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Note

The energy of graphs and matrices

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Abstract

Given a complex $m \times n$ matrix A, we index its singular values as $\sigma_1(A) \geqslant \sigma_2(A) \geqslant \cdots$ and call the value $\mathcal{E}(A) = \sigma_1(A) + \sigma_2(A) + \cdots$ the *energy* of A, thereby extending the concept of graph energy, introduced by Gutman. Let $2 \leqslant m \leqslant n$, A be an $m \times n$ nonnegative matrix with maximum entry α, and $\|A\|_1 \geqslant n\alpha$. Extending previous results of Koolen and Moulton for graphs, we prove that

$$\mathcal{E}(A) \leqslant \frac{\|A\|_1}{\sqrt{mn}} + \sqrt{(m-1)\left(\|A\|_2^2 - \frac{\|A\|_1^2}{mn}\right)} \leqslant \alpha \frac{\sqrt{n}(m+\sqrt{m})}{2}.$$

Furthermore, if A is any nonconstant matrix, then

$$\mathcal{E}(A) \geqslant \sigma_1(A) + \frac{\|A\|_2^2 - \sigma_1^2(A)}{\sigma_2(A)}.$$

Finally, we note that Wigner's semicircle law implies that

$$\mathcal{E}(G) = \left(\frac{4}{3\pi} + o(1)\right) n^{3/2}$$

for almost all graphs G.

Keywords: Graph energy; Graph eigenvalues; Singular values; Matrix energy; Wigner's semicircle law

Our notation is standard (e.g., see [3,4,9]); in particular, we write $M_{m,n}$ for the set of $m \times n$ matrices with complex entries, and A^* for the Hermitian adjoint of A. The singular values

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$\sigma_1(A) \geqslant \sigma_2(A) \geqslant \cdots$ of a matrix A are the square roots of the eigenvalues of AA^*. Note that if $A \in M_{n,n}$ is a Hermitian matrix with eigenvalues $\mu_1(A) \geqslant \cdots \geqslant \mu_n(A)$, then the singular values of A are the moduli of $\mu_i(A)$ taken in descending order.

For any $A \in M_{m,n}$, call the value $\mathcal{E}(A) = \sigma_1(A) + \cdots + \sigma_n(A)$ the *energy* of A. Gutman [7] introduced $\mathcal{E}(G) = \mathcal{E}(A(G))$, where $A(G)$ is the adjacency matrix of a graph G; in this narrow sense $\mathcal{E}(A)$ has been studied extensively (see, e.g., [2,8,10–14]). In particular, Koolen and Moulton [10] proved the following sharp inequalities for a graph G of order n and size $m \geqslant n/2$:

$$\mathcal{E}(G) \leqslant 2m/n + \sqrt{(n-1)\bigl(2m - (2m/n)^2\bigr)} \leqslant (n/2)(1+\sqrt{n}\,). \tag{1}$$

Moreover, Koolen and Moulton conjectured that for every $\varepsilon > 0$, for almost all $n \geqslant 1$, there exists a graph G with $\mathcal{E}(G) \geqslant (1-\varepsilon)(n/2)(1+\sqrt{n}\,)$.

In this note we give upper and lower bounds on $\mathcal{E}(A)$ and find the asymptotics of $\mathcal{E}(G)$ of almost all graphs G. We first generalize inequality (1) in the following way.

Theorem 1. *If $m \leqslant n$, A is an $m \times n$ nonnegative matrix with maximum entry α, and $\|A\|_1 \geqslant n\alpha$, then*

$$\mathcal{E}(A) \leqslant \frac{\|A\|_1}{\sqrt{mn}} + \sqrt{(m-1)\left(\|A\|_2^2 - \frac{\|A\|_1^2}{mn}\right)}. \tag{2}$$

From here we derive the following absolute upper bound on $\mathcal{E}(A)$.

Theorem 2. *If $m \leqslant n$ and A is an $m \times n$ nonnegative matrix with maximum entry α, then*

$$\mathcal{E}(A) \leqslant \alpha \frac{(m+\sqrt{m}\,)\sqrt{n}}{2}. \tag{3}$$

Note that Theorems 1 and 2 improve on the bounds for the energy of bipartite graphs given in [11].

