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On the Energy of a Graph and Its Vertex–Deleted Subgraphs

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Abstract

Gutman defined the energy $\mathcal{E}(G)$ of a simple graph G with vertex set $V = \{v_1, v_2, \ldots, v_n\}$ as the sum of the absolute values of eigenvalues of the adjacency matrix of G, which has been studied extensively in mathematical chemistry. Espinal and Rada (Graph energy change due to vertex deletion, MATCH Commun. Math. Comput. Chem. 92(2024), 89-103) proved that

$$(n-2)\mathcal{E}(G) \leq \sum_{i=1}^{n} \mathcal{E}(G - v_i).$$

In this paper, we generalize the above result by Espinal and Rada and prove that for any positive integer $k \leq n-2$, then

$$\binom{n-2}{k}\mathcal{E}(G) \leq \sum_{W \in \mathcal{G}_k} \mathcal{E}(G - W),$$

where $\mathcal{G}_k = \{W \subset V \,||W| = k\}$ and $G - W$ is the subgraph of G by deleting all vertices in W from G. Particularly, we show that if $n \geq 3$, then

$$\mathcal{E}(G) \leq \frac{2}{n-2}(2a + \sqrt{2}b + c),$$

where a, b and c are the numbers of triangles in G, induced subgraphs of G isomorphic to P_3 and $K_2 \cup K_1$, respectively.

1 Introduction

Suppose that $A(G) = (a_{ij})_{n\times n}$ is the adjacency matrix of a simple graph G with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$, where $a_{ij} = 1$ if $v_iv_j \in E(G)$ and $a_{ij} = 0$ otherwise. Note that $A(G)$ is a symmetric $(0,1)$-matrix and hence all eigenvalues of $A(G)$ (which are called the eigenvalues of G) are real numbers, denoted by $\lambda_1(G) \geq \lambda_2(G) \ldots \geq \lambda_n(G)$. Gutman [8] defined the energy $\mathcal{E}(G)$ of G as

$$\mathcal{E}(G) = |\lambda_1(G)| + |\lambda_2(G)| + \cdots + |\lambda_n(G)|,$$

which has been studied extensively in mathematical chemistry (see for example the book [10] and survey [9]).

If G_1 and G_2 are vertex disjoint graphs, we use $G_1 \cup G_2$ to denote the vertex disjoint union of G_1 and G_2. Suppose that G is a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. For a given vertex subset $V_1 \subset V(G)$ (resp. a given edge subset $E_1 \subset E(G)$), we use $G - V_1$ (resp. $G - E_1$) to denote the subgraph of G obtained from G by deleting all vertices in V_1 from G (resp. by deleting all edges in E_1 from G). Particularly, we use G_i to denote the vertex-deleted graph $G - v_i$. For any vertex $u \in V(G)$, we use $N_G(u)$ to denote the set of vertices of G incident with u and $d(u) = |N_G(u)|$. Let P_n, K_n and $K_{1,n-1}$ denote the path, complete graph and star with n vertices, respectively.

It is well known that to delete an edge e from a simple graph G may increase or decrease the energy. For example, if e is a cut edge of G, then $\mathcal{E}(G - e) < \mathcal{E}(G)$ (see [4]), and for any edge f in a complete multipartite graph $K_{n_1,n_2,\ldots,n_s}$, then (see [1])

$$\mathcal{E}(K_{n_1,n_2,\ldots,n_s} - f) > \mathcal{E}(G).$$

The energy of edge-deleted subgraphs of a graph has been studied extensively see for example [1, 2, 11–15].

It is very different from the edge-deleted case that to delete a non-isolated vertex v from a graph G will decrease the energy. That is, if v is a non-isolated vertex of G, then $\mathcal{E}(G - v) < \mathcal{E}(G)$. Recently, Espinal and

Rada [5] proved the following results:

Theorem 1 (Espinal and Rada, [5]). *Suppose that v is a vertex of a simple graph G with degree $d(v)$. Then*

$$0 \leq \mathcal{E}(G) - \mathcal{E}(G - v) \leq 2\sqrt{d(v)}$$

with the left equality if and only if v is an isolated vertex of G and with right equality if and only if the component of G containing vertex v is a star with center v.

In 2026, Espinal and Rada [6] studied the variation of the graph energy under the deletion of a set of vertices, which extends the above result. They proved that for any subset $S \in V(G)$, then

$$\mathcal{E}(G) - \mathcal{E}(G - S) \leq 2\sum_{v \in S} \sqrt{d(v)}. \tag{1}$$

Theorem 2 (Espinal and Rada, [5]). *Let G be a simple graph with vertex set $\{v_1, v_2, \ldots, v_n\}$. Then*

$$(n-2)\mathcal{E}(G) \leq \sum_{i=1}^{n} \mathcal{E}(G - v_i). \tag{2}$$

Espinal and Rada [5] posed also the question characterizing the graphs such that $(n-2)\mathcal{E}(G) = \sum_{i=1}^{n} \mathcal{E}(G - v_i)$.

In this short note, as an extension of Theorem 2, we consider the relation between the energies of G and all k-vertex-deleted subgraphs of G, and some new upper bounds of $\mathcal{E}(G)$ are obtained.

