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Published on: 01 Jan 2009 - Filomat (National Library of Serbia)

Topics: Incidence matrix

Faculty of Sciences and Mathematics, University of Niš, Serbia
Available at: `http://www.pmf.ni.ac.rs/filomat`

Filomat **23:3** (2009), 243–249 DOI:10.2298/FIL0903243S

ON THE ORIENTED INCIDENCE ENERGY AND DECOMPOSABLE GRAPHS*

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Abstract

Let G be a simple graph with n vertices and m edges. Let edges of G be given an arbitrary orientation, and let Q be the vertex-edge incidence matrix of such oriented graph. The oriented incidence energy of G is then the sum of singular values of Q. We show that for any $n \in N$, there exists a set of n graphs with $O(n)$ vertices having equal oriented incidence energy.

1 Introduction

Let $G = (V, E)$ be a finite, simple, undirected graph with vertices $V = \{1, 2, \ldots, n\}$ and $m = |E|$ edges. Let G have adjacency matrix A with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The energy of G was defined by Gutman in [1] as

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

and it has a long known chemical applications; for details see the surveys [2, 3, 4]. Recently, Nikiforov [5] generalized a concept of graph energy to arbitrary matrix M by defining the energy $E(M)$ to be the sum of singular values of M. The singular values of a real (not necessarily square) matrix M are the square roots of the eigenvalues of the (square) matrix MM^T, where M^T denotes the transpose of M.

Let edges of G be given an arbitrary orientation producing an oriented graph $\overrightarrow{G}$, and let Q be the vertex-edge incidence matrix of $\overrightarrow{G}$, whose (v, e) entry is equal to $+1$ if the vertex v is the head of the oriented edge e, -1 if v is the tail of e, and 0 otherwise. Then $QQ^T = L = D - A$ is the Laplacian matrix of G, where

*This work was supported by the research grant 144015G of Serbian Ministry of Science and in part by Grant 300563/94-9 of National Research Council of Brazil..

2000 *Mathematics Subject Classifications.* 05C50.

Key words and Phrases. Laplacian-like energy, Incidence energy, Decomposable graphs.

Received: October 20, 2009

Communicated by Dragan Stevanović

D is the diagonal matrix of vertex degrees [6, 7]. Suppose that L has eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$. The oriented incidence energy of G is then

$$OIE(G) = E(Q) = \sum_{i=1}^{n} \sqrt{\mu_i},$$

as observed in [8]. This invariant was introduced recently by Liu and Liu [9] under the name *the Laplacian energy-like invariant* and notation $LEL(G)$.

Due to its definition, it comes as no surprise that $OIE(G)$ has a number of properties analogous to $E(G)$ [9, 10]. $OIE(G)$ was suggested as a new molecular descriptor in [11]: a correlating study of OIE and topological indices provided by TOPOCLUJ software package [12], on thirteen properties of octanes, revealed that OIE describes well the properties which are well accounted by the Wiener-based molecular descriptors: octane number MON, entropy S, volume MV, or refraction MR, particularly the AF parameter, but also more difficult properties like boiling point BP, melting point MP and logP. In a second set of polycyclic aromatic hydrocarbons, OIE was proved to be as good as the Randić index and better than the Wiener index in correlations to BP, MP and logP.

A graph is *decomposable* if it can be contructed from isolated vertices by the operations of union and complement. The Laplacian spectrum of $G_1 \cup \cdots \cup G_k$ is the union of Laplacian spectra of $G_1, \ldots, G_k$, while the Laplacian spectrum of the complement of n-vertex graph G consists of values $n - \mu$, for each Laplacian eigenvalue μ of G, except for a single instance of eigenvalue 0 of G. Since the Laplacian spectrum of an isolated vertex consists of single eigenvalue 0, it is easy to conclude that the Laplacian spectrum of every decomposable graph consists of integers only [13, 14].

Much work on graph energy has appeared in literature, especially in the last decade, and a good deal of it studies graphs with equal energy [15]-[24]. Two graphs G_1 and G_2 of the same order, noncospectral with respect to L, are said to be *OIE-equienergetic* if $OIE(G_1) = OIE(G_2)$. Three pairs of connected OIE-equienergetic graphs were presented in [25] and, based on the computer search among small graphs, it was suggested that OIE-equienergetic graphs occur relatively rarely. However, note that the graphs G_{802}, G_{804} and G_{1202} from [25] are all decomposable graphs. Our goal here is to show that, for any given $n \in N$, there exists a set of n mutually OIE-equienergetic decomposable graphs with $O(n)$ vertices.

