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Laplacian energy of a graph

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Abstract

Let G be a graph with n vertices and m edges. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the adjacency matrix of G, and let $\mu_1, \mu_2, \ldots, \mu_n$ be the eigenvalues of the Laplacian matrix of G. An earlier much studied quantity $E(G) = \sum_{i=1}^{n} |\lambda_i|$ is the *energy* of the graph G. We now define and investigate the *Laplacian energy* as $LE(G) = \sum_{i=1}^{n} |\mu_i - 2m/n|$. There is a great deal of analogy between the properties of $E(G)$ and $LE(G)$, but also some significant differences.

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1. Introduction

In this paper we are concerned with simple graphs. Let G be such a graph, possessing n vertices and m edges. In what follows we say that G is an (n, m)-graph.

Let d_i be the degree of the ith vertex of G, $i = 1, 2, \ldots, n$.

The spectrum of the graph G, consisting of the numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$, is the spectrum of its adjacency matrix [3]. The Laplacian spectrum of the graph G, consisting of the numbers $\mu_1, \mu_2, \ldots, \mu_n$, is the spectrum of its Laplacian matrix [5,6,13,14].

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The ordinary and Laplacian graph eigenvalues obey the following well-known relations:

$$\sum_{i=1}^{n} \lambda_i = 0; \quad \sum_{i=1}^{n} \lambda_i^2 = 2m, \tag{1}$$

$$\sum_{i=1}^{n} \mu_i = 2m; \quad \sum_{i=1}^{n} \mu_i^2 = 2m + \sum_{i=1}^{n} d_i^2. \tag{2}$$

Furthermore, if the graph G has p components ($p \geqslant 1$), and if the Laplacian eigenvalues are labelled so that $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_n$, then

$$\mu_{n-i} = 0 \ \text{ for } i = 0, \ldots, p-1 \quad \text{and} \quad \mu_{n-p} > 0. \tag{3}$$

The energy of the graph G is defined as

$$E(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{4}$$

This quantity has a long known chemical application; for details see the surveys [7–9]. Recently much work on graph energy appeared also in the mathematical literature (see, for instance, [1,15–20]).

The following properties of the energy of a graph will be needed (for comparative purposes):

Note 1

(a) $E(G) \geqslant 0$; equality is attained if and only if $m = 0$.
(b) If the graph G consists of (disconnected) components G_1 and G_2, then $E(G) = E(G_1) + E(G_2)$.
(c) If one component of the graph G is G_1 and all other components are isolated vertices, then $E(G) = E(G_1)$.

Note 2 [12]. $E(G) \leqslant \sqrt{2mn}$ with equality holding if and only if G is regular of degree 0 or 1.

Note 3 [10,11]

$$E(G) \leqslant \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} \tag{5}$$

with equality holding if and only if G is either a regular graph of degree 0, 1, or $n-1$, or a non-complete connected strongly regular graph with two non-trivial eigenvalues both having absolute value $\sqrt{[2m - (2m/n)^2]/(n-1)}$.

Note 4 [2]. $2\sqrt{m} \leqslant E(G) \leqslant 2m$. If G has no isolated vertices, then the equality $E(G) = 2\sqrt{m}$ holds if and only if G is a complete bipartite graph. If G has no isolated vertices, then the equality $E(G) = 2m$ holds if and only if G is regular of degree 1.

2. The Laplacian energy concept

Our intention is to conceive a graph-energy-like quantity, that instead of Eq. (4) would be defined in terms of Laplacian eigenvalues, and that—hopefully—would preserve the main features of the original graph energy. Bearing in mind relations (1) and (2), we first introduce the auxiliary "eigenvalues" γ_i, $i = 1, 2, \ldots, n$, defined via

$$\gamma_i = \mu_i - \frac{2m}{n}. \tag{6}$$

Then, in analogy with Eq. (1) we have

$$\sum_{i=1}^{n} \gamma_i = 0; \quad \sum_{i=1}^{n} \gamma_i^2 = 2M, \tag{7}$$

where

$$M = m + \frac{1}{2} \sum_{i=1}^{n} \left(d_i - \frac{2m}{n} \right)^2. \tag{8}$$

Recall that $2m/n$ is the average vertex degree. Consequently, $M = m$ if and only if G is regular, and $M > m$ otherwise.