On the other hand, for every $A \in M_{m,n}$ $(m, n \geqslant 2)$, we have $\sigma_1^2(A) + \sigma_2^2(A) + \cdots = \operatorname{tr}(AA^*) = \|A\|_2^2$, and so

$$\|A\|_2^2 - \sigma_1^2(A) = \sigma_2^2 + \cdots + \sigma_m^2 \leqslant \sigma_2(A)\bigl(\mathcal{E}(A) - \sigma_1(A)\bigr).$$

Thus, if A is a nonconstant matrix, then

$$\mathcal{E}(A) \geqslant \sigma_1(A) + \frac{\|A\|_2^2 - \sigma_1^2(A)}{\sigma_2(A)}. \tag{4}$$

If A is the adjacency matrix of a graph, this inequality is tight up to a factor of 2 for almost all graphs. To see this, recall that the adjacency matrix $A(n, 1/2)$ of the random graph $G(n, 1/2)$ is a symmetric matrix with zero diagonal, whose entries a_{ij} are independent random variables with $E(a_{ij}) = 1/2$, $\operatorname{Var}(a_{ij}^2) = 1/4 = \sigma^2$, and $E(a_{ij}^{2k}) = 1/4^k$ for all $1 \leqslant i < j \leqslant n$, $k \geqslant 1$. The result of Füredi and Komlós [6] implies that, with probability tending to 1,

$$\sigma_1\bigl(G(n,1/2)\bigr) = \bigl(1/2 + o(1)\bigr)n,$$
$$\sigma_2\bigl(G(n,1/2)\bigr) < \bigl(2\sigma + o(1)\bigr)n^{1/2} = \bigl(1 + o(1)\bigr)n^{1/2}.$$

Hence, inequalities (1) and (4) imply that

$$\bigl(1/2 + o(1)\bigr)n^{3/2} > \mathcal{E}(G) > \bigl(1/2 + o(1)\bigr)n + \frac{(1/4 + o(1))n^2}{(1 + o(1))n^{1/2}} = \bigl(1/4 + o(1)\bigr)n^{3/2}$$

for almost all graphs G.

Moreover, Wigner's semicircle law [15] (we use the form given by Arnold [1, p. 263]), implies that

$$\mathcal{E}\big(A(n,1/2)\big)n^{-1/2} = n\left(\frac{2}{\pi}\int_{-1}^{1}|x|\sqrt{1-x^2}\,dx + o(1)\right) = \left(\frac{4}{3\pi}+o(1)\right)n,$$

and so $\mathcal{E}(G) = (\frac{4}{3\pi}+o(1))n^{3/2}$ for almost all graphs G.

Proof of Theorem 1. We adapt the proof of (1) in [10]. Letting $\mathbf{i}$ to be the all ones m-vector, Rayleigh's principle implies that $\sigma_1^2(A)m \geqslant \langle AA^*\mathbf{i},\mathbf{i}\rangle$; hence, after some algebra, $\sigma_1(A) \geqslant \|A\|_1/\sqrt{mn}$. The AM–QM inequality implies that

$$\mathcal{E}(A) - \sigma_1(A) \leqslant \sqrt{(m-1)\sum_{i=2}^{n}\sigma_i^2(A)} = \sqrt{(m-1)\big(\|A\|_2^2 - \sigma_1^2(A)\big)}.$$

The function $x \to x + \sqrt{(m-1)(\|A\|_2^2 - x^2)}$ is decreasing if $\|A\|_2/\sqrt{m} \leqslant x \leqslant \|A\|_2$; hence, in view of

$$\|A\|_2^2 = \sum_{j=1}^{n}\sum_{k=1}^{m}|a_{kj}|^2 = \sum_{j=1}^{n}\sum_{k=1}^{m}a_{kj}^2 \leqslant \alpha\sum_{j=1}^{n}\sum_{k=1}^{m}a_{kj} = \alpha\|A\|_1,$$

we find that $\|A\|_2/\sqrt{m} \leqslant \|A\|_1/\sqrt{mn}$, and inequality (2) follows. □

Proof of Theorem 2. If $\|A\|_1 \geqslant n\alpha$, then Theorem 1 and $\|A\|_2^2 \leqslant \alpha\|A\|_1$ imply that

$$\mathcal{E}(A) \leqslant \frac{\|A\|_1}{\sqrt{mn}} + \sqrt{(m-1)\left(\alpha\|A\|_1 - \frac{\|A\|_1^2}{mn}\right)}.$$

The right-hand side is maximal for $\|A\|_1 = (m+\sqrt{m})\alpha n/2$ and inequality (3) follows. If $\|A\|_1 < n\alpha$, we see that

$$\mathcal{E}(A) \leqslant \sqrt{m\|A\|_2^2} \leqslant \sqrt{m\alpha\|A\|_1} \leqslant \sqrt{mn}\alpha \leqslant \alpha\frac{(m+\sqrt{m})\sqrt{n}}{2},$$

completing the proof. □

Remarks.

(1) The bound (2) may be refined using more sophisticated lower bounds on $\sigma_1(A)$.
(2) Inequality (4) and the result of Friedman [5] can be used to obtain lower bounds for the energy of "almost all" d-regular graphs.

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