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Equality Cases for Energies of Vertex-Deleted Subgraphs

Juan Rada

Instituto de Matemáticas, Universidad de Antioquia, Medellín, Colombia
pablo.rada@udea.edu.co

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Abstract

Let G be a simple graph of order n, and let $\mathcal{E}(G)$ denote its energy. In a recent paper in *MATCH Commun. Math. Comput. Chem.*, Ye proved a lower bound for the sum of the energies of all induced subgraphs obtained by deleting a prescribed number of vertices. In this paper, we determine all equality cases in this inequality. More precisely, we prove that equality holds if and only if G is a disjoint union of copies of K_2 and isolated vertices. Our proof is based on the equality condition in the triangle inequality for the nuclear norm. As an application, we solve an open problem of Ye concerning an upper bound for graph energy in terms of the numbers of induced subgraphs isomorphic to K_3, P_3, and $K_2 \cup K_1$.

1 Introduction

Throughout this paper, all graphs are finite, simple, and undirected. We write $G \cong H$ to mean that G and H are isomorphic. Let G be a graph of order n, and let $A(G)$ be its adjacency matrix. If $\lambda_1(G), \ldots, \lambda_n(G)$ are the adjacency eigenvalues of G, then its energy is defined by

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

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Since $A(G)$ is real and symmetric, $\mathcal{E}(G)$ is the nuclear norm of its adjacency matrix:

$$\mathcal{E}(G) = \|A(G)\|_* .$$

The concept was introduced by Gutman [5] in connection with the Hückel molecular orbital approximation for the total π-electron energy of conjugated hydrocarbons. Since then, graph energy has become a widely studied invariant in mathematical chemistry and spectral graph theory. We refer to [6, 7] for historical background, fundamental results, and further references.

The quantity $\mathcal{E}(G)$ is a spectral invariant of the whole graph. Espinal and Rada [3] introduced a vertex-dependent quantity, the deletion-based local vertex energy, by setting

$$\mathcal{E}_G(v) = \mathcal{E}(G) - \mathcal{E}(G - v). \tag{1}$$

Thus, $\mathcal{E}_G(v)$ is defined by comparing the energies of G and $G - v$ and measures the change caused by deleting v. Several subsequent works have developed this deletion-based approach. Rakshith and Das [10] studied simultaneous deletion of vertices with a common neighborhood, obtained results for complete multipartite graphs, and derived bounds for the total local energy. Dede and Popat [2] introduced and investigated pairs of locally equienergetic graphs. Cruz, Franco, and Rada [1] determined extremal local vertices in broom and double-star trees, while Espinal and Rada [4] studied deletion of vertex sets and extended local energy to digraphs. Moon and Park [8] studied the change in Laplacian energy under vertex deletion, obtained a sharp upper bound and characterized its equality cases, and introduced a corresponding notion of local Laplacian energy, which they related to the Laplacian energy of the graph. Rada [9] subsequently proved that

$$\sum_{v \in V(G)} \mathcal{E}_G(v) \leq 2\mathcal{E}(G), \tag{2}$$

with equality if and only if every connected component of G is isomorphic to K_2 or K_1, and introduced an adjusted local vertex energy that yields an exact additive decomposition of $\mathcal{E}(G)$.

For a vertex set $W \subseteq V(G)$, we write $G - W$ for the graph obtained by deleting all vertices in W. For $0 \leq k \leq n$, define

$$\mathcal{V}_k(G) = \{W \subseteq V(G) : |W| = k\}.$$

Thus, $\mathcal{V}_k(G)$ is the family of all k-element subsets of $V(G)$.

In a recent paper in *MATCH Commun. Math. Comput. Chem.*, Ye [11] proved that

$$\binom{n-2}{k}\mathcal{E}(G) \leq \sum_{W \in \mathcal{V}_k(G)} \mathcal{E}(G - W), \qquad 1 \leq k \leq n-2. \tag{3}$$

The equality cases in (3) remained undetermined. In this paper, we characterize them completely and show that equality for one admissible value of k is equivalent to equality for every admissible value of k. The main structural step is to prove that equality for some admissible value of k implies equality for $k = 1$. Combining this reduction with the known equality characterization in (2), we obtain the following theorem.

