}. \tag{2}$$

and $-\lambda_{i,j} - 2$ for $i = 1, 2$ and $j = 2, 3, \ldots, n_i$. The eigenvalues given by (2) are both nonnegative: since G_1 and G_2 are not complete, we have $n_1 \geq r_1 + 2$ and $n_2 \geq r_2 + 2$, and so

$$(2n_1 - r_1 - 2)(2n_2 - r_2 - 2) \geq n_1 n_2.$$

Adding $((n_1 - r_1/2) - (n_2 - r_2/2))^2$ to both sides, we get

$$((n_1 - r_1/2) + (n_2 - r_2/2) - 2)^2 \geq ((n_1 - r_1/2) - (n_2 - r_2/2))^2 + n_1 n_2,$$

i.e., $n_1 + n_2 - 2 - \frac{r_1+r_2}{2} - \sqrt{\left(n_1 - n_2 - \frac{r_1-r_2}{2}\right)^2 + n_1 n_2} \geq 0$. Thus, the sum of absolute values of eigenvalues (2) is equal to $(2n_1 - r_1 - 2) + (2n_2 - r_2 - 2)$.

For the remaining eigenvalues of $G_1\nabla G_2$, from $\lambda_{i,j} \geq -2$ we have that $|-\lambda_{i,j} - 2| = \lambda_{i,j} + 2$ and therefore,

$$\begin{aligned}\sum_{j=2}^{n_1} |-\lambda_{1,j} - 2| + \sum_{j=2}^{n_1} |-\lambda_{2,j} - 2| &= \left(\sum_{j=2}^{n_1} \lambda_{1,j}\right) + 2(n_1 - 1) + \left(\sum_{j=2}^{n_2} \lambda_{2,j}\right) + 2(n_2 - 1) \\ &= -r_1 + 2(n_1 - 1) - r_2 + 2(n_2 - 1).\end{aligned}$$

We conclude that the distance energy of $G_1\nabla G_2$ is $2(2n_1 - r_1 - 2) + 2(2n_2 - r_2 - 2)$. $\square$

This result can be used to find new families of equienergetic graphs easily. For example, for constant sum $m + n$ we have the following sets of DE-equienergetic graphs:

$$DE\left(\bar{K}_m \nabla \frac{n}{2} K_2\right) = 4(m + n) - 10 \quad \text{for even } n,$$
$$DE\left(\bar{K}_m \nabla C_n\right) = 4(m + n) - 12,$$
$$DE\left(\frac{m}{2} K_2 \nabla \frac{n}{2} K_2\right) = 4(m + n) - 12, \quad \text{for even } m \text{ and } n,$$
$$DE\left(\frac{m}{2} K_2 \nabla C_n\right) = 4(m + n) - 14, \quad \text{for even } m,$$
$$DE\left(C_m \nabla C_n\right) = 4(m + n) - 16,$$

3. The join of a regular graph with the union of regular graphs

A computer search for pairs of DE-equienergetic graphs revealed that, among others, the wheel $W_9 \cong K_1\nabla C_8$ and $K_1\nabla(C_5 \cup K_3)$, which are DE-equienergetic by Theorem 5, are also DE-equienergetic to $K_1\nabla(C_4 \cup K_4)$. However, $C_4 \cup K_4$ is not regular, but rather a union of regular graphs. Motivated by this example, we consider the distance spectrum of the graph $G_0\nabla(G_1 \cup G_2)$, where G_0, G_1 and G_2 are regular graphs. If G_1 and G_2 have equal vertex degrees, then the distance spectrum of $G_0\nabla(G_1 \cup G_2)$ is given by Theorem 2. Thus, we consider the case when G_1 and G_2 have distinct vertex degrees only.