2 Main results

By using the singular-value inequality found by Fan [7], Day and So [3] proved that for any two Hermitian matrices A and B of order n, then

$$\mathcal{E}(A + B) \leq \mathcal{E}(A) + \mathcal{E}(B), \tag{3}$$

where $\mathcal{E}(A)$ is the sum of the absolute values of eigenvalues of A. By Ineq. (3), they proved that for any edge e of G, then

$$\mathcal{E}(G) \leq 2 + \mathcal{E}(G - e)$$

with equality if and only if e is one of components of G, which results in the following upper bound of $\mathcal{E}(G)$ [12]:

$$\mathcal{E}(G) \leq 2m \tag{4}$$

with equality if and only if $G = mK_2 \cup (n - 2m)K_1$, which is a previously known upper bound of $\mathcal{E}(G)$ in [2].

In this section, we prove mainly the following result.

Theorem 3. *Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, and let $\mathcal{G}_k$ be the set of all subsets W of $V(G)$ satisfying $|W| = k$ for some positive integer $1 \leq k \leq n - 2$. Then*

$$\binom{n-2}{k}\mathcal{E}(G) \leq \sum_{W \in \mathcal{G}_k} \mathcal{E}(G - W). \tag{5}$$

Proof. Let $A(G)$ be the adjacency matrix of G. For any $W \in \mathcal{G}_k$, we use G_W to denote the subgraph of G by delete all edges incident vertices in W. Hence G_W has vertex set $V(G_W) = V(G)$ and edge set $E(G_W) = E(G - W)$. We first prove that $A(G)$ and $\{A(G_W) | W \in \mathcal{G}_k\}$ satisfy the following equality:

$$\binom{n-2}{k}A(G) = \sum_{W \in \mathcal{G}_k} A(G_W). \tag{6}$$

Set

$$B = \binom{n-2}{k}A(G) = (b_{ij})_{n \times n}, \ C = \sum_{W \in \mathcal{G}_k} A(G_W) = (c_{ij})_{n \times n}.$$

It is obvious that if $v_iv_j \notin E(G)$, then $b_{ij} = c_{ij} = 0$. If $v_iv_j \in E(G)$, then $b_{ij} = \binom{n-2}{k}$. On the other hand, there exist $\binom{n-2}{k}$ subsets W in $\mathcal{G}_k$ such that $v_i, v_j \notin W$ and hence there exist exactly $\binom{n-2}{k}$ subgraphs G_W's in $\{G_W | W \in \mathcal{G}_k\}$ containing edge v_iv_j. So $c_{ij} = \binom{n-2}{k}$, and Eq.(5) holds.

Hence, by Ineq. (3) and Eq. (6),

$$\binom{n-2}{k}\mathcal{E}(G) \leq \sum_{W \in \mathcal{G}_k} \mathcal{E}(G_W). \tag{7}$$

Note that each vertex in W is an isolated vertex of G_W and so G_W and $G-W$ have the same energy. The theorem is immediate from Ineq. (7). ■

Remark. Set $k = 1$ or $k = n-2$ in Theorem 3. Then we can obtain Ineqs. (2) and (4), respectively.

The following corollary is immediate from Theorem 3.

Corollary 1. *Let G be a simple graph with n vertices. Then for any positive integer $1 \leq k \leq n-2$, then there exists a $W^* \in \mathcal{G}_k$ such that*

$$\mathcal{E}(G) \leq \frac{n(n-1)}{(n-k-1)(n-k)}\mathcal{E}(G - W^*).$$

Particularly, there exists a vertex $v \in V(G)$ such that

$$\mathcal{E}(G) \leq \frac{n}{n-2}\mathcal{E}(G - v).$$

Proof. Set $\mathcal{E}(G - W^*) = \max\{\mathcal{E}(G - W) | W \in \mathcal{G}_k\}$. Then the corollary is immediate. ■

Corollary 2. *Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ $(n \geq 3)$. Then*

$$\mathcal{E}(G) \leq \frac{2}{n-2}(2a + \sqrt{2}b + c),$$

where a, b and c are the numbers of triangles in G, induced subgraphs of G isomorphic to P_3 and $K_1 \cup K_2$, respectively. Particularly, if G is a *triangle-free graph, then*

$$\mathcal{E}(G) \leq \frac{2}{n-2}(\sqrt{2}b + c). \tag{8}$$

Proof. We only need to prove that the first inequality holds, which can directly result in Ineq. (8). Set $k = n - 3$ in Theorem 3. Then

$$\binom{n-2}{n-3}\mathcal{E}(G) \leq \sum_{W \in \mathcal{G}_{n-3}} \mathcal{E}(G - W),$$

that is,

$$(n-2)\mathcal{E}(G) \leq \sum_{W \in \mathcal{G}_{n-3}} \mathcal{E}(G - W). \tag{9}$$

