

# Note on Das–Mojallal Bound on Graph Energy

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## Abstract

In 2013, Das and Mojallal published a new upper bound on graph energy. We now comment on the proof of this bound, and show that it is inferior to McClelland's classic estimate.

## 1 Introduction

In this note we use the same notation and terminology as in the paper [1]. Thus,  $G$  is a simple graph, with vertex set  $\mathbf{V}(G) = \{v_1, v_2, \dots, v_n\}$  and edge set  $\mathbf{E}(G)$ , consisting of  $m$  edges. The edge of  $G$ , connecting the vertices  $v_j$  and  $v_k$  is denoted by  $v_j v_k$ .

The degree (= number of first neighbors) of the vertex  $v_i$  is  $d_i$ , and  $\min_{1 \leq i \leq n} d_i = \delta$ .

The eigenvalues of the adjacency matrix of  $G$  are  $\lambda_1, \lambda_2, \dots, \lambda_n$  and the energy of  $G$  is [2],

$$E(G) = \sum_{i=1}^n |\lambda_i|.$$

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Within the theory of graph energy [2], numerous lower and upper bounds on  $E(G)$  were discovered. Among these, we mention here the McClelland bound [3]

$$E(G) \leq \sqrt{2mn}$$

in which equality holds if and only if  $G$  is either edgeless or 1-regular (i.e., for connected graphs, if and only if  $n = 2$  and  $G \cong K_2$ ).

In [1], the following upper bound for graph energy was claimed to hold (as Theorem 3.1):

$$E(G) \leq \sqrt{2m(n - \delta) + 4\sqrt{m^3(1 - 1/\omega)}} \quad (1)$$

where  $\omega$  denotes the clique number.

## 2 Concerning the proof of inequality (1)

Proving inequality (1) (i.e., proving their Theorem 3.1), the authors of [1] used the relations

$$\sum_{v_j v_k \notin \mathbf{E}(G)} |\lambda_j \lambda_k| \leq (n - 1 - \delta)m$$

and

$$\sum_{v_j v_k \in \mathbf{E}(G)} |\lambda_j \lambda_k| \leq \sqrt{4m^3(1 - 1/\omega)}$$

(formulas no. (4) and (5) in [1]). Unfortunately, these relations are ill-defined. The indices  $j, k$  in the terms  $v_j v_k \in \mathbf{E}(G)$  and  $v_j v_k \notin \mathbf{E}(G)$  refer to vertices of  $G$ . On the other hand, there is no canonical mapping between eigenvalues and vertices (i.e., between  $v_j$  and  $\lambda_j$ ), and thus the sums

$$\sum_{v_j v_k \notin \mathbf{E}(G)} |\lambda_j \lambda_k| \quad \text{and} \quad \sum_{v_j v_k \in \mathbf{E}(G)} |\lambda_j \lambda_k|$$

are not mathematically meaningful. In other words, if for  $j = 1, 2, \dots, n$ , the eigenvalue  $\lambda_j$  is associated with the vertex  $v_j$ , then the numerical values of above sums depend on the numbering of vertices of the graph  $G$ ,

i.e., these sums are not graph invariants.

By this, the proof of formula (1) in [1] is either inconceivable or invalid.

Analyzing the proof of Theorem 3.1 in [1], several other mathematical inconsistencies could be noticed. These will not be specified here.

### 3 Analysis of inequality (1)

We now show that (1) is weaker than the classical McClelland upper bounds  $E(G) \leq \sqrt{2mn}$  [2, 3].

**Theorem 1.** *Let  $G$  be a connected graph of order  $n$ , with  $m$  edges, with minimum degree  $\delta$ , and clique number  $\omega$ . Then*

$$E(G) \leq \sqrt{2mn} < \sqrt{2m(n - \delta) + 4\sqrt{m^3(1 - 1/\omega)}}.$$

*The Das–Mojallal part of the inequality is strict.*

*Proof.* For any connected graph,  $\omega \geq 2$ . Therefore,

$$\begin{aligned} & \sqrt{2m(n - \delta) + 4\sqrt{m^3(1 - 1/\omega)}} \geq \sqrt{2m(n - \delta) + 4\sqrt{m^3(1 - 1/2)}} \\ & = \sqrt{2m(n - \delta) + 2m\sqrt{2m}} = \sqrt{2m(n + \sqrt{2m} - \delta)}. \end{aligned}$$

We now need to show that  $\sqrt{2m} > \delta$ . Since  $2m$  is equal to the sum of vertex degrees, its minimal value will be achieved if all vertices of the graph  $G$  have degree  $\delta$ . Then  $2m = n\delta$ . Therefore, it is sufficient to show that  $\sqrt{n\delta} > \delta$  i.e.,  $n\delta > \delta^2$  i.e.,  $n > \delta$ .

In simple graphs of order  $n$ , the greatest possible vertex degree is  $n - 1$ . Therefore,  $\delta \leq n - 1$ , i.e.,  $n > \delta$ . Thus

$$\sqrt{2m(n + \sqrt{2m} - \delta)} > \sqrt{2mn}$$

which completes the proof of Theorem 1. ■

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## 4 Concluding remarks

It is remarkable that the paper [1] passed the referee check and could be published in its present form. Equally remarkable is that over 10 years passed before the obvious flaws in [1] were noticed.

## References

- [1] K. C. Das, S. A. Mojallal, Upper bounds for the energy of graphs *MATCH Commun. Math. Comput. Chem.* **70** (2013) 657–662.
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- [3] B. J. McClelland, Properties of the latent roots of a matrix: The estimation of  $\pi$ -electron energies, *J. Chem. Phys.* **54** (1971) 640–643.