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LARGE SETS OF NONCOSPECTRAL GRAPHS WITH EQUAL LAPLACIAN ENERGY¹

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Abstract

Several alternative definitions to graph energy have appeared in literature recently, the first among them being the Laplacian energy, defined by Gutman and Zhou in [Linear Algebra Appl. 414 (2006), 29–37]. We show here that Laplacian energy apparently has small power of discrimination among threshold graphs, by showing that, for each n, there exists a set of n mutually noncospectral connected threshold graphs with equal Laplacian energy with $O(\sqrt{n})$ vertices only. Nevertheless, situation becomes opposite when trees are considered, as it turns out that, up to 20 vertices, there exists no pair of noncospectral trees with equal Laplacian energies.

1 Introduction

Let G = (V, E) be a finite, simple, undirected graph with vertices $V = \{1, 2, ..., n\}$ and m = |E| edges. The degree of a vertex $u \in V$ will be denoted by d_u . Let G have adjacency matrix A with eigenvalues $\lambda_1 \ge \lambda_2 \ge ... \ge \lambda_n$, and Laplacian matrix L = D - A, where D is the diagonal matrix of vertex degrees, with eigenvalues $\mu_1 \ge \mu_2 \ge ... \ge \mu_n = 0$.

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Additional details on the theory of graph spectra may be found in [1]. These eigenvalues obey the following well-known relations:

$$\sum_{i=1}^{n} \lambda_i = 0, \qquad \sum_{i=1}^{n} \mu_i = 2m.$$
 (1)

The energy and the Laplacian energy of G are now defined as follows

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|, \qquad LE = LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|.$$
(2)

The energy of a graph was defined by Gutman in [2] and it has a long known chemical applications; for details see the surveys [3, 4, 5]. Much work has appeared in literature, especially in the last decade. On the other hand, the Laplacian energy was defined in [6] only recently, with some further properties found in [7]-[10].

From (1) and (2) we can observe that both energies represent the absolute deviation of corresponding eigenvalues from their average value. Thus, we can introduce the following

Definition 1 The energy of a given matrix M, denoted as M-energy, is the absolute deviation of eigenvalues of M from their average value.

This way, the energy of a graph is its A-energy and the Laplacian energy of a graph is its L-energy. Other types of energy can be defined in the same way, the difference being only in the matrix under consideration: for example, the energy of a distance matrix is studied in [11, 12]. Among those found in literature, it is the Laplacian-like energy only, defined by Liu and Liu [13], that does not fit this setting (which, at the end, may happen to be to its advantage, as a number of extremal problems for Laplacian-like energy can be solved by considering the coefficients of characteristic polynomial of L and finding transformations which are monotone on these coefficients [14, 15, 16]).

On the other hand, Nikiforov [17] has recently introduced another concept of the energy of a complex matrix M as the sum of the singular values of M, which made possible to determine the energy of random graphs.

A feasible use of energies, as numerical invariants, is to distinguish nonisomorphic graphs from each other. In that respect, for a given type of graph matrix M, graphs having equal M-energy will be called M-equienergetic. Of course, since M-energy is calculated from spectrum of M, M-cospectral graphs will trivially have the same M-energy. Thus,

Definition 2 For a given type of graph matrix M, two graphs G and H will be called M-equienergetic if they are not M-cospectral, yet have equal M-energies.

A number of results on A-equienergetic graphs have appeared recently [18]-[27]. In principle, most of these results show that A-equienergetic graphs exist in various classes of graphs, and in some cases, sets of n such graphs can be found (e.g., see [21]), although on very large number of vertices (of order 5^n in [21]).

When it comes to Laplacian energy, it appears that it might not be well suited to distinguish among nonisomorphic graphs, as there exists a triplet of L-equienergetic graphs on four vertices already:



Our main task here is to show that the above example is not a coincidence. In particular, we show that for any $n \in \mathbf{N}$ there exists a set of *n L*-equienergetic threshold graphs on $O(\sqrt{n})$ vertices only. It turns out that these graphs have equal number of edges as well. We find them in the class of threshold graphs.

2 Threshold graphs

Threshold graphs are a simple class of graphs, which due to their wide applicability, keeps reappearing under various names. A good survey on the properties of threshold graphs is [28].