Theorem 1. *Let G be a graph of order $n \geq 3$. Equality holds in* (3) *for some integer k with $1 \leq k \leq n-2$ if and only if*

$$G \cong rK_2 \cup (n-2r)K_1$$

for some integer r with $0 \leq r \leq \lfloor n/2 \rfloor$.

As a consequence, we solve an open problem posed by Ye [11]. More precisely, Corollary 1, applied to (3) with $k = n-3$, shows that, for $n \geq 4$, equality in

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

holds if and only if G is a disjoint union of copies of K_2 and isolated vertices. Here a, b, and c denote the numbers of induced subgraphs of G isomorphic to K_3, P_3, and $K_2 \cup K_1$, respectively.

2 Preliminaries

Let $M_n(\mathbb{R})$ be the space of real $n \times n$ matrices and $\mathrm{O}(n)$ the orthogonal group. For $M \in M_n(\mathbb{R})$, $\|M\|_*$ is the sum of its singular values.

A matrix $X \in M_n(\mathbb{R})$ is called positive semidefinite, denoted by $X \succeq 0$, if $X = X^\mathsf{T}$ and $x^\mathsf{T} X x \geq 0$ for all $x \in \mathbb{R}^n$.

We first recall the variational characterization of the nuclear norm, together with its equality condition. This is a standard form of von Neumann's trace theorem; see [9, Theorem 2.1].

Theorem 2 (von Neumann's trace theorem)**.** *For every $M \in M_n(\mathbb{R})$,*

$$\|M\|_* = \max_{Q \in \mathrm{O}(n)} \mathrm{tr}(QM).$$

Moreover, for $Q \in \mathrm{O}(n)$,

$$\mathrm{tr}(QM) = \|M\|_* \quad \Longleftrightarrow \quad QM \succeq 0.$$

The equality condition in Theorem 2 concerns a single matrix. In the reduction argument below, however, we shall need one orthogonal matrix that realizes equality simultaneously for an entire family of symmetric matrices. The following finite-family real symmetric formulation provides precisely such a common orthogonal factor; see [9, Lemma 2.3].

Lemma 1. *Let $X_1, \ldots, X_s \in M_n(\mathbb{R})$ be symmetric matrices. If*

$$\left\| \sum_{i=1}^{s} X_i \right\|_* = \sum_{i=1}^{s} \|X_i\|_* ,$$

then there exists a symmetric orthogonal matrix $P \in \mathrm{O}(n)$ such that

$$PX_i \succeq 0 \quad \textit{and} \quad PX_i = X_i P, \qquad i = 1, \ldots, s.$$

Remark. Theorem 2 and Lemma 1 will play complementary roles. The lemma converts equality in the triangle inequality for the nuclear norm into simultaneous positive semidefiniteness. By summing suitable subfamilies of the deleted adjacency matrices, we shall transfer this positivity from

deletion of k vertices to deletion of a single vertex. The theorem will then convert the resulting positive semidefinite relations into nuclear-norm identities. This is the mechanism behind the reduction principle proved in the next section. Only the simultaneous positive semidefiniteness assertion of Lemma 1 is needed in this argument.

3 Deletion of k vertices

In this section we prove Theorem 1. The first step is the reduction from an arbitrary admissible value of k to the case $k = 1$.

Let $A = A(G)$. For each $W \subseteq V(G)$, let B_W be the $n \times n$ matrix obtained from A by replacing the rows and columns indexed by W with zero rows and columns. Thus, B_W is permutation-similar to $A(G - W) \oplus 0_{|W|}$, and hence

$$\|B_W\|_* = \mathcal{E}(G - W). \tag{4}$$

If $W = \{v\}$, we simply write B_v instead of $B_{\{v\}}$.

We first record a simple counting identity. Every edge of G survives in $G - W$ for exactly $\binom{n-2}{k}$ sets $W \in \mathcal{V}_k(G)$. Therefore,

$$\sum_{W \in \mathcal{V}_k(G)} B_W = \binom{n-2}{k} A. \tag{5}$$

Entrywise, each edge $\{u, v\}$ contributes the two symmetric entries $A_{uv} = A_{vu} = 1$. Both entries survive precisely when $W \cap \{u, v\} = \varnothing$, which occurs for exactly $\binom{n-2}{k}$ choices of W. The zero entries of A remain zero. Identity (5) underlies Ye's proof of (3). By (4) and the triangle inequality for the nuclear norm,

$$\begin{aligned}\binom{n-2}{k}\mathcal{E}(G) = \binom{n-2}{k}\|A\|_* &= \left\| \sum_{W \in \mathcal{V}_k(G)} B_W \right\|_* \\ &\leq \sum_{W \in \mathcal{V}_k(G)} \|B_W\|_* = \sum_{W \in \mathcal{V}_k(G)} \mathcal{E}(G - W).\end{aligned}$$

This gives (3). More importantly for our purposes, it shows that equality

in (3) holds if and only if equality holds in the triangle inequality above.