For any $W \in \mathcal{G}_{n-3}$, since $|W| = n - 3$, $G - W$ is an induced subgraph of G with three vertices, which is isomorphic to one in $\{K_3, P_3, K_1 \cup K_2, K_1 \cup K_1 \cup K_1\}$. Note that

$$\mathcal{E}(K_3) = 4,\ \mathcal{E}(P_3) = 2\sqrt{2},\ \mathcal{E}(K_1 \cup K_2) = 2,\ \mathcal{E}(K_1 \cup K_1 \cup K_1) = 0.$$

The corollary is immediate from Ineq. (9). ■

Theorem 4. *Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$ such that for any edge $e = uv$ of G, $d(u) + d(v) = k + 2$ is a constant. Then*

$$\mathcal{E}(G) \leq \frac{1}{m-k}\left[\sum_{uv \in E(G)} \mathcal{E}(G - u - v) + 2m\right]. \tag{10}$$

Proof. For any vertex $v_i \in V(G)$, let E_{v_i} be the set of edges of G incident with vertex v_i. Given any $f = uv \in E(G)$, we set $E_f = E_{uv} = (E_u \cup E_v) \setminus \{f\}$ and $G_f = G - E_f$. Obviously, G_f is a spanning subgraph of G with vertex set $V(G)$ and edge set $E(G) \setminus E_f$. Particularly, the subgraph of G induced by edge $f = uv$ is one component of G_f. Hence

$$\mathcal{E}(G_f) = \mathcal{E}(G - u - v) + 2. \tag{11}$$

We now prove that $A(G)$ and $\{A(G_f)|f \in E(G)\}$ satisfy the following equality:

$$(m-k)A(G) = \sum_{f=uv \in E(G)} A(G_f). \tag{12}$$

Set

$$P = (m-k)A(G) = (p_{ij})_{n\times n}$$

and

$$Q = \sum_{f=uv \in E(G)} A(G_f) = (q_{ij})_{n\times n}.$$

It is obvious that if $v_iv_j \notin E(G)$, then $p_{ij} = q_{ij} = 0$. If $v_iv_j \in E(G)$, then $p_{ij} = m - k$. On the other hand, for any $f \in E_{v_iv_j}$, $v_iv_j \notin E(G_f)$, and for any $f \in E(G) \setminus E_{v_iv_f}$, $v_iv_j \in E(G_f)$. Hence

$$q_{ij} = |E(G)| - |E_{v_iv_j}| = m - [d(v_i) - 1 + d(v_j) - 1] = m - k.$$

Hence we have proved that Eq. (12) holds.

So the theorem is immediate from Ineq. (3) and Eqs. (11) and (12). ■

The following result is a direct corollary of the theorem above.

Corollary 3. *Let G be a simple graph with n vertices and m edges such that for any edge $e = uv$ of G, $d(u) + d(v) = k + 2$ is a constant. Let $st \in E(G)$ satisfying $\mathcal{E}(G - s - t) = \max\{\mathcal{E}(G - u - v)|e = uv \in E(G)\}$. Then*

$$\mathcal{E}(G) \leq \frac{m}{m-k}\left[\mathcal{E}(G - s - t) + 2\right]. \tag{13}$$

Particularly, if G is an edge-transive graph. Then, for any edge uv of G,

$$\mathcal{E}(G) \leq \frac{m}{m-k}\left[\mathcal{E}(G - u - v) + 2\right]. \tag{14}$$

Remark. Suppose that a graph G is r-regular or (a, b)-semiregular. Let $k = 2r - 2$ or $k = a + b - 2$. Then G is a graph satisfying that for any edge $e = uv$, $d(u) + d(v) = k$. Hence there exist many graphs satisfying the condition in Theorem 4 and Corollary 3.

3 Discussion

In this note, we mainly consider the relation between the energy $\mathcal{E}(G)$ of a simple graph G with n vertices ($n \geq 3$) and m edges and the energies of all k-vertex-deleted subgraphs of G, which is different from the Espinal-Rada result (1). In fact, Espinal and Rada considered the relation between $\mathcal{E}(G)$ and $\mathcal{E}(G-S)$ for some $S \in V(G)$.

Moreover, we obtain an upper bound of $\mathcal{E}(G)$ in Corollary 2 as follows:

$$\mathcal{E}(G) \leq \frac{2}{n-2}(2a + \sqrt{2}b + c), \tag{15}$$

where a, b and c are the numbers of triangles in G, induced subgraphs of G isomorphic to P_3 and $K_1 \cup K_2$, respectively. It is not difficult to show that if $G = K_3$ or $G = mK_2 \cup (n-2m)K_1$, then equality in Ineq. (15) holds. So a natural problem is:

Problem 1. Determine the graphs G with n vertices satisfying

$$\mathcal{E}(G) = \frac{2}{n-2}(2a + \sqrt{2}b + c).$$

On the other hand, if G is a simple graph with m edges and any for any edge $e = uv \in E(G)$, $d(u) + d(v) = k + 2$ is a constant, then, by Theorem 4, Ineq. (10) holds. Note that if $G = mK_2 \cup (n-2m)K_1$, then equality in Ineq. (10) holds. Hence the following problem is interesting:

Problem 2. Determine the graphs G with m edges such that the equality in Ineq. (10) holds.

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