Basically, a threshold graph is obtained in a recursive process, where one starts with an isolated vertex and at each step either a new isolated vertex is added or a new vertex adjacent to all previous vertices is added. This construction process can be encoded with a sequence of 0s and 1s, where 0 represents addition of an isolated vertex, while 1 represents addition of a vertex adjacent to all previous vertices. Thus, an *n*-vertex threshold graph can be encoded with a sequence of n - 1 symbols. For our purposes, we will extend this encoding with an arbitrary initial element (0 or 1) that will correspond to the starting isolated vertex. Thus, in our case, an *n*-vertex threshold graph will be encoded with a sequence of *n* symbols, where symbol at position *k* describes the nature of vertex *k*. It is immediate to see from this encoding that two threshold graphs are isomorphic if and only if they have the same encoding sequence (without initial element).

Suppose that G is a threshold graph with encoding sequence $a_1a_2...a_n \in \{0,1\}^n$, and let $d_1 \geq d_2 \geq ... \geq d_n$ be its degree sequence. The degree sequence can be represented via its Ferrers diagram, as shown by example in Fig. 1.

A particularly nice property of a class of threshold graphs is that

Lemma 1 ([28]) The Laplacian spectrum of a threshold graph G is the conjugate of its degree sequence.

Thus, Laplacian spectrum of G consists of eigenvalues

$$\mu_i = |\{j : d_j \ge i\}|, \qquad i = 1, 2, \dots, n.$$
(3)

Let us now study the effects of two particular operations on the encoding sequence of a threshold graph:

Operation A. Changing 01 with 10 in encoding sequence.

Suppose $a_i = 0$ and $a_{i+1} = 1$ and form a new threshold graph G' encoded by a sequence $a_1 \ldots a_{i-1} 10a_{i+2} \ldots a_n$. Then G' is obtained by removing edge $\{i, i+1\}$ from G, so that the degrees of i and i+1 decrease by one, while the degrees of all other vertices remain



Encoding sequence 01010101

L-spectrum [8, 7, 6, 5, 3, 2, 1, 0]



intact. Then from (3) we see that, in the Laplacian spectrum of G', the eigenvalues $\mu_{d'}$ and $\mu_{d''}$ decrease by one, while other eigenvalues remain intact.

Operation B. Changing 10 with 01 in encoding sequence.

Suppose $a_i = 1$ and $a_{i+1} = 0$ and form a new threshold graph G'' encoded by a sequence $a_1 \ldots a_{i-1} 01 a_{i+2} \ldots a_n$. Then G'' is obtained by adding edge $\{i, i+1\}$ to G, so that the degrees of i and i+1 increase by one, while the degrees of all other vertices remain intact. Then from (3) we see that, in the Laplacian spectrum of G'', the eigenvalues $\mu_{d'+1}$ and $\mu_{d''+1}$ increase by one, while other eigenvalues remain intact.

3 A particular threshold graph and its mates

If we apply just one of operations A and B to a threshold graph G, then its number of edges changes, and so, the term 2m/n in the formula for L-energy changes as well. In such case, if we wish to know how does L-energy change, we first need to know how many eigenvalues of L fall into each of intervals [0, 2(m-1)/n], [2(m-1)/n, 2m/n] and $[2m/n, +\infty]$. However, we can work around this problem if we simultaneously apply both operations to G, as then the number of edges remain the same.

The threshold graph G_k , $k \geq 3$, that will be used to generate a large set of *L*-equienergetic graphs, has encoding sequence

$$\underbrace{010101\dots010101}_{k \text{ times}}.$$
(4)

For example, G_5 is the first graph shown in Fig. 2.

From its encoding sequence, it is easy to see that G_k has 2k vertices with degrees, given in the same order as vertices,

$$k, k, k-1, k+1, k-2, k+2, \ldots, 1, 2k-1,$$

where the vertex at position 2i - 1, corresponding to 0 in (4), has degree k - i + 1, while the vertex at position 2i, corresponding to 1 in (4), has degree k + i - 1, i = 1, 2, ..., k. From (3), its Laplacian spectrum is

$$[2k, 2k-1, \ldots, k+2, k+1, k-1, k-2, \ldots, 1, 0]$$

The average degree of G_k is exactly k, and thus, its Laplacian energy is equal to k(k+1).

Let us now apply operation **A** to pair 01 at positions 2i - 1 and 2i, $1 \le i \le k$, and operation **B** to pair 10 at positions 2j and 2j + 1, $1 \le j \le k - 1$, in the encoding sequence (4) (assuming that $\{2i - 1, 2i\} \cap \{2j, 2j + 1\} = \emptyset$). Then the degrees of vertices 2i - 1 and 2i decrease by one, while those of vertices 2j and 2j + 1 increase by one, so that the new degree sequence becomes

$$\underbrace{k,k,\ldots,k-i+2,k+i-2}_{\text{vertices 1 to }2i-2}, \quad \mathbf{k}-\mathbf{i},\mathbf{k}+\mathbf{i}-2, \quad \underbrace{k-i,k+i,\ldots,k-j+1}_{\text{vertices }2i+1 \text{ to }2j-1}, \\ \mathbf{k}+\mathbf{j},\mathbf{k}-\mathbf{j}+1, \quad \underbrace{k+j,\ldots,1,2k-1}_{\text{vertices }2j+2 \text{ to }2k}.$$

