dMFA

ARS MATHEMATICA CONTEMPORANEA

Also available at http://amc.imfm.si
ISSN 1855-3966 (printed edn.), ISSN 1855-3974 (electronic edn.)
ARS MATHEMATICA CONTEMPORANEA 2 (2009) 35–40

Large sets of long distance equienergetic graphs*

Dragan Stevanović

University of Primorska — FAMNIT, Glagoljaška 8, 6000 Koper, Slovenia
and
Mathematical Institute, Serbian Academy of Science and Arts,
Knez Mihajlova 36, 11000 Belgrade, Serbia

Received 2 December 2008, accepted 2 January 2009, published online 11 March 2009

Abstract

Distance energy of a graph is a recent energy-type invariant, defined as the absolute deviation of the eigenvalues of the distance matrix of the graph. Two graphs of the same order are said to be distance equienergetic if they have equal distance energy, while they have distinct spectra of their distance matrices. Examples of pairs of distance equienergetic graphs appear in the literature already, but most of them have diameter two only.

We describe here the distance spectrum of a special composition of regular graphs, and, as an application, we show that for any $n \geq 3$, there exists a set of $n+1$ distance equienergetic graphs which have order $6n$ and diameter $n-1$ each.

Keywords: Distance spectrum, distance energy, join, regular graphs.

Math. Subj. Class.: 05C50

1 Introduction

Let $G = (V, E)$ be a simple graph with n vertices $V = \{v_1, v_2, \ldots, v_n\}$. The energy of a graph $E = E(G) = \sum_{i=1}^{n} |\lambda_i|$, where λ_i, $i = 1, \ldots, n$ are the eigenvalues of an adjacency matrix of G, has well-known chemical applications [3, 4, 5, 6]. Following the recent definition of the Laplacian energy in [7], 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. Let $d_G(v_i, v_j)$ denote the length of the shortest path between the vertices v_i and v_j of G. The matrix $D(G) = (d_G(v_i, v_j))$, indexed by the vertices of G, is the *distance matrix* of G. Since its trace is zero, we can define the *distance energy* $DE(G)$ of G as the sum of absolute values of the eigenvalues of the distance matrix $D(G)$. The distance energy, together with a handful of other invariants, has been studied by Consonni and

*This work was supported by the research program P1-0285 of the Slovenian Agency for Research and the research grant 144015G of the Serbian Ministry of Science.

E-mail address: dragan.stevanovic@upr.si (Dragan Stevanović)

Todeschini [1] for possible use in QSPR modelling. Their study reveals that the distance energy is a useful molecular descriptor: the values $DE(G)$ or $DE(G)/n$ appear among the best univariate models for the motor octane number of the octane isomers or the water solubility of polychlorobiphenyls.

Two graphs of the same order are said to be distance equienergetic if they have equal distance energy, while they have distinct distance spectra. Examples of distance equienergetic graphs appear in the literature [8, 9, 10], but most of them have diameter two only. We show here that new pairs of distance equienergetic graphs can be constructed as compositions of regular graphs.

The particular composition that we consider is defined as follows. Let $G_i = (V_i, E_i)$, $i = 1, \ldots, n$ be arbitrary finite graphs. The *joined union* $G[G_1, \ldots, G_n]$ is the graph $H = (W, F)$ with:

$$\begin{aligned} W &= \bigcup_{i=1}^{n} V_i, \\ F &= \bigcup_{i=1}^{n} E_i \cup \bigcup_{(v_i,v_j)\in E} V_i \times V_j. \end{aligned}$$

In other words, the joined union is obtained from the union of graphs $G_1, \ldots, G_n$ by joining with an edge each pair of a vertex from G_i and a vertex from G_j whenever v_i and v_j are adjacent in G. For example, the usual join of two graphs G and H is a special case of the joined union: $K_2[G, H]$, where K_2 is the complete graph on two vertices.

In the next section, we describe the distance spectrum of the joined union of regular graphs in the terms of their adjacency spectrum and the eigenvalues of the auxiliary matrix, determined by the graph G. Then in Section 3 we show that the sets of graphs with equal distance energy can be constructed as a joined union of regular graphs for which all adjacency eigenvalues are at least -2. As an example, we show that for any $n \geq 3$, there exists a set of $n + 1$ distance equienergetic graphs which have order $6n$ and diameter $n - 1$ each.