Definition. If G is an (n, m)-graph, and its Laplacian eigenvalues are $\mu_1, \mu_2, \ldots, \mu_n$, then the *Laplacian energy* of G, denoted by $LE(G)$, is equal to $\sum_{i=1}^{n} |\gamma_i|$, i.e.,

$$LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|. \tag{9}$$

That the above definition is well chosen is seen from the following bounds, that should be compared with Notes 2–4:

$$LE(G) \leqslant \sqrt{2Mn}, \tag{10}$$

$$LE(G) \leqslant \frac{2m}{n} + \sqrt{(n-1)\left[2M - \left(\frac{2m}{n}\right)^2\right]}, \tag{11}$$

$$2\sqrt{M} \leqslant LE(G) \leqslant 2M. \tag{12}$$

In the subsequent section we discuss Eqs. (10)–(12) in more detail and provide proofs thereof.

3. The main results

Lemma 1. *If the graph G is regular, then* $LE(G) = E(G)$.

Proof. If an (n, m)-graph is regular of degree r, then $r = 2m/n$ and [3]

$$\mu_i - 2m/n = -\lambda_{n-i+1}, \quad i = 1, 2, \ldots, n \tag{13}$$

and Lemma 1 follows from (9). □

Theorem 2. *Inequality* (10) *holds for any* (n, m)*-graph* G, *where* M *is given via Eq.* (8). *Equality is attained if and only if* G *is either regular of degree* 0 *or consists of* α *copies of complete graphs of order* k *and* $(k-2)\alpha$ *isolated vertices*, $\alpha \geqslant 1, k \geqslant 2$. (*Recall that in the case* $k = 2$, G *is regular of degree* 1.)

Proof. Consider the sum

$$S = \sum_{i=1}^{n} \sum_{j=1}^{n} (|\gamma_i| - |\gamma_j|)^2. \tag{14}$$

By direct calculation

$$S = 2n \sum_{i=1}^{n} \gamma_i^2 - 2 \left(\sum_{i=1}^{n} |\gamma_i| \right) \left(\sum_{j=1}^{n} |\gamma_j| \right) = 4nM - 2LE(G)^2.$$

Since $S \geqslant 0$, we have $4nM - 2LE(G)^2 \geqslant 0$, which directly leads to Eq. (10).

Consider now the graphs for which $LE(G) = \sqrt{2Mn}$, i.e., for which $S = 0$. From (14) it is evident that $S = 0$ if and only if all $|\gamma_i|$-values are mutually equal. By (3) and (6), $\gamma_n = -2m/n$. Consequently, $\gamma_i \in \{-2m/n, +2m/n\}$ for all $i = 1, 2, \ldots, n$. Then from (6) we conclude that G has at most two distinct Laplacian eigenvalues: 0 and $4m/n$.

If all Laplacian eigenvalues of G are equal to zero, then G has no edges, i.e., G is regular of degree 0. Then $M = LE(G) = 0$ and the equality in Eq. (10) holds.

Suppose, therefore, that G has exactly two distinct Laplacian eigenvalues.

A connected graph has exactly two distinct Laplacian eigenvalues if and only if its diameter is equal to unity, i.e., if it is a complete graph, cf. Theorem 2.5 in [13]. Therefore, our graph G must consist of components that are mutually isomorphic complete graphs (say, of order k) and isolated vertices.

Let G consist of α components isomorphic to K_k and β isolated vertices. Then the Laplacian spectrum of G consists of numbers k [$(k-1)\alpha$ times] and 0 [$\alpha + \beta$ times]. Because $n = k\alpha + \beta$ and $2m = k(k-1)\alpha$, it is

$$\gamma_i = \begin{cases} k - k(k-1)\alpha/(k\alpha + \beta) & \text{for } i = 1, 2, \ldots, (k-1)\alpha, \\ -k(k-1)\alpha/(k\alpha + \beta) & \text{for} i = (k-1)\alpha + 1, \ldots, k\alpha + \beta. \end{cases}$$

Now, in order that all $|\gamma_i|$-values be mutually equal, it must be

$$k - \frac{k(k-1)\alpha}{k\alpha+\beta} = \frac{k(k-1)\alpha}{k\alpha+\beta}$$

i.e., $\beta = (k-2)\alpha$. □

Theorem 3. *Let G be an (n, m)-graph and p, the number of its components* $(p \geqslant 1)$. *Then*

$$LE(G) \leqslant \frac{2m}{n}p + \sqrt{(n-p)\left[2M - p\left(\frac{2m}{n}\right)^2\right]}. \tag{15}$$

For $p = 1$ *equality in* (15) *is attained for the graphs specified in Note* 3, *but also for other graphs. For* $p = n$, *G consists of isolated vertices*, $LE(G) = 0$, *and equality in* (15) *holds in a trivial manner. For any* p, *equality in* (15) *holds for the graphs consisting of* α *copies of complete graphs of order k and* $(k-2)\alpha$ *isolated vertices*, $\alpha \geqslant 1, k \geqslant 2$, *provided* $(k-1)\alpha = p$. (*Recall that in this case* $p = n/2$; *if* $k = 2$, *then G is regular of degree* 1.)

