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ORIENTED INCIDENCE ENERGY AND THRESHOLD 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 $n \geq 9$, there exists at least $\binom{\lfloor n/9 \rfloor}{2} + 1$ distinct pairs of graphs on 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

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

for which chemical applications have long been known; for details see the surveys [2, 3, 4]. Recently, Nikiforov [5] generalized the concept of graph energy to an 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

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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.

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 [13]-[21]. 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 [22] and, based on the computer search among small graphs, it was suggested that OIE-equienergetic graphs occur relatively rarely. Our goal here is to show that for any $n \geq 9$, there exists at least $\binom{\lfloor n/9 \rfloor + 1}{2}$ distinct pairs of noncospectral graphs on n vertices having equal oriented incidence energy. Such pairs are found among threshold graphs.

2 Properties of threshold graphs

A threshold graph is obtained in a recursive process, starting with an isolated vertex 0 and adding at step i, $i \geq 1$, a new vertex i which is either isolated or adjacent to all vertices $0, \ldots, i-1$. This process may be encoded by a sequence of 0s and 1s, where 0 represents addition of an isolated vertex, while 1 represents addition of a vertex adjacent to previous vertices. Thus, an n-vertex threshold graph is encoded with a sequence of $n-1$ symbols. For our purposes, we extend this encoding with an arbitrary initial element, denote it by x, corresponding to vertex 0. Thus, we encode an n-vertex threshold graph with a sequence of n symbols. It is immediate to see that two threshold graphs are isomorphic if and only if they have same encoding sequences. A good survey on the properties of threshold graphs is [23].

A few simple properties of a degree sequence of a threshold graph are described next.

Lemma 1. *Let G be a threshold graph with an encoding sequence $A = xa_1 \ldots a_{n-1}$, and let d_i be the degree of vertex i, $i = 0, \ldots, n-1$. Then, for $1 \leq i \leq n-1$:*

i) if $a_i = 0$*, then* $d_0 \geq d_i$*;*

ii) if $a_i = 1$*, then* $d_0 \leq d_i$*;*

iii) if $a_i = a_j = 0$ *and* $i < j$*, then* $d_i \geq d_j$*;*

iv) if $a_i = a_j = 1$ *and* $i < j$*, then* $d_i \leq d_j$*.*

Proof. Vertex 0 is adjacent only to the vertices in G encoded by 1 in A. Thus, the number of 1s in A is equal to d_0.

Suppose that $a_i = 0$ for some $i \geq 1$. A vertex i is adjacent only to the vertices encoded by 1 in A whose index is larger than i. Thus, each neighbor of i is also a neighbor of 0, and so $d_0 \geq d_i$. Further, if $a_j = 0$ for some $j > i$, each neighbor of j is also a neighbor of i, and so $d_i \geq d_j$.

Now, suppose that $a_i = 1$ for some $i \geq 1$. A vertex i is adjacent to vertices $0, \ldots, i-1$ and those vertices encoded by 1 in A whose index is larger than i. In particular, it is adjacent to all vertices encoded by 1 in A, except itself, and also to vertex 0, so that $d_i \geq (d_0 - 1) + 1 = d_0$.

Next, let $a_j = 1$ for some $j \geq i+1$. Let k be the number of 1s among positions $i+1, \ldots, j-1$ in A, so that $k \leq j-i-1$, and let l be the number of 1s among positions $j+1, \ldots, n-1$ in A. Then $d_i = i+k+1+l$, $d_j = j+l$, and from $k+i+1 \leq j$, it follows that $d_j \geq d_i$. □

Threshold graphs also satisfy the following

Theorem 1 ([23])**.** *The Laplacian spectrum of a threshold graph G is the conjugate of its degree sequence.*

Thus, Laplacian spectrum of G consists of eigenvalues

$$\mu_j = |\{i : \ d_i \geq j\}|, \qquad j = 1, 2, \ldots, n. \tag{2}$$

Next, we are interested in the effect that selected operations on a threshold graph have on its Laplacian spectrum and oriented incidence energy.