These operations decrease or increase by one corresponding Laplacian eigenvalues of G_k , so that their new values are

$$\mu'_{k-i+1} = k+i-1, \tag{5}$$

$$\mu'_{k-j+1} = k+j+1, \tag{6}$$

$$\mu'_{k+i-1} = k - i, \tag{7}$$

$$\mu'_{k+j} = k - j + 1, \tag{8}$$

while the rest of the *L*-spectrum remains intact. Thus, two *L*-eigenvalues that were larger than k increase and decrease by one, respectively, and two *L*-eigenvalues that were smaller than k increase and decrease by one, respectively. Since the average degree remains k in a newly obtained graph, we see that the *L*-energy does not change, and so, G_k and a newly obtained graph are *L*-equienergetic.

Next, notice that operation \mathbf{A} can be applied to G_k in k-1 ways (we do not apply it to last pair 01 in the encoding sequence, as it results in a disconnected graph). If \mathbf{A} is applied to the first pair 01, then operation \mathbf{B} can be applied in k-2 ways, while in other cases, \mathbf{B} can be applied in k-3 ways. Thus, we can apply them simultaneously in $k^2 - 4k + 4$ ways. Since all these threshold graphs have distinct encoding sequences, no two of them are isomorphic. Moreover, it is easy to see from (5)-(8) that no two of them may be *L*-cospectral as well. Thus, we have just shown

Theorem 1 For each $k \ge 3$, there exists a set of $k^2 - 4k + 5$ L-equienergetic graphs on 2k vertices.

The construction of such set is exemplified for k = 5 in Fig. 2.

4 Concluding remarks

We see from Theorem 1 that there exist arbitrariy large sets of L-equienergetic graphs, with a relatively small number of vertices, and moreover with the same number of edges, all of which show that L-energy is not well suited to distinguish threshold graphs from each other. This conclusion may extend to connected graphs as well, as it turns out that there exists



Sequence 0101010101[10, 9, 8, 7, 6, 4, 3, 2, 1, 0]



Sequence 0011011001[10, 8, 8, 7, 7, 5, 3, 1, 1, 0]



Sequence 0011100101 [10, 9, 7, 7, 7, 5, 2, 2, 1, 0]





Sequence 0100111001 [10, 8, 8, 8, 6, 4, 4, 1, 1, 0]



Sequence 0101100011 [10, 10, 7, 7, 6, 4, 2, 2, 2, 0]



Sequence 1000110101[10, 9, 8, 8, 4, 4, 4, 2, 1, 0]

Sequence 0110001101 [10, 9, 9, 6, 6, 3, 3, 3, 1, 0]



Sequence 1001001101[10, 9, 9, 7, 4, 4, 3, 3, 1, 0]

Sequence 0110010011 [10, 10, 8, 6, 6, 3, 3, 2, 2, 0]



Sequence 1001010011 [10, 10, 8, 7, 4, 4, 3, 2, 2, 0]

Figure 2: $k^2 - 4k + 5 = 10$ L-equienergetic graphs on 2k = 10 vertices, with encoding sequence and Laplacian spectrum below each graph.

- $\bullet\,$ 297 pairs of noncospectral $L\text{-}{\rm equienergetic}$ graphs among 853 connected graphs on seven vertices,
- 13044 pairs among 11117 connected graphs on eight vertices (implying, in fact, existence of a large number of *L*-equienergetic sets containing at least four graphs each), and
- 39304 pairs among 261080 connected graphs on nine vertices.

Nevertheless, *L*-energy may be fit for business in more restricted graph classes. For example, our computer search employing first a Java-based program that puts trees in hash map with *L*-energy as keys, calculated using Colt library (available from http://acs.lbl.gov/~hoschek/colt/), and then checking the findings with Wolfram's Mathematica, revealed that

there is not a single pair of L-equienergetic trees up to 20 vertices!

There is a large number of trees whose *L*-energy differs by less than 10^{-11} , but no two of them are really *L*-equienergetic. This is in sharp contrast with the fact that there are already 120 pairs of equienergetic trees on 20 vertices (which was checked by the same programs, except that *A*-energy was calculated instead of *L*-energy).

