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Graph Energy Change on Edge Deletion

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Abstract

The energy $\mathcal{E}(G)$ of a graph G is the sum of the absolute values of all eigenvalues of G. An interesting and "hard-to-crack" problem about graph energy was mentioned by Gutman in [The energy of a graph: old and new results]: *characterize the graphs G and their edges e for which $\mathcal{E}(G-e) < \mathcal{E}(G)$.* In this paper, we give a new sufficient condition for $\mathcal{E}(G-e) < \mathcal{E}(G)$ where e is not necessarily to be a cut-edge set or a cut edge. This work can be used to generalize some well-known results.

1 Introduction

In this paper we are concerned with undirected simple graphs. Let $G = (V, E)$ be such a graph with n vertices and m edges, and $V = \{v_1, \ldots, v_n\}$. Denote $N(v)$ the neighbors of vertex v in G. Let $A(G)$ be the adjacency matrix of G whose (i, j)-entry is 1 if the vertices v_i and v_j are adjacent and 0 otherwise. Let $\lambda_i(\cdot)$ be the eigenvalues of a matrix of order n, and labelled in a non-increasing manner: $\lambda_1(\cdot) \geq \lambda_2(\cdot) \geq \cdots \geq \lambda_n(\cdot)$. The

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energy of graph is defined [6,7] as

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i(A(G))| = 2\sum_{+} \lambda_i(A(G))$$

with $\sum_+$ indicating summation over all positive-valued eigenvalues.

In theoretical chemistry, the energy of a graph has been extensively studied since it is related to the total π-electron energy of the molecule represented by that graph (see, e.g., [5,10,12]).

An interesting "hard-to-crack" problem about graph energy was mentioned by Gutman [7] in 2001: *characterize the graphs G and their edges e for which $\mathcal{E}(G-e) < \mathcal{E}(G)$.* This problem and related problems are called *graph energy change* in [15]. Day and So [3] studied the maximum amount of change of graph energy with edges deleted. Moreover, they gave a sufficient condition for $\mathcal{E}(G-e) \leq \mathcal{E}(G)$, that is, e a cut-edge set or a cut edge in [4]. A similar sufficient condition for weighted graph was pointed out by Gutman and Shao [10]. When G is a complete multipartite graph, the conditions for the sign of $\mathcal{E}(G-e)-\mathcal{E}(G)$ were determined in [1,14]. Additionally, the effects on the energy for adding edges among pendent vertices was explored by Rojo [13]. Even though some partial results along these lines have been obtained, the complete solution of this problem is still far from known.

In this paper, we determine a new sufficient condition for $\mathcal{E}(G-e) < \mathcal{E}(G)$ where e is not necessarily to be a cut-edge set or a cut edge, which can generalize some well-known results.

2 Preliminaries

As usual, let K_n be a complete graph of order n, and G^c be the complement of G. A *k-partite graph* is one whose vertices can be partitioned into k parts such that no edge has both ends in the same part. A *complete k-partite graph* is one whose any two vertices in different parts are adjacent. When $k = 2$, the graph is called complete bipartite graph and denoted by $K_{a,a}$ with $a = n/2$. A *complete k-partite graph* on n vertices whose parts are of equal or almost equal sizes (that is, $\lfloor n/k \rfloor$ or $\lceil n/k \rceil$) is called a *Turán graph* and denoted by $T_{k,n}$.

Let T be real $n \times n$ matrix with nonnegative entries. T is called irreducible if for all i, j there is a k such that $(T^k)_{ij} > 0$. If graph G is connected, then it is easy to check that $A(G)$ is irreducible.

Let $x_1, \ldots, x_n$ be n vectors, and $\text{span}\{x_1, \ldots, x_n\}$ be the vector space spanned by those vectors. Let X be a vector space, and let $\dim X$ denote the dimension of X.

3 Main Results

Theorem 1. *Suppose G is a graph of order n with a given vertex set U such that induced subgraph $G[U]$ is a complete bipartite graph $K_{a,a}$, and $N(v) \setminus U = N(u) \setminus U$ for any $v, u \in U$. Then $\mathcal{E}(G) > \mathcal{E}(G - E(G[U]))$, i.e., deleting all edges of $G[U]$ from G will decrease $\mathcal{E}(G)$.*

Proof. It may be assumed that G is connected, otherwise we only have to consider the component containing vertex set U since the energy of a graph equals to the sum of all its components' energy.

Let $G' = G - E(G[U])$. Let $r = |N(v) \setminus U|$ for $v \in U$. If $r = 0$, then $G = G[U]$, so $\mathcal{E}(G) > 0 = \mathcal{E}(G')$. We may therefore assume that $r > 0$, then G' is connected because G is connected.

Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ with $U = \{v_1, \ldots, v_{2a}\}$, and $H = G - U$. Let $X = \begin{pmatrix} \mathbf{0}_{a\times a} & J_{a\times a} \\ J_{a\times a} & \mathbf{0}_{a\times a} \end{pmatrix}$, $Y = \begin{pmatrix} J_{2a\times r} & \mathbf{0}_{2a\times(n-2a-r)} \end{pmatrix}$, and $B = \begin{pmatrix} X & \mathbf{0}_{2a\times(n-2a)} \\ \mathbf{0}_{(n-2a)\times 2a} & \mathbf{0}_{(n-2a)\times(n-2a)} \end{pmatrix}$, where $J_{i\times j}$ is an $i \times j$ matrix whose entries are all 1. Now we can write $A(G)$ and $A(G')$ as

$$A(G') = \begin{pmatrix} \mathbf{0}_{2a\times 2a} & Y \\ Y^T & A(H) \end{pmatrix}, \qquad A(G) = A(G') + B.$$

Note that G can always be relabelled to make $A(G)$ to have this form.

Let $\{p_i\}_{i=1}^n$, $\{q_i\}_{i=1}^n$ and $\{w_i\}_{i=1}^n$ be orthonormal lists of eigenvectors of $A(G'), B$ and $A(G)$, arranged as the same order as eigenvalues. Note that the eigenvalues of B are $\{a, 0^{n-2}, -a\}$, and the eigenvector of $-a$ is $q_n = \frac{1}{\sqrt{2a}} \begin{pmatrix} J_{1\times a} & -J_{1\times a} & \mathbf{0}_{1\times(n-2a)} \end{pmatrix}^T$. It can be verified that $A(G')q_n = \mathbf{0}$, that is, q_n is also an eigenvector of $\lambda_k(A(G')) = 0$. We may assume that $\lambda_k(A(G'))$ is the first eigenvalue of $A(G')$ to be zero, i.e., $\lambda_i(A(G')) > 0$ for $i < k$, and $\lambda_i(A(G')) \le 0$ otherwise.

For a given $1 \le j < k$, let $S_1 = \operatorname{span}\{p_1, \dots, p_j\}$, $S_2 = \operatorname{span}\{q_1, \dots, q_{n-1}\}$, and $S_3 = \operatorname{span}\{w_j, \dots, w_n\}$. Since $q_n \in \operatorname{span}\{p_{j+1}, \dots, p_n\}$, that is $q_n \notin S_1$ and q_n is orthogonal to S_1, hence

$$\begin{aligned}\dim(S_1 \cap S_2) + \dim S_3 &= \dim(S_1 \cap \operatorname{span}\{q_1, \dots, q_n\}) + \dim S_3 \\ &= \dim S_1 + \dim S_3 = j + (n - j + 1) = n + 1 > n.\end{aligned}$$

So there is a unit vector $x \in (S_1 \bigcap S_2) \bigcap S_3$, and by appealing to Rayleigh Theorem [11, Theorem 4.2.2] three times, we get

$$\begin{aligned}\lambda_j(A(G)) &= w_j^T A(G) w_j \ge x^T A(G) x = x^T A(G') x + x^T B x \\ &\ge p_j^T A(G') p_j + q_{n-1}^T B q_{n-1} \\ &= \lambda_j(A(G')) + \lambda_{n-1}(B) = \lambda_j(A(G')).\end{aligned}$$

Furthermore, $A(G')$ is irreducible and nonnegative since G' is connected. By Perron-Frobenius Theorem [11, Theorem 8.4.4], all entries of p_1 are positive. Therefore

$$\begin{aligned}\lambda_1(A(G)) - \lambda_1(A(G')) &\ge p_1^T A(G) p_1 - p_1^T A(G') p_1 \\ &= p_1^T B p_1 > 0. \qquad \text{(since } r > 0\text{)}\end{aligned}$$

So we have

$$\begin{aligned}\mathcal{E}(G') = 2\sum_{+} \lambda_i(A(G')) &= 2\left(\lambda_1(A(G')) + \sum_{j=2}^{k-1} \lambda_j(A(G'))\right) \\ &< 2\left(\lambda_1(A(G)) + \sum_{j=2}^{k-1} \lambda_j(A(G))\right) \le \mathcal{E}(G),\end{aligned}$$

that is, $\mathcal{E}(G') < \mathcal{E}(G)$ holds as desired. ■

Set $K_{a,a} = K_{1,1}$, and we have the following corollary immediately.

Corollary 1. *Suppose G is a graph with a given edge uv such that $N(v) \setminus \{u\} = N(u) \setminus \{v\}$, then $\mathcal{E}(G) > \mathcal{E}(G - uv)$, i.e., deleting edge uv will decrease the energy of G.*

4 Applications

As an example, the assertion that $\mathcal{E}(K_n) > \mathcal{E}(K_n - e)$ for any edge e of K_n can be found in [4,9]. The following lemmas generalize this result.