Proposition 1. *Let* G *be a threshold graph with an encoding sequence* $A = xa_1 \ldots a_{n-1}$*, the Laplacian eigenvalues* $\mu_1 \geq \cdots \geq \mu_n = 0$ *given by (2), and the degree sequence* $d'_1 \geq d'_2 \geq \cdots \geq d'_n$ *sorted in nonincreasing order. Further, let* m *be the number of 1s in* A *among positions* $k+1, \ldots, n-1$*,* $m \geq 1$*.*

For $k, l \geq 0$*, let* $G_{k,l}$ *be the threshold graph with an encoding sequence*

$$xa_1 \ldots a_k \underbrace{0 \ldots 0}_{l} a_{k+1} \ldots a_{n-1}.$$

Then the Laplacian eigenvalues of $G_{k,l}$ *are given by*

$$\mu'_j = \begin{cases} \mu_j + l & \text{for } 1 \leq j \leq m, \\ \mu_j + |\{i : \ j-1 \geq d'_i \geq j-l, 1 \leq i \leq m\}| & \text{for } m+1 \leq j \leq n-1, \\ |\{i : \ d'_i \geq j-l, \ 1 \leq i \leq m\}| & \text{for } n \leq j \leq n+l. \end{cases}$$

Proof. Graph $G_{k,l}$ is obtained from G by inserting l new vertices, denote them by $-l,\dots,-2,-1$, each of them adjacent to all vertices encoded by 1 in A whose index is larger than k. Thus, the degree of vertices $-l,\dots,-1$ is equal to m.

On the other hand, the degree of each vertex encoded by 1 in A whose index is larger than k has been increased by l. By Lemma 1, these vertices have m largest degrees in G, so that

$$d'_1 + l \geq \cdots \geq d'_m + l > d'_{m+1} \geq \cdots \geq d'_n, \underbrace{m,\dots,m}_{l}$$

is the degree sequence of $G_{k,l}$. The degree of vertex 0 in G is at least m, then by Lemma 1.ii), $d'_i \geq m$ for $i = 1,\dots,m$.

For $1 \leq j \leq m$, we have from (2),

$$\begin{aligned}
\mu'_j &= |\{i:\ d'_i + l \geq j,\ 1 \leq i \leq m\}| + |\{i:\ d'_i \geq j,\ m+1 \leq i \leq n\}| \\
&\quad + |\{-i : m \geq j,\ -l \leq i \leq -1\}| \\
&= m + |\{i:\ d'_i \geq j,\ m+1 \leq i \leq n\}| + l \\
&= \mu_j + l.
\end{aligned}$$

For $m+1 \leq j \leq n+l$, we have

$$\begin{aligned}
\mu'_j &= |\{i:\ d'_i + l \geq j,\ 1 \leq i \leq m\}| + |\{i:\ d'_i \geq j,\ m+1 \leq i \leq n\}| \\
&= |\{i:\ d'_i \geq j-l,\ 1 \leq i \leq m\}| - |\{i:\ d'_i \geq j,\ 1 \leq i \leq m\}| \\
&+ |\{i:\ d'_i \geq j,\ 1 \leq i \leq m\}| + |\{i:\ d'_i \geq j,\ m+1 \leq i \leq n\}| \\
&= |\{i:\ j-1 \geq d'_i \geq j-l,\ 1 \leq i \leq m\}| + \mu_j.
\end{aligned}$$

From above for $n \leq j \leq n+l$, from $\mu_j = 0$ and $d'_i \leq n-1$ we have

$$\mu'_j = |\{i:\ d'_i \geq j-l,\ 1 \leq i \leq m\}|. \qquad \square$$

Proposition 2. *Let G and H be n-vertex threshold graphs whose encoding sequences both end with $n-k-1$ symbols 1, for some $k < n$. Then for any $l \geq 1$,*

$$OIE(G) = OIE(H) \quad \Rightarrow \quad OIE(G_{k,l}) = OIE(H_{k,l}).$$

Proof. Let $xg_1 \dots g_{n-1}$ and $xh_1 \dots h_{n-1}$ be encoding sequences of G and H, such that $g_i = h_i = 1$ for $k+1 \leq i \leq n-1$. Denote by $m = n-k-1$ the number of 1s in common ending of encoding sequences of G and H. Next, let $\mu_1,\dots,\mu_n$ be the Laplacian eigenvalues of G and $\lambda_1,\dots,\lambda_n$ the Laplacian eigenvalues of H given by equation (2), and let $\mu'_1,\dots,\mu'_{n+l}$ be the Laplacian eigenvalues of $G_{k,l}$ and $\lambda'_1,\dots,\lambda'_{n+l}$ the Laplacian eigenvalues of $H_{k,l}$, given by Proposition 1.

First we show that

$$\mu_j = \lambda_j, \qquad \text{for } j = 1,\dots,m. \tag{3}$$

Vertices $1,\dots,k$ have degree at least m (they are adjacent to m 1s in the common ending), thus these vertices contribute k to the eigenvalues μ_j and λ_j, $j \leq m$.