Theorem 6. *For $i = 0, 1, 2$, let G_i be an r_i-regular graph with n_i vertices and eigenvalues $\lambda_{i,1} = r_i \geq \lambda_{i,2} \geq \lambda_{i,2} \geq \cdots \geq \lambda_{i,n_i}$ of the adjacency matrix A_{G_i}. If $r_1 \neq r_2$, then the distance spectrum of $G_0\nabla(G_1 \cup G_2)$ consists of eigenvalues $-\lambda_{i,j} - 2$ for $i = 0, 1, 2$ and $j = 2, 3, \ldots, n_i$ and three more eigenvalues which are solutions of the cubic equation in ν:*

$$(2n_0 - r_0 - 2 - \nu)(\nu + r_1 + 2)(\nu + r_2 + 2) + [2(\nu + r_0 + 2) - 3n_0][n_1(\nu + r_2 + 2) + n_2(\nu + r_1 + 2)] = 0. \tag{3}$$

Proof. The distance matrix of $G_0\nabla(G_1 \cup G_2)$ has the form

$$D = \begin{bmatrix} 2(J - I) - A_{G_0} & J & J \\ J & 2(J - I) - A_{G_1} & 2J \\ J & 2J & 2(J - I) - A_{G_2} \end{bmatrix}.$$

By analogy to the proof of Theorem 2, to every eigenvalue λ of A_{G_i} with corresponding eigenvector x, such that $j^{\top}x = 0$, there corresponds an eigenvalue $-\lambda - 2$ of D with eigenvector of D obtained by putting vector x at the coordinates corresponding to G_i and zeros at the remaining coordinates. The $n_0 + n_1 + n_2 - 3$ eigenvectors so obtained are mutually orthogonal, and also orthogonal to the vectors $\left(j\, 0_{n_1\times 1}\, 0_{n_2\times 1}\right)^{\top}$, $\left(0_{n_0\times 1}\, j\, 0_{n_2\times 1}\right)^{\top}$, $\left(0_{n_0\times 1}\, 0_{n_1\times 1}\, j\right)^{\top}$. Thus, the three remaining eigenvectors of D have the form $(\alpha j\ \beta j\ \gamma j)^{\top}$ for some $(\alpha, \beta, \gamma) \neq (0, 0, 0)$.

If ν is an eigenvalue of D with an eigenvector $(\alpha j\ \beta j\ \gamma j)^{\top}$, from $D\,(\alpha j\ \beta j\ \gamma j)^{\top} = \nu\,(\alpha j\ \beta j\ \gamma j)^{\top}$, and $A_{G_i}j = r_i j$ for $i = 0, 1, 2$, we get the system

$$\alpha(2n_0 - r_0 - 2) + \beta n_1 + \gamma n_2 = \nu\alpha, \tag{4}$$

$$\alpha n_0 + \beta(2n_1 - r_1 - 2) + 2\gamma n_2 = \nu\beta, \tag{5}$$

$$\alpha n_0 + 2\beta n_1 + \gamma(2n_2 - r_2 - 2) = \nu\gamma. \tag{6}$$

Assuming $\alpha = 0$ in (4)–(6), after simplifying, leads to $(r_1 - r_2)\gamma = (r_1 - r_2)\beta = 0$, which, due to $r_1 \neq r_2$, implies that $\beta = \gamma = 0$, a contradiction.

Suppose, without loss of generality, that $\alpha = 1$. Solving for β and γ and substituting solutions back into (4) yields a cubic equation (3) whose solutions, as easily seen, represent the three remaining eigenvalues of D. □

The cubic equation (3), provided $n_0 > r_0 + 2$, $n_1 \geq r_1 + 2$ and $r_1 > r_2$, has a positive solution between 0 and $2n_0 - r_0 - 2$, and a negative solution between $-r_1 - 2$ and $-r_2 - 2$. Thus, one cannot find $|\nu_1| + |\nu_2| + |\nu_3|$ without explicitly knowing the values of ν_1, ν_2 and ν_3.