Of course, it is hard to believe that there exists no pair of L-equienergetic trees at all, and they probably do exist on a larger number of vertices. Thus, we close this paper by leaving the following

Open problem. Find a pair of L-equienergetic trees.

References

- D. Cvetković, M. Doob and H. Sachs, Spectra of Graphs—Theory and Application, 3rd edition, Johann Ambrosius Barth Verlag, 1995.
- [2] I. Gutman, The energy of a graph, Ber. Math.Statist. Sekt. Forschungsz. Graz 103 (1978), 1-22.
- [3] I. Gutman, Total π-electron energy of benzenoid hydrocarbons, Topics Curr. Chem. 162 (1992), 29–63.
- [4] I. Gutman, The energy of a graph: old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (eds.), Algebraic Combinatorics and Applications, Springer-Verlag, Berlin, 2001, pp. 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, B. Zhou, Laplacian energy of a graph, Linear Algebra Appl. 414 (2006), 29–37.
- [7] H. Wang, H. Hua, Note on Laplacian Energy of Graphs, MATCH Commun. Math. Comput. Chem. 59 (2008), 373–380.
- [8] T. Aleksić, Upper Bounds for Laplacian Energy of Graphs, MATCH Commun. Math. Comput. Chem. 60 (2008), 435–439.
- [9] B. Zhou, I. Gutman, T. Aleksić, A Note on Laplacian Energy of Graphs, MATCH Commun. Math. Comput. Chem. 60 (2008), 441–446.
- [10] N.M.M. de Abreu, C.T.M. Vinagre, A.S. Bonifacio, I. Gutman, *The Laplacian Energy of Some Laplacian Integral Graphs*, MATCH Commun. Math. Comput. Chem. 60 (2008), 447–460.

- [11] G. Indulal, I. Gutman, A. Vijayakumar, On Distance Energy of Graphs MATCH Commun. Math. Comput. Chem. 60 (2008), 461–472.
- [12] H.S. Ramane, I. Gutman, D.S. Revankar, *Distance Equienergetic Graphs*, MATCH Commun. Math. Comput. Chem. 60 (2008), 473–484.
- [13] J. Liu, B. Liu, A Laplacian-Energy-Like Invariant of a Graph, MATCH Commun. Math. Comput. Chem. 59 (2008), 355–372.
- [14] D. Stevanović, Laplacian-like energy of trees, MATCH Commun. Math. Comput. Chem. 61 (2009), 407–417.
- [15] D. Stevanović, A. Ilić, Maximum Laplacian-like energy of unicyclic graphs, preprint.
- [16] A. Ilić, D. Stevanović, Minimum Laplacian-like energy of unicyclic graphs, preprint.
- [17] V. Nikiforov, The energy of graphs and matrices, J. Math. Anal. Appl. 326 (2007), 1472–1475.
- [18] V. Brankov, D. Stevanović, I. Gutman, *Equienergetic chemical trees*, J. Serb. Chem. Soc. 69 (2004), 549–554.
- [19] R. Balakrishnan, The energy of a graph, Linear Algebra Appl. 387 (2004), 287-295.
- [20] H.S. Ramane, H.B. Walikar, S.B. Rao, B.D. Acharya, I. Gutman, P.R. Hampiholi, S.R. Jog, *Equienergetic graphs*, Kragujevac. J. Math. 26 (2004), 5–13.
- [21] D. Stevanović, Energy and NEPS of graphs, Linear Multilinear Algebra 53 (2005), 67–74.
- [22] H.S. Ramane, H.B. Walikar, S.B. Rao, B.D. Acharya, P.R. Hampiholi, S.R. Jog, I. Gutman, Spectra and energies of iterated line graphs of regular graphs, Appl. Math. Lett. 18 (2005), 679–682.
- [23] G. Indulal, A. Vijayakumar, On a pair of equienergetic graphs, MATCH Commun. Math. Comput. Chem. 55 (2006), 83–90.
- [24] H.S. Ramane, H.B. Walikar, Construction of equienergetic graphs, MATCH Commun. Math. Comput. Chem. 57 (2007), 203-210.
- [25] L. Xu, Y. Hou, Equienergetic bipartite graphs, MATCH Commun. Math. Comput. Chem. 57 (2007), 363–370.
- [26] G. Indulal, A. Vijayakumar, A Note on Energy of Some Graphs, MATCH Commun. Math. Comput. Chem. 59 (2008), 269–274.
- [27] J. Liu, B. Liu, Note on a Pair of Equienergetic Graphs, MATCH Commun. Math. Comput. Chem. 59 (2008), 275–278.
- [28] R. Merris, Degree maximal graphs are Laplacian integral, Linear Algebra Appl. 199 (1994), 381–389.