Vertices $k+1,\dots,n-1$ have same degrees in both G and H, so they contribute same value to both eigenvalues μ_j and λ_j, $j \le m$. From Proposition 1, we see that also

$$\mu'_j = \lambda'_j, \qquad \text{for } j = 1,\dots,m. \tag{4}$$

Next, the eigenvalues $\mu'_n,\dots,\mu'_{n+l}$ and $\lambda'_n,\dots,\lambda'_{n+l}$ are determined by m largest degrees in G and H, which are the degrees of vertices $k+1,\dots,n-1$. In particular, these vertices have degree $n-1$ each, so that

$$\mu'_j = \lambda'_j = m \text{ for } n \le j \le n+l-1, \text{ while } \mu'_{n+l} = \lambda'_{n+l} = 0. \tag{5}$$

Further, the m largest degrees in G and H being equal to $n-1$ each, implies by Proposition 1 that,

$$\mu'_j = \mu_j \text{ and } \lambda'_j = \lambda_j \quad \text{for } m+1 \le j \le n-1. \tag{6}$$

Finally, suppose that $OIE(G) = OIE(H)$. Equation (3) implies $0 = OIE(G) - OIE(H) = \sum_{j=m+1}^{n} \sqrt{\mu_j} - \sum_{j=m+1}^{n} \sqrt{\lambda_j}$. Then from (4), (5) and (6) above and $\mu_n = \lambda_n = 0$, we have

$$\begin{aligned} OIE(G_{k,l}) - OIE(H_{k,l}) &= \left(\sum_{j=1}^{m} \sqrt{\mu_j + l} + \sum_{j=m+1}^{n-1} \sqrt{\mu_j} + \sum_{j=n}^{n+l-1} \sqrt{m} \right) \\ &- \left(\sum_{j=1}^{m} \sqrt{\lambda_j + l} + \sum_{j=m+1}^{n-1} \sqrt{\lambda_j} + \sum_{j=n}^{n+l-1} \sqrt{m} \right) \\ &= \sum_{j=m+1}^{n-1} \sqrt{\mu_j} - \sum_{j=m+1}^{n-1} \sqrt{\lambda_j} = OIE(G) - OIE(H) = 0. \end{aligned}$$

□

Proposition 3. *Let G be a threshold graph with encoding sequence $xg_1 \dots g_{n-1}$. For $q \ge 1$ and $g_0 \in \{0,1\}$, let G^{q,g_0} be the threshold graph with encoding sequence*

$$x \underbrace{g_0 \cdots g_0}_{q-1} \underbrace{g_1 \cdots g_1}_{q} \cdots \underbrace{g_{n-1} \cdots g_{n-1}}_{q}.$$

If $\mu_1 \ge \cdots \ge \mu_{n-1} \ge \mu_n = 0$ are the Laplacian eigenvalues of G given by (2), then the Laplacian eigenvalues of G^{q,g_0} are

$$\underbrace{q\mu_1,\dots,q\mu_1}_{q},\ \dots,\ \underbrace{q\mu_{n-1},\dots,q\mu_{n-1}}_{q},\ \underbrace{qm,\dots,qm}_{q-1}, 0,$$

where m is the number of 1s in the encoding sequence of G plus g_0, $m \ge 1$. In particular, $OIE(G^{q,g_0}) = q\sqrt{q}\, OIE(G) + (q-1)\sqrt{qm}$.

Proof. Note that each vertex i of G, $0 \le i \le n-1$, corresponds to the set of vertices $\{qi, qi+1, \dots, qi+q-1\}$ in G^{q,g_0}. Let d_i be the degree of vertex i in G.

If $g_i = 0$, the degree of vertices $qi, \dots, qi+q-1$ in G^{q,g_0} is equal to qd_i, while if $g_i = 1$, the degree of vertices $qi, \dots, qi+q-1$ in G^{q,g_0} is equal to $qd_i + q - 1$.

Let $d'_1 \geq d'_2 \geq \cdots \geq d'_n$ be the degree sequence of G, sorted in nonincreasing order. Since any vertex encoded by symbol 1 has degree larger than any vertex encoded by symbol 0 in G by Lemma 1, the degree sequence of G^{q,g_0} is

$$qd'_1 + q - 1 \geq \cdots \geq qd'_m + q - 1 \geq qd'_{m+1} \geq \cdots \geq qd'_n,$$

where each degree appears q times.