Even so, Theorem 6 can be used to provide new families of sets of *DE*-equienergetic graphs. The main points to observe are, firstly, that the graphs G_0, G_1 and G_2 need not be connected (the only fact used in the proofs of Theorems 2 and 6 is that these graphs have the all-one vector j as an eigenvector of adjacency matrix), and, secondly, that the solutions of (3) depend only on $n_0, r_0, n_1, r_1, n_2, r_2$, and not on the structure of G_0, G_1 and G_2. Thus, we can create a set of *DE*-equienergetic graphs whenever we can iterate one of the graphs, say G_1, through a set of regular graphs with fixed values of n_1 and r_1.

For example, let G be an arbitrary, but fixed, regular graph with least eigenvalue at least -2. Further, for fixed $n \in \mathbf{N}$, let $\mathcal{P}_n$ be the set of integer partitions of n into parts of size at least 3. For $P = \{p_1, \ldots, p_k\} \in \mathcal{P}_n$, we denote by $\mathcal{C}_P$ the union of cycles with sizes $p_1, \ldots, p_k$. Now, Theorem 6 implies the following:

Corollary 7. *Graphs $K_1 \nabla (\mathcal{C}_P \cup G)$, $P \in \mathcal{P}_n$, form a set of DE-equienergetic graphs.*

Proof. Let G be an r-regular graph with m vertices and eigenvalues of the adjacency matrix $\lambda_1 = r \geq \lambda_2 \geq \cdots \geq \lambda_m$. For $P \in \mathcal{P}_n$, the graph $\mathcal{C}_P$ is 2-regular with n vertices. From Theorem 6, the distance eigenvalues of $K_1 \nabla (\mathcal{C}_P \cup G)$ are the solutions of the cubic equation

$$-\nu(\nu + 4)(\nu + r + 2) + (2\nu + 1)[n(\nu + r + 2) + m(\nu + 4)] = 0, \tag{7}$$

the values $-\lambda_i - 2$ for $i = 2, 3, \ldots, m$, and the values $-2\cos\frac{\pi j}{p_i} - 2$, for $p_i \in P$, $0 \leq j \leq p_i$ and $(i, j) \neq (1, 0)$ (to exclude an eigenvalue of $\mathcal{C}_P$ corresponding to the all-one eigenvector).

Let $f(n, m, r)$ be the sum of absolute values of the three solutions of (7). From the proof of Theorem 5 we know that $\sum_{i=2}^{m} |-\lambda_i - 2| = 2m - r - 2$, while the sum of $|-2\cos\frac{\pi j}{p_i} - 2|$ for $p_i \in P$ and $j = 0, \ldots, p_i$, $(i, j) \neq (1, 0)$, is equal to $2n - 4$. Thus, $DE(K_1 \nabla (\mathcal{C}_P \cup G)) = f(n, m, r) + 2n + 2m - r - 6$, regardless of the partition $P \in \mathcal{P}_n$. □

4. Concluding remarks

We have seen that the compositions of regular graphs based on the join of graphs yield a number of families containing large sets of *DE*-equienergetic graphs. However, the families presented here consist of dense graphs. Among sparse graphs, it is natural to start looking among trees for examples of *DE*-equienergetic graphs. We were surprised to find that

There exists no pair of noncospectral DE-equienergetic trees up to 20 *vertices.*

Trees have exactly one positive distance eigenvalue [11,12]. Other classes of graphs with exactly one positive distance eigenvalue include the hypermetric graphs and the graphs of negative type [13], connected bipartite graphs that are hypercube embeddable, as well as median graphs, which are the retracts of hypercubes and can be recognized in polynomial time [14].

Hence, the distance energy of a tree is twice the unique positive distance eigenvalue. The above observation then leads to the question of whether the positive distance eigenvalue determines the whole distance spectrum of a tree. More generally, to what extent does the positive distance eigenvalue characterize a tree?

Acknowledgement

The authors are indebted to an anonymous referee whose comments led to an improved presentation of the results.

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