Proof. If G has p components, then according to (3) and (6), $\gamma_{n-i} = -2m/n$ for $i = 0, \ldots, p-1$. Bearing this in mind, consider the non-negative sum

$$S' = \sum_{i=1}^{n-p}\sum_{j=1}^{n-p}(|\gamma_i| - |\gamma_j|)^2. \tag{16}$$

In an analogous manner as in the proof of Theorem 2, we arrive at $2(n-p)[2M - p(2m/n)^2] - 2[LE(G) - p(2m/n)]^2 \geqslant 0$, from which Eq. (15) follows.

With regard to the graphs for which

$$LE(G) = \frac{2m}{n}p + \sqrt{(n-p)\left[2M - p\left(\frac{2m}{n}\right)^2\right]} \tag{17}$$

we first observe that any regular graph for which (5) is an equality, also satisfies (17). These graphs are specified in Note 3.

Using the same reasoning as in the proof of Theorem 2, we conclude that if (17) holds, then G has at most three distinct Laplacian eigenvalues.

If G has only two distinct Laplacian eigenvalues, then in a same manner as in the proof of Theorem 2 we arrive at the conclusion that G consists of α copies of complete graphs of order k and $(k-2)\alpha$ isolated vertices, $\alpha \geqslant 1, k \geqslant 2$, provided $(k-1)\alpha = p$. □

If the graph satisfying (17) has three distinct Laplacian eigenvalues then, for instance, it may consist of α_1 copies of complete graphs of order k_1, α_2 copies of complete graphs of order k_2, and β isolated vertices, provided $k_1 > k_2 \geqslant 2$, $\alpha_1, \alpha_2 \geqslant 1$, and β,

$$\beta = \frac{(k_1^2 - 2k_1 - k_1k_2)\alpha_1 + (k_2^2 - 2k_2 - k_1k_2)\alpha_2}{k_1 + k_2}$$

is a non-negative integer. (Examples: $G = K_6 \cup K_2$ and $G = 9K_7 \cup 9K_2 \cup 7K_1$.)

The characterization of all (m, n)-graphs for which (17) holds seems to be difficult and remains a task for the future.

Relation (11) is the special case of (15) for $p = 1$. Setting $p = 0$ into the right-hand side of (15) we obtain (10). It can be shown that the right-hand side of (15) is a monotonously decreasing function of the parameter p. In particular, the upper bound (11) is better than (10).

Theorem 4. *The left-hand side inequality* (12) *holds for any* (n, m)*-graph, where* M *is given via Eq.* (8). *Equality* $LE(G) = 2\sqrt{M}$ *is attained if and only if* G *is the complete bipartite graph* $K_{n/2,n/2}$. *The right-hand side inequality* (12) *holds for graphs without isolated vertices. For such graphs, the equality* $LE(G) = 2M$ *is attained if and only if* G *is regular of degree* 1.

For graphs without edges, $LE(G) = M = 0$ and (12) is satisfied in a trivial manner. Therefore in what follows we assume that $m > 0$ and thus $n \geqslant 2$.

Proof of the left-hand side inequality. From

$$\left(\sum_{i=1}^{n} \gamma_i\right)^2 = 0$$

by taking into account (7) and the fact that $M > 0$, we obtain

$$2M = -2\sum_{i<j} \gamma_i \gamma_j = 2\left|\sum_{i<j} \gamma_i \gamma_j\right|$$

and thus

$$2M \leqslant 2\sum_{i<j} |\gamma_i||\gamma_j|. \tag{18}$$

Now, by (7) and (9),

$$LE(G)^2 = 2M + 2\sum_{i<j} |\gamma_i||\gamma_j|,$$

which combined with (18) yields $LE(G)^2 \geqslant 4M$.

It is easy to check that equality in (18) is obeyed by graphs with two vertices. Therefore we assume that $n \geqslant 3$.

Equality in (18) holds if and only if there is at most one positive-valued and at most one negative-valued γ_i, i.e.,

$$\gamma_1 > 0, \gamma_2 = \cdots = \gamma_{n-1} = 0, \gamma_n = -\frac{2m}{n} < 0. \tag{19}$$

From (19) and the fact that $n \geqslant 3$ follows that $\mu_{n-1} = 2m/n$.

