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Note

On a conjecture about the Randić index

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Abstract

A conjecture of Delorme, Favaron and Rautenbach [On the Randić index, Discrete Math. 257 (2002) 29–38] about the Randić index of a graph, in relation to its order and minimum degree, is refuted by the AutoGraphiX 2 system. Moreover, a modified conjecture is derived from presumably extremal graphs obtained with that system.

MSC: 05C35

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Let $G=(V,E)$ denote a simple connected graph, of order $n=|V|$, with vertex degrees $d_1, d_2, \ldots, d_n$. The Randić (or connectivity) index [10] $R(G)$ is defined by

$$R(G)=\sum_{ij\in E}\frac{1}{\sqrt{d_i d_j}}. \tag{1}$$

This index was extensively studied in mathematical chemistry. More recently study of its mathematical properties has progressed, spurred by a paper of Bollobas and Erdös [2]. These authors showed that for a connected G

$$R(G)\geqslant\sqrt{n-1}, \tag{2}$$

the bound is tight if and only if G is a star. A stronger result, due to Delorme, et al. [6], holds if the minimum degree is greater or equal to 2:

$$R(G)\geqslant\frac{2n-4}{\sqrt{2n-2}}+\frac{1}{n-1}, \tag{3}$$

and the bound is tight if and only if $G\equiv SK_{2,n-2}$, i.e., a complete split graph is obtained by joining all vertices of a clique K_2 to all vertices of an independent set S_{n-2}. The proof uses graph theoretic arguments. For another proof using a linear programming technique, introduced in [3], see Pavlović [7].

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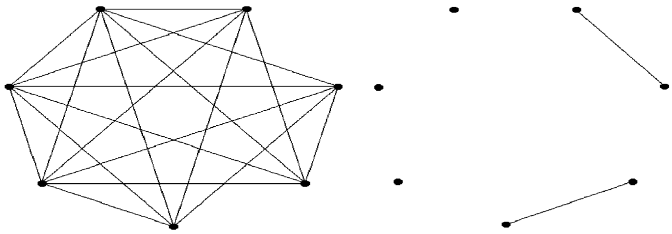

Fig. 1. The smallest counter-example (left) found and its complement (right).

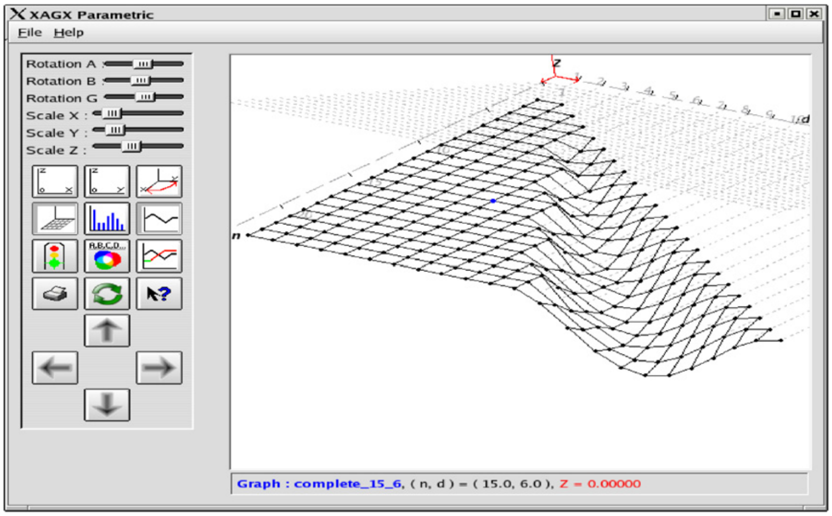

Fig. 2. The expression of the left-hand side of (4) for $5 \leqslant n \leqslant 24$ and $1 \leqslant \delta \leqslant n-1$.

Delorme et al. [6] also formulated a conjecture which includes (2) and (3) as particular cases. Setting $R = R(G)$ and $\delta = \delta(G)$, for a connected graph G,

$$R(G) - \frac{\delta(n-\delta)}{\sqrt{\delta(n-1)}} - \frac{\delta(\delta-1)}{2}\frac{1}{n-1} \geqslant 0, \tag{4}$$

and the bound is tight if and only if $G \equiv SK_{\delta,n-\delta}$.

Using again linear programming, Pavlovic [8] proved that (4) holds when $\delta = (n-1)/2$ or $\delta = n/2$ (see also [9] for further results proved by quadratic programming).

In this note, we show that (4) does not hold in general and propose a modified conjecture.

First, counter-examples were sought for, by minimizing heuristically the left-hand side of (4) using the AutoGraphiX 2 (AGX 2) system [1,4,5] in automated mode. For several graphs, negative values were obtained. The smallest counter-example found is represented in Fig. 1. It has $n = 7$ vertices, minimum degree $\delta = 5$, $R = 3.49089$ and a value for the left-hand side of (4) of -0.00151829.