Let $A = \{a_1, \ldots, a_k\}$ be a multiset of positive integers such that $a_i \geq 3$, $i = 1, \ldots, k$. The graph S_A^*, formed from the union of stars $S_{a_1-1}, S_{a_2-1}, \ldots, S_{a_k-1}$ by adding a vertex adjacent to all other vertices, has $n = \left(\sum_{i=1}^{k} a_i\right) - k + 1$ vertices and $m = 2n - k - 2$ edges. It is decomposable since it can be represented as

$$S_A^* = \overline{K_1 \cup \overline{\bigcup_{i=1}^{k} \overline{K_1 \cup \overline{a_{i-2}K_1}}}}$$

and its Laplacian spectrum is given by

$$[n, a_1, \dots, a_k, 2^{n-2k-1}, 1^{k-1}, 0],$$

where exponents denote multiplicities. Thus,

$$OIE(S_A^*) = \sqrt{n} + \sum_{i=1}^{k} \sqrt{a_i} + (n-2k-1)\sqrt{2} + k - 1. \qquad (2)$$

Let $\mathcal{S}$ be the set of of finite multisets of positive integers each of which is at least three. Let ρ be an equivalence relation on $\mathcal{S}$ defined by

$$A\,\rho\,B \quad \Leftrightarrow \quad |A| = |B|, \sum_{i=1}^{k} a_i = \sum_{i=1}^{k} b_i \text{ and } \sum_{i=1}^{k} \sqrt{a_i} = \sum_{i=1}^{k} \sqrt{b_i}.$$

From (2) we see that

$$A\,\rho\,B \quad \Rightarrow \quad OIE(S_A^*) = OIE(S_B^*).$$

Moreover, if A and B are distinct equivalent multisets, then the graphs S_A^* and S_B^* are noncospectral, while they have the same order and size.

Therefore, in order to construct sets of OIE-equienergetic decomposable graphs, we need to find nontrivial equivalence classes of ρ in $\mathcal{S}$. Construction of equivalence classes containing pairs of triplets is given in Section 2, while operations for constructing large equivalence classes in $\mathcal{S}/\rho$ are discussed in Section 3. A few nontrivial equivalence classes found by initial computer search are given in Table 1.

$\sum_i a_i = \sum_i b_i$	$\{a_1, \dots, a_k\}$	$\{b_1, \dots, b_k\}$	$\sum_i \sqrt{a_i} = \sum_i \sqrt{b_i}$
37	{25,6,6}	{24,9,4}	$5 + 2\sqrt{6}$
40	{27,9,4}	{25,12,3}	$5 + 3\sqrt{3}$
24	{12,4,4,4}	{9,9,3,3}	$6 + 2\sqrt{3}$
42	{20,9,9,4}	{16,16,5,5}	$8 + 2\sqrt{5}$
43	{27,4,4,4,4}	{25,9,3,3,3}	$8 + 3\sqrt{3}$

Table 1: A few equivalence classes in $\mathcal{S}$.

2 Equivalence classes containing triplets

Proposition 1. *Let a, b, c, d, e, f be positive integers such that $abc = def$. Then*

$$\{a^2c, b^2c, (d+e)^2 f\} \;\rho\; \{(a+b)^2 c, d^2 f, e^2 f\}.$$

Proof. Both multisets have three elements and the sum of square roots of their elements is equal to $(a+b)\sqrt{c}+(d+e)\sqrt{f}$. From $abc=def$ it follows that the sum of their elements are also equal,

$$(a^2+b^2)c+(d^2+e^2)f+2def=(a^2+b^2)c+2abc+(d^2+e^2)f,$$

so that these two triplets belong to the same equivalence class of ρ. ∎

For example, the first pair of triplets in Table 1 is obtained by setting $(a,b,c,d,e,f)=(1,1,6,2,3,1)$, while the second pair of triplets is obtained for $(a,b,c,d,e,f)=(2,3,1,2,1,3)$. We can construct infinitely many new pairs of triplets from Proposition 1 by taking distinct factorizations of positive integers into three factors a,b,c and d,e,f. For example, 10 can be factorized in distinct ways as

$$10=2\cdot 5\cdot 1=1\cdot 1\cdot 10,$$

which gives a new pair of equivalent triplets

$$(4,25,40) \text{ and } (49,10,10).$$

Previous proposition can be easily generalized:

Proposition 2. *For a given $k\in N$, let a_i,b_i,c_i,d_i,e_i,f_i be positive integers such that*

$$\sum_{i=1}^{k} a_ib_ic_i=\sum_{i=1}^{k} d_ie_if_i.$$

Then the multisets

$$A=\{a_i^2c_i, b_i^2c_i, (d_i+e_i)^2f_i\colon i=1,\ldots,k\}$$

and

$$B=\{(a_i+b_i)^2c_i, d_i^2f_i, e_i^2f_i\colon i=1,\ldots,k\}$$

belong to the same equivalence class of ρ.