2 The distance spectrum of the joined union

Theorem 2.1. *Let $G = (V, E)$ be a simple graph with n vertices $v_1, \ldots, v_n$, and for $i = 1, \ldots, n$, let $G_i = (V_i, E_i)$ be an r_i-regular graph of order m_i and eigenvalues of the adjacency matrix A_{G_i}: $\lambda_{i,1} = r_i \geq \lambda_{i,2} \geq \cdots \geq \lambda_{i,m_i}$. The distance spectrum of the joined union $G[G_1, \ldots, G_n]$ consists of the eigenvalues $-\lambda_{i,j} - 2$ for $i = 1, \ldots, n$ and $j = 2, 3, \ldots, m_i$ and the eigenvalues of the matrix*

$$\begin{bmatrix} 2m_1 - r_1 - 2 & d_G(v_1, v_2)m_2 & d_G(v_1, v_3)m_3 & \ldots & d_G(v_1, v_n)m_n \\ d_G(v_2, v_1)m_1 & 2m_2 - r_2 - 2 & d_G(v_2, v_3)m_3 & \ldots & d_G(v_2, v_n)m_n \\ d_G(v_3, v_1)m_1 & d_G(v_3, v_2)m_2 & 2m_3 - r_3 - 2 & \ldots & d_G(v_3, v_n)m_n \\ \ldots & \ldots & \ldots & & \ldots \\ d_G(v_n, v_1)m_1 & d_G(v_n, v_2)m_2 & d_G(v_n, v_3)m_3 & \ldots & 2m_n - r_n - 2 \end{bmatrix}. \quad (2.1)$$

Proof. The distance matrix $D(H)$ of the joined union $H = G[G_1, \ldots, G_n]$ is a block

matrix of the form

$$D(H) = \begin{bmatrix} 2(J-I) - A_{G_1} & d_G(v_1,v_2)J & \dots & d_G(v_1,v_n)J \\ d_G(v_2,v_1)J & 2(J-I) - A_{G_2} & \dots & d_G(v_2,v_n)J \\ \dots & \dots & \dots & \dots \\ d_G(v_n,v_1)J & d_G(v_n,v_2)J & \dots & 2(J-I) - A_{G_n} \end{bmatrix},$$

where I and J are the unit and the all-one matrices of corresponding orders.

First, let $i \in \{1,\dots,n\}$. As a regular graph, G_i has all-one vector j as an eigenvector of the adjacency matrix A_{G_i} corresponding to the eigenvalue r_i, while other eigenvectors are orthogonal to j. (Note that G_i need not be connected, and thus, r_i need not be a simple eigenvalue of G_i.) Let λ be an arbitrary eigenvalue of A_{G_i} with the corresponding eigenvector x, such that $j^T x = 0$. Then the vector y, given by

$$y_u = \begin{cases} x_u, & u \in V_i \\ 0, & u \notin V_i \end{cases}$$

is an eigenvector of $D(H)$ corresponding to the eigenvalue $-\lambda - 2$: since y has zeros at coordinates corresponding to $\bigcup_{j\neq i} V_j$, we have

$$D(H)y = \begin{bmatrix} d_G(v_1,v_i)J \\ \dots \\ d_G(v_{i-1},v_i)J \\ 2(J-I) - A_{G_i} \\ d_G(v_{i+1},v_i)J \\ \dots \\ d_G(v_n,v_i)J \end{bmatrix} x = \begin{pmatrix} d_G(v_1,v_i)Jx \\ \dots \\ d_G(v_{i-1},v_i)Jx \\ 2Jx - 2x - A_{G_i}x \\ d_G(v_{i+1},v_i)Jx \\ \dots \\ d_G(v_n,v_i)Jx \end{pmatrix} = -(2+\lambda)y.$$

There exists a total of $(\sum_{i=1}^n |V_i|) - n$ mutually orthogonal eigenvectors of $D(H)$ of this form. Moreover, they are all orthogonal to the vectors

$$(j^i)_u = \begin{cases} 1, & u \in V_i \\ 0, & u \notin V_i \end{cases} \qquad i = 1,\dots,n.$$

In particular, this means that the vectors j^1, j^2, …, j^n are spanned by the n remaining eigenvectors of $D(H)$, which, due to the fact that j^1, j^2, …, j^n are linearly independent, implies that the remaining eigenvectors of $D(H)$ have the form $\sum_{i=1}^n \alpha_i j^i$ for suitable coefficients α_1,…,α_n.

Let ν be an eigenvalue of $D(H)$ with an eigenvector of the form $\sum_{i=1}^n \alpha_i j^i$. Then from $A_{G_i} j = r_i j$, $i = 1,\dots,n$, we have

$$\begin{aligned} D(H)\sum_{i=1}^n \alpha_i j^i &= \sum_{i=1}^n \alpha_i D(H) j^i = \sum_{i=1}^n \alpha_i \begin{bmatrix} d_G(v_1,v_i)J \\ \dots \\ d_G(v_{i-1},v_i)J \\ 2(J-I) - A_{G_i} \\ d_G(v_{i+1},v_i)J \\ \dots \\ d_G(v_n,v_i)J \end{bmatrix} j \\ &= \sum_{i=1}^n \alpha_i \left((2m_i - r_i - 2)j^i + \sum_{k\neq i} d_G(v_k,v_i) m_i j^k \right) \end{aligned}$$

$$= \sum_{i=1}^{n} \left((2m_i - r_i - 2)\alpha_i + \sum_{k \neq i} d_G(v_i, v_k) m_k \alpha_k \right) j^i = \nu \sum_{i=1}^{n} \alpha_i j^i.$$