Note that conditions (19) are not satisfied by complete graphs with more than two vertices, for which $\mu_{n-1} = n \neq 2m/n$. If G is not a complete graph, then by [4], $\delta \geqslant \mu_{n-1}$, where δ is the minimum vertex degree of G. On the other hand, $\delta \geqslant 2m/n$ implies that G is a regular graph, and then $M = m$. Then by Lemma 1 and Note 4, $LE(G) = 2\sqrt{M}$ if and only if G is the complete bipartite graph $K_{n/2,n/2}$. □

Proof of the right-hand side inequality. We start with relation (10). For a graph with m edges and no isolated vertex, $n \leqslant 2m$. Therefore,

$$LE(G) \leqslant \sqrt{2Mn} \leqslant \sqrt{2M(2m)} = 2\sqrt{Mm}.$$

Because $M \geqslant m$, we arrive at $\sqrt{Mm} \leqslant M$.

All inequalities occurring in the above reasoning become equalities in the case of regular graphs of degree 1. Consequently, $LE(G) = 2M$ holds for regular graphs of degree 1. For all other graphs $M = m$ and $n = 2m$ cannot hold at the same time. Therefore $LE(G) = 2M$ holds only for regular graphs of degree 1. □

By this the proof of Theorem 4 is completed. □

4. Dissimilarities between energy and Laplacian energy

In Note 1 three elementary properties of the graph energy are stated. Of these, only (a) has its direct analog for Laplacian energy. Indeed, from (9) is evident that $LE(G) \geqslant 0$ and we already know (from the proof of Theorem 2) that $LE(G) = 0$ if $m = 0$. If the graph G has at least one edge, then $\gamma_n = -2m/n$ is non-zero and, consequently, $LE(G) > 0$.

Observation 5 (*To be compared with Note* 1(b)). If the graph G consists of (disconnected) components G_1 and G_2, and if G_1 and G_2 have equal average vertex degrees, then $LE(G) = LE(G_1) + LE(G_2)$. Otherwise, the latter equality needs not be satisfied.

Proof. Let G, G_1, and G_2 be (n, m)-, (n_1, m_1)-, and (n_2, m_2)-graphs, respectively. Then from $2m_1/n_1 = 2m_2/n_2$ follows $2m/n = 2m_i/n_i$, $i = 1, 2$, implying

$$\begin{aligned} LE(G) &= \sum_{i=1}^{n_1+n_2} \left| \gamma_i - \frac{2m}{n} \right| = \sum_{i=1}^{n_1} \left| \gamma_i - \frac{2m_1}{n_1} \right| + \sum_{i=n_1+1}^{n_1+n_2} \left| \gamma_i - \frac{2m_2}{n_2} \right| \\ &= LE(G_1) + LE(G_2). \qquad \square \end{aligned}$$

If the condition $2m_1/n_1 = 2m_2/n_2$ is not obeyed, then it may be either $LE(G) > LE(G_1) + LE(G_2)$ or $LE(G) < LE(G_1) + LE(G_2)$ or, exceptionally, $LE(G) =$

$LE(G_1) + LE(G_2)$. It remains as an open problem to characterize the graphs satisfying each of these relations.

Consider now a graph G consisting of an (n_1, m)-graph G_1 (which, in addition, may have p components, $p \geqslant 1$) and of additional n_2 isolated vertices. Then

$$LE(G) = \sum_{i=1}^{n_1-p} \left| \mu_i(G_1) - \frac{2m}{n_1+n_2} \right| + (p+n_2)\frac{2m}{n_1+n_2}.$$

Observation 6 (*To be compared with Note* 1(c)). If n_2 is sufficiently large, then

$$LE(G) = 4m\frac{p+n_2}{n_1+n_2} < 4m. \tag{20}$$

Thus, in this case the Laplacian energy is independent of any other structural features of the graph G. In addition,

$$\lim_{n_2\to\infty} LE(G) = 4m.$$

Proof. For $i = 1, \ldots, n_1 - p$, and sufficiently large n_2,

$$\mu_i > \frac{2m}{n_1+n_2}$$

and therefore

$$LE(G) = \sum_{i=1}^{n_1-p} \left(\mu_i - \frac{2m}{n_1+n_2} \right) + (p+n_2)\,\frac{2m}{n_1+n_2},$$

which, in view of $\sum_{i=1}^{n_1-p} \mu_i = 2m$, is transformed into Eq. (20). □

What is "sufficiently large" in the above observation remains another open problem, to be resolved in the future.

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