Next, let $\mu'_1, \dots, \mu'_{qn}$ be the Laplacian eigenvalues of G^{q,g_0} given by (2). Then for $1 \leq j \leq qd'_{m+1}$,

$$\begin{aligned} \mu'_j &= q\,|\{i:\, qd'_i + q - 1 \geq j,\ 1 \leq i \leq m\}| + q\,|\{i:\, qd'_i \geq j,\ m+1 \leq i \leq n\}| \\ &= qm + q\,|\{i:\, d'_i \geq \lceil j/q \rceil,\ m+1 \leq i \leq n\}| \\ &= q\mu_{\lceil j/q \rceil}, \end{aligned}$$

for $qd'_{m+1} + 1 \leq j \leq qd'_{m+1} + q - 1$,

$$\begin{aligned} \mu'_j &= q\,|\{i:\, qd'_i + q - 1 \geq j,\ 1 \leq i \leq m\}| + q\,|\{i:\, qd'_i \geq j,\ m+1 \leq i \leq n\}| \\ &= qm, \end{aligned}$$

and for $qd'_{m+1} + q \leq j \leq qn$,

$$\begin{aligned} \mu'_j &= q\,|\{i:\, qd'_i + q - 1 \geq j,\ 1 \leq i \leq m\}| + q\,|\{i:\, qd'_i \geq j,\ m+1 \leq i \leq n\}| \\ &= q\left|\{i:\, d'_i \geq \lceil \frac{j-q+1}{q} \rceil,\ 1 \leq i \leq m\}\right| \\ &= q\mu_{\lceil \frac{j-q+1}{q} \rceil}. \qquad \Box \end{aligned}$$

Corollary 1. *Let G and H be threshold graphs with $OIE(G) = OIE(H)$. If the numbers of 1s in the encoding sequences of G and H differ by at most one, then there exists $g_0, h_0 \in \{0,1\}$ such that $OIE(G^{q,g_0}) = OIE(H^{q,h_0})$ for any $q \geq 1$.*

Proof. Let m_G and m_H be the number of 1s in the encoding sequences of G and H, respectively. Since $|m_G - m_H| \leq 1$, we can choose $g_0, h_0 \in \{0,1\}$ such that $m_G + g_0 = m_H + h_0$. Then from Proposition 3

$$\begin{aligned} OIE(G^{q,g_0}) &= q\sqrt{q}\,OIE(G) + (q-1)\sqrt{q(m_G + g_0)} \\ &= q\sqrt{q}\,OIE(H) + (q-1)\sqrt{q(m_H + h_0)} = OIE(H^{q,h_0}). \end{aligned}$$

3 Many pairs of OIE-equienergetic threshold graphs

Proposition 2 and Corollary 1 provide us with means of constructing new pairs of OIE-equienergetic threshold graph from existing ones. In order to find small pairs of such graphs, we performed a computer search on threshold graphs up to 17 vertices and found several pairs of OIE-equienergetic threshold graphs to which these results may be applied. Their symbols are given in Table 1.

We are now in position to prove

n	Symbol	Symbol
9	x10000101	x00000011
16	x100100000100011	x011010001010001
16	x101000011010001	x010010000100011
16	x101010011001001	x010101000010011
17	x1101010110001001	x1010101000010101

Table 1: Pairs of small OIE-equienergetic threshold graphs.

Proposition 4. *For any $n \geq 9$, there exists at least $\binom{\lfloor n/9 \rfloor}{2} + 1$ distinct pairs of graphs on n vertices having equal oriented incidence energy.*

Proof. Let q be such that $9q \leq n$. Let X and Y be threshold graphs with symbols $x10000101$ and $x00000011$. Since $OIE(X) = OIE(Y)$, from Corollary 1 we have that $OIE(X^{q,0}) = OIE(Y^{q,1})$. Next, for any $0 \leq k \leq q-1$, from Proposition 2 we have that $OIE(X^{q,0}_{8q+k,n-9q}) = OIE(Y^{q,1}_{8q+k,n-9q})$.

Graphs $X^{q,0}_{8q+k,n-9q}$ and $Y^{q,1}_{8q+k,n-9q}$ are mutually nonisomorphic graphs on n vertices, each with distinct Laplacian spectrum. For each q with $9q < n$, there exists q such pairs, while when $9q = n$, there exists one such pair. In total, they form at least $\binom{\lfloor n/9 \rfloor}{2} + 1$ such pairs. □

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