From the last equality we get the system of equations in $\alpha_1, \ldots, \alpha_n$:

$$(2m_i - r_i - 2 - \nu)\alpha_i + \sum_{k \neq i} d_G(v_i, v_k) m_k \alpha_k = 0, \qquad i = 1, \ldots, n, \tag{2.2}$$

which may have a nontrivial solution only if its determinant is equal to zero, i.e., only if ν is an eigenvalue of (2.1). Further, it is obvious from above that any nontrivial solution of (2.2) forms an eigenvector of $D(H)$ corresponding to eigenvalue ν. Since all n remaining eigenvectors of $D(H)$ must be formed in this way, we conclude that each eigenvalue of (2.1) is an eigenvalue of $D(H)$ as well. □

For example, let G be an r_1-regular graph of order n_1 and the eigenvalues $\lambda_1 = r_1 \geq \lambda_2 \geq \cdots \geq \lambda_{n_1}$ of its adjacency matrix, and let H be an r_2-regular graph of order n_2 and the eigenvalues $\mu_1 = r_2 \geq \mu_2 \geq \cdots \geq \mu_{n_2}$ of its adjacency matrix. From the previous theorem, the distance spectrum of the join $G \nabla H$, which is the same as $K_2[G, H]$, consists of the eigenvalues $-\lambda_i - 2$ for $i = 2, \ldots, n_1$, then $-\mu_j - 2$ for $j = 2, \ldots, n_2$, and two eigenvalues $(m_1 - r_1/2) + (m_2 - r_2/2) - 2 \pm \sqrt{((m_1 - r_1/2) - (m_2 - r_2/2))^2 + m_1 m_2}$.

3 Long distance equienergetic graphs

Sets of graphs with equal distance energy can be constructed as a joined union of regular graphs for which all adjacency eigenvalues are at least -2, when the corresponding eigenvalues $-\lambda - 2$ of the distance matrix are always negative. Such graphs are, for example, the empty graph $\overline{K}_m$, the complete graph K_m, the cycle C_m, as well as regular line graphs [2] (which are itself 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 0 (see, e.g., [2]) in order to determine the distance energy of the joined union.

Theorem 3.1. *Let $G = (V, E)$ be a simple graph with n vertices $v_1, \ldots, v_n$, and for $i = 1, \ldots, n$, let G_i and H_i be r_i-regular graphs of order m_i whose smallest eigenvalue of the adjacency matrix is at least -2. Then*

$$DE(G[G_1, \ldots, G_n]) = DE(G[H_1, \ldots, H_n]).$$

Proof. Since graphs G_i and H_i, $i = 1, \ldots, n$, have the same order m_i and the degree r_i, both joined unions $G[G_1, \ldots, G_n]$ and $G[H_1, \ldots, H_n]$ have the same auxiliary matrix

$$\begin{bmatrix} 2m_1 - r_1 - 2 & d_G(v_1, v_2)m_2 & d_G(v_1, v_3)m_3 & \ldots & d_G(v_1, v_n)m_n \\ d_G(v_2, v_1)m_1 & 2m_2 - r_2 - 2 & d_G(v_2, v_3)m_3 & \ldots & d_G(v_2, v_n)m_n \\ d_G(v_3, v_1)m_1 & d_G(v_3, v_2)m_2 & 2m_3 - r_3 - 2 & \ldots & d_G(v_3, v_n)m_n \\ \ldots & \ldots & \ldots & & \ldots \\ d_G(v_n, v_1)m_1 & d_G(v_n, v_2)m_2 & d_G(v_n, v_3)m_3 & \ldots & 2m_n - r_n - 2 \end{bmatrix},$$

so that the corresponding part of their distance spectra is equal, and adds the same amount M to the distance energy of joined unions.

