The Energy of Graphs and Matrices

Vladimir Nikiforov
Department of Mathematical Sciences, University of Memphis,
Memphis TN 38152, USA, e-mail: vnikifrv@memphis.edu

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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 $\mathcal{E}(A) = \sigma_1(A) + \sigma_2(A) + \ldots$ 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

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

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

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

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], 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 $\mu_1(A) \geq \ldots \geq \mu_n(A)$, 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 $\mathcal{E}(A) = \sigma_1(A) + \ldots + \sigma_n(A)$ the energy of $A$. Gutman 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], [3], [10], [11], [12], [13], and [14]). In particular, Koolen and Moulton 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

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

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 $\sigma_1^2(A) + \sigma_2^2(A) + \ldots = tr(AA^*)$, and so

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

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

$$\mathcal{E}(A) \geq \sigma_1(A) + \frac{tr(AA^*) - \sigma_1^2(A)}{\sigma_2(A)} \tag{4}.$$
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 \cite{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

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

for almost all graphs $G$.

Moreover, Wigner’s semicircle law \cite{15} (we use the form given by Arnold \cite{1}, p. 263), implies that

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

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

**Proof of Theorem 1** We adapt the proof of (1) in \cite{10}. Letting $i$ to be the all ones $m$-vector, Rayleigh’s principle implies that $\sigma_1^2(A) m \geq \langle AA^* i, i \rangle$; 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 $x \to x + \sqrt{(m - 1)(tr(AA^*) - x^2)}$ is decreasing if $\sqrt{tr(AA^*)}/m \leq x \leq \sqrt{tr(AA^*)}$; hence, in view of

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

we find that $\sqrt{tr(AA^*)}/m \leq ||A||_1 / \sqrt{mn}$, and inequality (2) follows.
Proof of Theorem 2: If \( \|A\|_1 \geq n\alpha \), then Theorem 1 and \( \text{tr}(AA^*) \leq \alpha \|A\|_1 \) 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

\[
\mathcal{E}(A) \leq \sqrt{m\text{tr}(AA^*)} \leq \sqrt{m\alpha \|A\|_1} \leq \sqrt{mn\alpha} \leq \alpha \frac{(m + \sqrt{m}) \sqrt{n}}{2},
\]

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.

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