To analyze the equality case, we shall need a second counting identity. Fix $v \in V(G)$. Every edge not incident with v survives for exactly $\binom{n-3}{k-1}$ sets $W \in \mathcal{V}_k(G)$ containing v. It follows that

$$\sum_{\substack{W \in \mathcal{V}_k(G) \\ v \in W}} B_W = \binom{n-3}{k-1} B_v. \tag{6}$$

Proposition 3. *Let G be a graph of order $n \geq 3$. If equality holds in (3) for some integer k with $1 \leq k \leq n-2$, then*

$$(n-2)\mathcal{E}(G) = \sum_{v \in V(G)} \mathcal{E}(G - v). \tag{7}$$

Proof. Suppose that equality holds in (3) for some integer k with $1 \leq k \leq n-2$, and fix such a k. By the preceding nuclear-norm argument, equality must hold in the triangle inequality for the family $\{B_W : W \in \mathcal{V}_k(G)\}$. Hence

$$\left\| \sum_{W \in \mathcal{V}_k(G)} B_W \right\|_* = \sum_{W \in \mathcal{V}_k(G)} \|B_W\|_* .$$

Applying Lemma 1, we obtain a symmetric orthogonal matrix $P \in \mathrm{O}(n)$ such that

$$PB_W \succeq 0 \qquad \text{for every } W \in \mathcal{V}_k(G). \tag{8}$$

We next transfer this positive semidefiniteness to the matrices corresponding to single-vertex deletions. Fix $v \in V(G)$. Multiplying (6) on the left by P gives

$$\binom{n-3}{k-1} PB_v = \sum_{\substack{W \in \mathcal{V}_k(G) \\ v \in W}} PB_W.$$

Every matrix on the right-hand side is positive semidefinite by (8), and hence so is their sum. Therefore,

$$\binom{n-3}{k-1} PB_v \succeq 0.$$

Since $0 \le k-1 \le n-3$, we have $\binom{n-3}{k-1} > 0$. Consequently,

$$PB_v \succeq 0 \qquad \text{for every } v \in V(G). \tag{9}$$

We now show that the same orthogonal matrix also makes PA positive semidefinite. Applying (5) with $k = 1$ yields

$$\sum_{v \in V(G)} B_v = (n-2)A.$$

Multiplying this identity on the left by P and using (9), we obtain

$$(n-2)PA = \sum_{v \in V(G)} PB_v \succeq 0.$$

Since $n \ge 3$, we have $n - 2 > 0$, and therefore

$$PA \succeq 0.$$

Since $P \in \mathrm{O}(n)$, the equality condition in Theorem 2, applied first to each B_v and then to A, gives

$$\operatorname{tr}(PB_v) = \|B_v\|_* \qquad \text{for every } v \in V(G),$$

and

$$\operatorname{tr}(PA) = \|A\|_* .$$

Using these identities together with (4), we conclude that

$$\begin{aligned} \sum_{v \in V(G)} \mathcal{E}(G-v) &= \sum_{v \in V(G)} \operatorname{tr}(PB_v) \\ &= \operatorname{tr}\left(P \sum_{v \in V(G)} B_v \right) = (n-2)\operatorname{tr}(PA) = (n-2)\mathcal{E}(G). \end{aligned}$$ ■

We can now prove our main characterization.

Proof of Theorem 1. Assume first that equality holds in (3) for some integer k with $1 \le k \le n-2$. By Proposition 3, equality holds in (7). In

terms of (1), this gives

$$\begin{aligned}\sum_{v\in V(G)}\big(\mathcal{E}(G)-\mathcal{E}(G-v)\big) &= n\mathcal{E}(G)-\sum_{v\in V(G)}\mathcal{E}(G-v)\\ &= n\mathcal{E}(G)-(n-2)\mathcal{E}(G)\\ &= 2\mathcal{E}(G).\end{aligned}$$

The known equality characterization in (2) [9, Theorem 2.8] now implies that every connected component of G is isomorphic to K_2 or K_1. Thus

$$G \cong rK_2 \cup (n-2r)K_1$$

for some $0 \le r \le \lfloor n/2 \rfloor$.