Next, for $i = 1, \ldots, n$, let G_i has eigenvalues of the adjacency matrix $\lambda_{i,1} = r_i \geq \lambda_{i,2} \geq \cdots \geq \lambda_{i,m_i} \geq -2$, and let H_i has eigenvalues of the adjacency matrix $\mu_{i,1} = r_i \geq \mu_{i,2} \geq \cdots \geq \mu_{i,m_i} \geq -2$. The remaining distance eigenvalues of $G[G_1, \ldots, G_n]$ are of the form $-\lambda_{i,j} - 2$ for $i = 1, \ldots, n$ and $j = 2, \ldots, m_i$. Since $\lambda_{i,j} \geq -2$ we have that $|-\lambda_{i,j} - 2| = \lambda_{i,j} + 2$. Then from $\sum_{j=1}^{m_i} \lambda_{i,j} = 0$, we get

$$\sum_{i=1}^{n} \sum_{j=2}^{m_i} |-\lambda_{i,j} - 2| = \sum_{i=1}^{n} \left(\sum_{j=2}^{m_i} \lambda_{i,j} \right) + 2(m_i - 1) = \sum_{i=1}^{n} -r_i + 2(m_i - 1).$$

For the remaining distance eigenvalues $-\mu_{i,j} - 2$ of $G[H_1, \ldots, H_n]$, $i = 1, \ldots, n$, $j = 2, \ldots, m_i$, we similarly get

$$\sum_{i=1}^{n} \sum_{j=2}^{m_i} |-\mu_{i,j} - 2| = \sum_{i=1}^{n} -r_i + 2(m_i - 1).$$

Therefore,

$$DE(G[G_1, \ldots, G_n]) = M + \sum_{i=1}^{n} 2m_i - r_i - 2 = DE(G[H_1, \ldots, H_n]). \qquad \square$$

In the above theorem, the graphs $G[G_1, \ldots, G_n]$ and $G[H_1, \ldots, H_n]$ share the auxiliary matrix and have a common part of the distance spectra. Therefore, in order for these graphs to be distance equienergetic, it is necessary that the union of adjacency spectra of $G_1, \ldots, G_n$, with vertex degree being deleted from each adjacency spectrum, is different from the union of adjacency spectra of $H_1, \ldots, H_n$.

Example

Let P_n and C_n be the path and the cycle of order n, respectively. As an application of Theorem 3.1, we observe that, for each $n \geq 3$, the following is a set of $n + 1$ distance equienergetic graphs of order $6n$ and diameter $n - 1$:

$$\begin{aligned}
\{ \quad & P_n[C_6, C_6, \ldots, C_6, C_6], \\
& P_n[C_6, C_6, \ldots, C_6, C_3 \cup C_3], \\
& P_n[C_6, C_6, \ldots, C_3 \cup C_3, C_3 \cup C_3], \\
& \ldots, \\
& P_n[C_6, C_3 \cup C_3, \ldots, C_3 \cup C_3, C_3 \cup C_3], \\
& P_n[C_3 \cup C_3, C_3 \cup C_3, \ldots, C_3 \cup C_3, C_3 \cup C_3] \qquad \}.
\end{aligned}$$

Since both C_6 and $C_3 \cup C_3$ are 2-regular graphs of order 6, all graphs above have the same auxiliary matrix (2.1), and thus, share this part of the distance spectra. The remaining part of the distance spectrum of $P_n[\underbrace{C_6, \ldots, C_6}_{k}, \underbrace{C_3 \cup C_3, \ldots, C_3 \cup C_3}_{n-k}]$, $0 \leq k \leq n$, is

$$[-4^{n-k}, -3^{2k}, -1^{4n-2k}, 0^k],$$

with exponents denoting the multiplicities, showing that no two graphs above are cospectral.

References

[1] V. Consonni and R. Todeschini, New Spectral Indices for Molecule Description, *MATCH Commun. Math. Comput. Chem.* **60** (2008), 3–14.

[2] D. Cvetković, M. Doob and H. Sachs, Spectra of Graphs—Theory and Application, 3rd edition, Johann Ambrosius Barth Verlag, 1995.

[3] I. Gutman, The energy of a graph, *Ber. Math. Statist. Sekt. Forschungsz. Graz* **103** (1978), 1–22.

[4] I. Gutman, The energy of a graph: old and new results, in: A. Betten, A. Kohnert, R. Laue and A. Wassermann (eds.), *Algebraic Combinatorics and Applications*, Springer-Verlag, Berlin, 2001, 196–211.

[5] I. Gutman, Topology and stability of conjugated hydrocarbons. The dependence of total π-electron energy on molecular topology, *J. Serb. Chem. Soc.* **70** (2005), 441–456.

[6] I. Gutman, Total π-electron energy of benzenoid hydrocarbons, *Topics Curr. Chem.* **162** (1992), 29–63.

[7] I. Gutman and B. Zhou, Laplacian energy of a graph, *Linear Algebra Appl.* **414** (2006), 29–37.

[8] G. Indulal and I. Gutman, On the distance spectra of some graphs, *Math. Commun.—Univ. of Croatia* **13** (2008), 123–131.

[9] G. Indulal, I. Gutman and A. Vijayakumar, On Distance Energy of Graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008), 461–472.

[10] H. S. Ramane, I. Gutman and D. S. Revankar, Distance Equienergetic Graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008), 473–484.