



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  $\alpha$ , 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  $m \geq n/2$ :

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

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  $\alpha$ , and  $\|A\|_1 \geq n\alpha$ , then*

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

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  $\alpha$ , then*

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

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  $A \in M_{m,n}$  ( $m, n \geq 2$ ), 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

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

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  $E(a_{ij}) = 1/2$ ,  $\text{Var}(a_{ij}^2) = 1/4 = \sigma^2$ , 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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