Proof. Both A and B have $3k$ elements and the sum of square roots of their elements is equal to $\sum_{i=1}^{k}(a_i+b_i)c_i+(d_i+e_i)f_i$. For the sum of elements of A and B, we have

$$\begin{aligned}\sum_{x\in A} x &= \sum_{i=1}^{k}(a_i^2+b_i^2)c_i+(d_i^2+e_i^2)f_i+2d_ie_if_i\\ &= \sum_{i=1}^{k}(a_i^2+b_i^2)c_i+(d_i^2+e_i^2)f_i+2a_ib_ic_i=\sum_{y\in B} y.\end{aligned}$$ ∎

This proposition has even more freedom than Proposition 1. For example, 10 can be written in distinct ways as

$$10=1\cdot 1\cdot 4+2\cdot 3\cdot 1=1\cdot 1\cdot 5+1\cdot 1\cdot 5,$$

yielding $(a_1,b_1,c_1,a_2,b_2,c_2)=(1,1,4,2,3,1)$ and $(d_1,e_1,f_1,d_2,e_2,f_2)=(1,1,5,1,1,5)$. Proposition 2 now gives equivalent multisets

$$\{4,4,20,4,9,20\} \quad \text{and} \quad \{16,5,5,25,5,5\}.$$

3 Operations in $\mathcal{S}/\rho$

We can introduce two operations to $\mathcal{S}$ which agree with ρ to construct equivalence classes with more than two multisets. First, declare *scalar* to be a positive integer. Then for scalar α and multiset $A \in \mathcal{S}$, the product αA is defined as

$$\alpha A = \{\alpha a \colon a \in A\}.$$

The second operation is the union $A \uplus B$ of multisets A and B, which preserves multiplicities of their elements: if a appears m times in A and n times in B, then a appears $m + n$ times in $A \cup B$.

Proposition 3. *For any $\alpha \in N$ and $A, B, C, D \in \mathcal{S}$,*

$$\begin{aligned} A \ \rho \ B &\Rightarrow \alpha A \ \rho \ \alpha B, \\ A \ \rho \ B, C \ \rho \ D &\Rightarrow A \uplus C \ \rho \ B \uplus D. \end{aligned}$$

Proof. The sum of elements in αA is α times the sum of elements in A. Similarly, the sum of square roots of elements in αA is $\sqrt{\alpha}$ times the sum of square roots of elements in A. Thus, from $A \ \rho \ B$ it follows that $\alpha A \ \rho \ \alpha B$.

Next, we have

$$\sum_{x \in A \uplus C} x = \sum_{x \in A} x + \sum_{x \in C} x = \sum_{x \in B} x + \sum_{x \in D} x = \sum_{x \in B \uplus D} x,$$

and, similarly,

$$\sum_{x \in A \uplus C} \sqrt{x} = \sum_{x \in A} \sqrt{x} + \sum_{x \in C} \sqrt{x} = \sum_{x \in B} \sqrt{x} + \sum_{x \in D} \sqrt{x} = \sum_{x \in B \uplus D} \sqrt{x}.$$

Thus, $A \uplus C \ \rho \ B \uplus D$. ∎

These two operations now provide a simple way to create arbitrarily large equivalence classes. Namely, for any $A \ \rho \ B$, $n \in N$ and $\alpha_1, \ldots \alpha_n \in N$, it follows from Proposition 3 that

$$\begin{aligned} & \alpha_1 A \uplus \alpha_2 A \uplus \cdots \uplus \alpha_{n-1} A \uplus \alpha_n A \\ \rho \quad & \alpha_1 B \uplus \alpha_2 A \uplus \cdots \uplus \alpha_{n-1} A \uplus \alpha_n A \\ \rho \quad & \alpha_1 B \uplus \alpha_2 B \uplus \cdots \uplus \alpha_{n-1} A \uplus \alpha_n A \\ \rho \quad & \ldots \\ \rho \quad & \alpha_1 B \uplus \alpha_2 B \uplus \cdots \uplus \alpha_{n-1} B \uplus \alpha_n A \\ \rho \quad & \alpha_1 B \uplus \alpha_2 B \uplus \cdots \uplus \alpha_{n-1} B \uplus \alpha_n B. \end{aligned}$$

Thus, this equivalence class contains at least $n+1$ multisets, each of them containing $n|A|$ elements.

In particular, take $A = \{25, 6, 6\}$, $B = \{24, 9, 4\}$ and $\alpha_1 = \cdots = \alpha_n = 1$. Then for any $n \in N$, we have a set of $n+1$ OIE-equienergetic noncospectral decomposable graphs

$$S^*_{A \uplus A \uplus \cdots \uplus A}, S^*_{B \uplus A \uplus \cdots \uplus A}, S^*_{B \uplus B \uplus \cdots \uplus A}, \ldots, S^*_{B \uplus B \uplus \cdots \uplus B},$$

each of which has $34n + 1$ vertices and $65n$ edges.

4 Concluding remarks

Our last example shows that for any $n \in N$, there exists a set of n OIE-equienergetic noncospectral graphs with $O(n)$ vertices. Propositions 1, 2 and 3 provide means to construct an abundance of further examples of OIE-equienergetic noncospectral graphs. It should be noted, however, that all these graphs have more vertices than what can be reached by a computer search on modern day computers, so that our finding, in fact, should not be considered contradictory to the conclusion from [25] that OIE-equienergetic graphs occur relatively rarely.

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