

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 $\sigma_1(A) \geq \sigma_2(A) \geq \dots$ and call the value $\mathcal{E}(A) = \sigma_1(A) + \sigma_2(A) + \dots$ the *energy* of A , thereby extending the concept of graph energy, introduced by Gutman. Let $2 \leq m \leq n$, A be an $m \times n$ nonnegative matrix with maximum entry α , and $\|A\|_1 \geq n\alpha$. Extending previous results of Koolen and Moulton for graphs, we prove that

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

Furthermore, if A is any nonconstant matrix, then

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

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 .

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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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$\sigma_1(A) \geq \sigma_2(A) \geq \dots$ 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 $\mu_1(A) \geq \dots \geq \mu_n(A)$, 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 $\mathcal{E}(A) = \sigma_1(A) + \dots + \sigma_n(A)$ 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 $m \geq n/2$:

$$\mathcal{E}(G) \leq 2m/n + \sqrt{(n-1)(2m - (2m/n)^2)} \leq (n/2)(1 + \sqrt{n}). \quad (1)$$

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

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 $m \leq n$, A is an $m \times n$ nonnegative matrix with maximum entry α , and $\|A\|_1 \geq n\alpha$, then*

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

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

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

$$\mathcal{E}(A) \leq \alpha \frac{(m + \sqrt{m})\sqrt{n}}{2}. \quad (3)$$

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 $A \in M_{m,n}$ ($m, n \geq 2$), we have $\sigma_1^2(A) + \sigma_2^2(A) + \dots = \text{tr}(AA^*) = \|A\|_2^2$, and so

$$\|A\|_2^2 - \sigma_1^2(A) = \sigma_2^2 + \dots + \sigma_m^2 \leq \sigma_2(A)(\mathcal{E}(A) - \sigma_1(A)).$$

Thus, if A is a nonconstant matrix, then

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

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 $E(a_{ij}) = 1/2$, $\text{Var}(a_{ij}^2) = 1/4 = \sigma^2$, and $E(a_{ij}^{2k}) = 1/4^k$ for all $1 \leq i < j \leq n$, $k \geq 1$. The result of Füredi and Komlós [6] implies that, with probability tending to 1,

$$\begin{aligned} \sigma_1(G(n, 1/2)) &= (1/2 + o(1))n, \\ \sigma_2(G(n, 1/2)) &< (2\sigma + o(1))n^{1/2} = (1 + o(1))n^{1/2}. \end{aligned}$$

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

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

for almost all graphs G .

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

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

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 $\sigma_1^2(A)m \geq \langle AA^*\mathbf{i}, \mathbf{i} \rangle$; hence, after some algebra, $\sigma_1(A) \geq \|A\|_1/\sqrt{mn}$. The AM–QM inequality implies that

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

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

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

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

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

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

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

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

completing the proof. \square

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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