Conversely, suppose that $G \cong rK_2 \cup (n-2r)K_1$, and let k be any integer with $1 \le k \le n-2$. For $W \in \mathcal{V}_k(G)$, let $q(W)$ be the number of copies of K_2 whose two vertices lie outside W. Since graph energy is additive over disjoint unions, while $\mathcal{E}(K_2) = 2$ and $\mathcal{E}(K_1) = 0$, we have

$$\mathcal{E}(G-W) = 2q(W).$$

Each of the r copies of K_2 survives for exactly $\binom{n-2}{k}$ choices of W. Double counting the pairs consisting of a surviving copy of K_2 and a set $W \in \mathcal{V}_k(G)$ gives

$$\sum_{W\in\mathcal{V}_k(G)} q(W) = r\binom{n-2}{k}.$$

Therefore,

$$\sum_{W\in\mathcal{V}_k(G)} \mathcal{E}(G-W) = 2r\binom{n-2}{k} = \binom{n-2}{k}\mathcal{E}(G).$$

Since k was arbitrary, equality holds in (3) for every admissible value of k, and hence for some admissible value of k. ■

The preceding proof shows, in particular, that equality for some admissible k is equivalent to equality for every admissible k. This yields the following formulation.

Corollary 1. *For a graph G of order $n \geq 3$, the following statements are equivalent:*

(i) equality holds in (3) *for some $k \in \{1, \ldots, n-2\}$;*

(ii) equality holds in (3) *for every $k \in \{1, \ldots, n-2\}$;*

(iii) every connected component of G is isomorphic to K_2 or K_1.

4 An open problem of Ye

Let a, b, and c denote, respectively, the numbers of induced subgraphs of G isomorphic to K_3, P_3, and $K_2 \cup K_1$. Ye [11, Corollary 2] proved that every graph G of order $n \geq 3$ satisfies

$$\mathcal{E}(G) \leq \frac{2}{n-2}\big(2a + \sqrt{2}\,b + c\big), \tag{10}$$

and posed the problem of determining all equality cases.

The connection with Corollary 1 follows by considering all induced subgraphs of order three. Indeed, the map

$$W \longmapsto V(G) \setminus W$$

is a bijection between $\mathcal{V}_{n-3}(G)$ and the three-element subsets of $V(G)$. Every induced subgraph of order three is isomorphic to exactly one of

$$K_3, \qquad P_3, \qquad K_2 \cup K_1, \qquad 3K_1,$$

whose energies are, respectively,

$$4, \qquad 2\sqrt{2}, \qquad 2, \qquad 0.$$

Consequently,

$$\sum_{W \in \mathcal{V}_{n-3}(G)} \mathcal{E}(G - W) = 4a + 2\sqrt{2}\,b + 2c. \tag{11}$$

We can now solve the problem of Ye.

Corollary 2. *Let G be a graph of order $n \geq 3$. If $n = 3$, then equality holds in* (10) *for every graph G. If $n \geq 4$, then equality holds in* (10) *if and only if*

$$G \cong rK_2 \cup (n-2r)K_1$$

for some integer r with $0 \leq r \leq \lfloor n/2 \rfloor$.

Proof. If $n = 3$, then G is isomorphic to one of K_3, P_3, $K_2 \cup K_1$, or $3K_1$. Their energies are, respectively, 4, $2\sqrt{2}$, 2, and 0, so equality follows directly from (10).

Now assume that $n \geq 4$. The integer $k = n - 3$ then satisfies $1 \leq k \leq n - 2$. The factorization

$$\begin{aligned}\frac{2}{n-2}\big(2a + \sqrt{2}\,b + c\big) &= \frac{1}{n-2}\big(4a + 2\sqrt{2}\,b + 2c\big) \\ &= \frac{1}{n-2}\sum_{W \in \mathcal{V}_{n-3}(G)} \mathcal{E}(G - W)\end{aligned}$$

follows from (11). Therefore, equality in (10) is equivalent to

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

This is equality in (3) for $k = n - 3$, so Corollary 1 applies. ■

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