Lemma 1. *Suppose M_1 and M_2 are two matchings of K_n with $n \geq 2$. If $|M_1| < |M_2|$, then $\mathcal{E}(K_n - M_1) > \mathcal{E}(K_n - M_2)$.*

Proof. First consider the case $M_1 \subset M_2$, and let $M_2 \setminus M_1 = \{v_1u_1, \ldots, v_ku_k\}$ with $k > 0$. Let $G_0 = K_n - M_1$, and $G_i = G_{i-1} - v_iu_i$ for $i = 1, \ldots, k$. Note that $G_k = K_n - M_1 - (M_2 \setminus M_1) = K_n - M_2$. And it is not difficult to check that $N(v_i) \setminus \{u_i\} = N(u_i) \setminus \{v_i\}$ in G_{i-1} for $i = 1, \ldots, k$. Hence $\mathcal{E}(G_{i-1}) > \mathcal{E}(G_i)$ by Corollary 1. Therefore, we have $\mathcal{E}(K_n - M_1) > \mathcal{E}(K_n - M_2)$.

If $M_1 \not\subset M_2$, we claim that $K_n - M_1$ is isomorphic to $K_n - M_1'$ for any $M_1' \subset M_2$ with $|M_1| = |M_1'|$. To prove this, we relabel $K_n - M_1$ and $K_n - M_1'$ in the following way: first label all vertices of degree $n-1$, then label any vertex v of degree $n-2$ with the one not adjacent to v until all vertices are labelled. Now it is not hard to check that the vertices with the same label in $K_n - M_1$ and $K_n - M_1'$ have neighbors with the same labels. Therefore $\mathcal{E}(K_n - M_1) = \mathcal{E}(K_n - M_1') > \mathcal{E}(K_n - M_2)$. So the proof is complete. ■

Remark. Take $M_1 = \emptyset, |M_2| = 1$, and we get the original result.

Lemma 2. *Suppose $U = \{v_1, v_2, v_3, v_4\}$ is a subset of vertices of K_n with $n \geq 4$. Then $\mathcal{E}(K_n) > \mathcal{E}(K_n - \{v_1v_2, v_3v_4\}) > \mathcal{E}(K_n - E(K_n[U]))$.*

Proof. Since $\{v_1v_2, v_3v_4\}$ is a matching of K_n, then by Lemma 1 we have $\mathcal{E}(K_n) > \mathcal{E}(K_n - \{v_1v_2, v_3v_4\})$.

Let $G = K_n - \{v_1v_2, v_3v_4\}$, then $K_n - E(K_n[U]) = G - G[U]$. Note that $G[U]$ is a $K_{2,2}$, and $N(v) \setminus U = V(K_n) \setminus U$ for each $v \in U$. By appealing to Theorem 1, we obtain $\mathcal{E}(K_n - \{v_1v_2, v_3v_4\}) = \mathcal{E}(G) > \mathcal{E}(G - G[U]) = \mathcal{E}(K_n - E(K_n[U])$. Therefore it follows the result clearly. ■

Corollary 1 can be restated from the view of edge addition.

Lemma 3. *Suppose G is a graph with two non-adjacent vertices u and v such that $N(v) = N(u)$, then $\mathcal{E}(G) < \mathcal{E}(G + uv)$, i.e., adding edge uv to G will increase the energy of G.*

Analogously to Lemma 1, we can establish the following relation for *complete k-partite graph* and matchings of its complement.

Lemma 4. *Let G be a complete k-partite graph with $k \geq 2$. Suppose M_1 and M_2 are two matchings of G^c. If $M_1 \subset M_2$, then $\mathcal{E}(G + M_1) < \mathcal{E}(G + M_2)$.*

Proof. Let $M_2 \setminus M_1 = \{v_1u_1, \ldots, v_ku_k\}$ with $k > 0$. Let $G_0 = G + M_1$, and $G_i = G_{i-1} + v_iu_i$ for $i = 1, \ldots, k$. Note that $G_k = G + M_1 + (M_2 \setminus M_1) = G + M_2$. For $i = 1, \ldots, k$, we have $N(v_i) \setminus \{u_i\} = N(u_i) \setminus \{v_i\}$ in G_i. Hence $\mathcal{E}(G_{i-1}) < \mathcal{E}(G_i)$ by Corollary 1. Therefore, we have $\mathcal{E}(G + M_1) < \mathcal{E}(G + M_2)$. ■

Remark. It is not hard to see that Lemma 4 holds when G is a star or a *Turán graph*.

In 2015, Wang and So [15] suggested following conjecture.

Conjecture 1. *There is no graph G such that $\mathcal{E}(G) = \mathcal{E}(G - e)$ for each edge e.*

They noted that: *since the deletion of a cut-edge from a graph decreases its energy, a counterexample to Conjecture 1 cannot have any cut-edge.* Then it is easy to see that a counterexample to Conjecture 1 cannot have an edge uv such that $N(v) \setminus \{u\} = N(u) \setminus \{v\}$. This may be helpful to solve the conjecture.

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