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 $\sigma_1(A) \geq \sigma_2(A) \geq \ldots$ and call the value $E(A) = \sigma_1(A) + \sigma_2(A) + \ldots$ 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

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

Furthermore, if $A$ is any nonconstant matrix, then

$$E(A) \geq \sigma_1(A) + \frac{\text{tr}(AA^*) - \sigma_2^2(A)}{\sigma_2(A)}.$$ 

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

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

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], and [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 $\sigma_1(A) \geq \sigma_2(A) \geq \ldots$ of a matrix $A$ are the square roots of the eigenvalues of
Note that if $A \in M_{n,n}$ is a Hermitian matrix with eigenvalues $\mu_1 (A) \geq ... \geq \mu_n (A)$, 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 $E (A) = \sigma_1 (A) + ... + \sigma_n (A)$ the energy of $A$. Gutman [7] introduced $E (G) = E (A (G))$, where $A (G)$ is the adjacency matrix of a graph $G$; in this narrow sense $E (A)$ has been studied extensively (see, e.g., [2], [8], [10], [11], [12], [13], and [14]). In particular, Koolen and Moulton [10] proved the following sharp inequalities for a graph $G$ of order $n$ and size $m \geq n/2$,

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

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

In this note we give upper and lower bounds on $E (A)$ and find the asymptotics of $E (G)$ 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

$$E (A) \leq \|A\|_1 \sqrt{mn} + \sqrt{(m-1) (\text{tr} (AA^*) - \|A\|_1^2/\text{mn})} \quad (2).$$

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

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

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

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 $\sigma_1^2 (A) + \sigma_2^2 (A) + ... = \text{tr} (AA^*)$, and so

$$\text{tr} (AA^*) - \sigma_1^2 (A) = \sigma_2^2 + ... + \sigma_m^2 \leq \sigma_2 (A) (E (A) - \sigma_1 (A)).$$

Thus, if $A$ is a nonconstant matrix, then

$$E (A) \geq \sigma_1 (A) + \frac{\text{tr} (AA^*) - \sigma_1^2 (A)}{\sigma_2 (A)} \quad (4).$$
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 $E(a_{ij}) = 1/2$, $Var(a_{ij}^2) = 1/4 = \sigma^2$, and $E(a_{i,j}^{2k}) = 1/4^k$ 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,

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

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

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

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

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

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

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

$$tr(AA^*) = \sum_{j=1}^{m} \sum_{k=1}^{n} |a_{kj}|^2 = \sum_{j=1}^{m} \sum_{k=1}^{n} a_{kj}^2 \leq \alpha \sum_{j=1}^{m} \sum_{k=1}^{n} a_{kj} = \alpha \|A\|_1,$$

we find that $\sqrt{tr(AA^*) / m} \leq \|A\|_1 / \sqrt{mn}$, and inequality (2) follows. \qed
Proof of Theorem 2 If $\|A\|_1 \geq n\alpha$, then Theorem 1 and $tr(AA^*) \leq \alpha \|A\|_1$ imply that
\[
E(A) \leq \frac{\|A\|_1}{\sqrt{mn}} + \sqrt{(m-1) \left( \alpha \|A\|_1 - \frac{\|A\|_1^2}{mn} \right)}.
\]
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
\[
E(A) \leq \sqrt{mtr(AA^*)} \leq \sqrt{m\alpha \|A\|_1} \leq \sqrt{mn\alpha} \leq \alpha \frac{(m + \sqrt{m}) \sqrt{n}}{2},
\]
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.

References