Then the interactive mode of AGX 2 was used to obtain families of graphs with (presumably) minimum R, taking n and δ as parameters. Values of the difference are represented in Fig. 2 and some extremal graphs for which (4) does not hold in Fig. 3.

It is then easy to see that for given n and $\delta \geqslant \delta_n$, the graph that minimizes the left-hand side of (4) is the complement of a graph $G_{n,p,\delta}$ composed of a $(n-\delta-1)$-regular graph on p vertices together with $n-p$ isolated vertices,

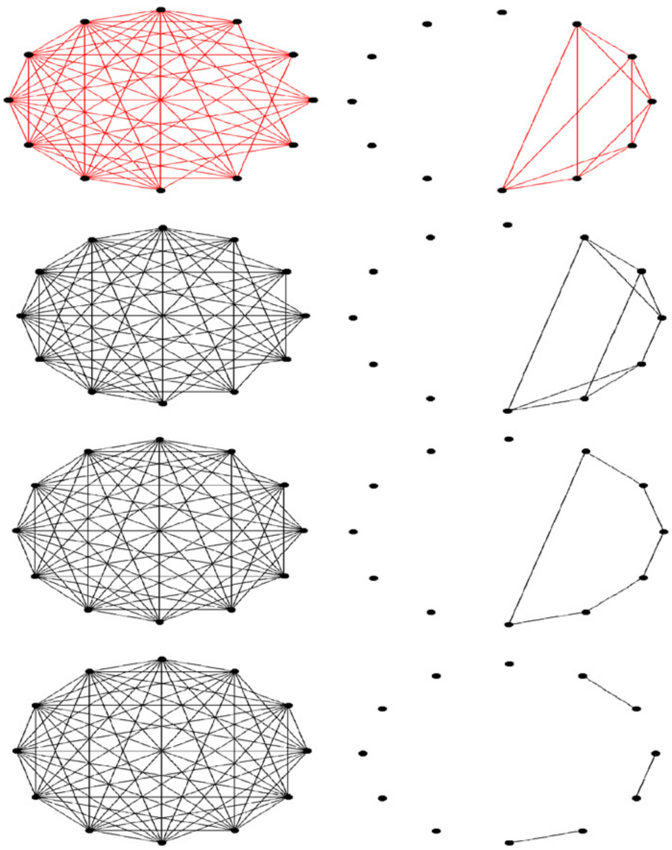

Fig. 3. Counter-examples (left) and their complements (right) for $n = 12$ and $7 \leqslant \delta \leqslant 10$.

where

$$\delta_n = \begin{cases} \dfrac{n+2}{2} & \text{if } n \equiv 0[4] \\ \dfrac{n+3}{2} & \text{if } n \equiv 1[4] \\ \dfrac{n+4}{2} & \text{if } n \equiv 2[4] \\ \dfrac{n+3}{2} & \text{if } n \equiv 3[4] \end{cases} \quad \text{and} \quad p = \begin{cases} \dfrac{n-2}{2} & \text{if } n \equiv 2[4] \text{ and } \delta \text{ is even,} \\ \left\lceil \dfrac{n}{2} \right\rceil & \text{if } n \equiv 3[4], \\ \left\lfloor \dfrac{n}{2} \right\rfloor & \text{otherwise.} \end{cases} \tag{5}$$

For such a graph, we have

$$R = \frac{(n-p)(n-p-1)}{2(n-1)} + \frac{p(p+\delta-n)}{2\delta} + \frac{p(n-p)}{\sqrt{\delta(n-1)}}.$$

Using these results the conjecture of Delorme, et al. becomes the following:

Conjecture. Let $G = (V, E)$ be a graph of order n with Randić index R and minimum degree δ. Then,

$$R \geqslant \begin{cases} \dfrac{\delta(n-\delta)}{\sqrt{\delta(n-1)}} + \dfrac{\delta(\delta-1)}{2} \cdot \dfrac{1}{n-1} & \text{if } \delta < \delta_n, \\ \dfrac{(n-p)(n-p-1)}{2(n-1)} + \dfrac{p(p+\delta-n)}{2\delta} + \dfrac{p(n-p)}{\sqrt{\delta(n-1)}} & \text{if } \delta_n \leqslant \delta \leqslant n-2 \end{cases}$$

where δ_n and p are given in (5), with equality if and only if G is a complete split graph $SK_{\delta,n-\delta}$ for $\delta < \delta_n$, and if and only if G is the complement of $G_{n,p,\delta}$ (described above) for $\delta \geqslant \delta_n$.

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