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Note

Corrections of proofs for Hansen and Mélot's two theorems☆

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Abstract

The Randić index $R(G)$ of a (chemical) graph G is also called connectivity index. Hansen and Mélot [Variable neighborhood search for extremal graphs 6: analyzing bounds for the connectivity index, J. Chem. Inf. Comput. Sci. 43 (2003) 1–14] in their paper, characterized the chemical trees of given order and number of pendent vertices which have the minimum and maximum Randić index, respectively. In this note, we point out the mistakes in the proofs of their results Theorems 8 and 10, while we still believe that the two theorems are true, and then we give their corrected proofs.

Keywords: Chemical tree; Pendent path; Randić index; Connectivity index

1. Introduction

The *Randić index* $R(G)$ of a graph G, also called connectivity index, was introduced by the chemist Milan Randić under the name "*branching index*" in 1975 [21] as the sum of $1/\sqrt{d(u)d(v)}$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G, i.e.,

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{d(u)d(v)}}.$$

It is well known that the Randić index was introduced as one of the many graph-theoretical parameters derived from the graph underlying some molecule. The research background of Randić index together with its generalization appears in chemistry or mathematical chemistry and can be found in the literature, see [2–4,13–17,21]. There are also many results about trees with given order and number of pendent vertices, see [12,19,22]. For a comprehensive survey of its mathematical properties, see the book of Li and Gutman "*Mathematical Aspects of Randić-Type Molecular Structure Descriptors*" [18].

In order to discuss the Randić index of chemical trees, we first introduce some terminology and notations of graphs. Let $G = (V, E)$ be a graph. For a vertex x of G, we denote the neighborhood and the degree of x by $N(x)$ and $d(x)$, respectively. A *chemical tree* is a tree with maximum degree at most 4. A vertex with degree one is called a *pendent vertex*. A path $v_1 v_2 \cdots v_{s-1} v_s$ is called a *pendent path*, if $d(v_1)=1$, $d(v_s) \geqslant 3$ and $d(v_2)=\cdots=d(v_{s-1})=2$. Undefined terminology and notations can be found in [5].

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2. Mistakes in [12]

In [12], the authors introduced two classes of chemical trees $L_e(n, n_1)$ and $U(n, n_1)$, which were founded by the system *AutoGraphix* (*AGX*) of Caporossi and Hansen (further papers describing mathematical applications of *AGX* are in [1,6,7,10,11]). The structure of $L_e(n, n_1)$ (n_1 is even) is depicted in Fig. 1. These trees are composed of subgraphs that are stars S_5, and these stars are connected by paths (the dotted lines in the figure), whose lengths can be 0. The Randić index of $L_e(n, n_1)$ is

$$R(L_e(n, n_1)) = \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2}.$$

$U(n, n_1)$ has a subgraph of $n_1 - 2$ vertices of degree 3 which is a tree; we denote its vertex set by V_3. In Fig. 2, the vertices of V_3 are on a path, but in general case this may be different. All these vertices are connected to another vertex of V_3 or to a path of length at least 2. The number of paths adjacent to the vertices of V_3 is $|V_3| + 2$, and the number of vertices of degree 2 is $n - 2n_1 + 2$. The Randić index of $U(n, n_1)$ is

$$R(U(n, n_1)) = \frac{n}{2} + n_1\left(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}} - \frac{7}{6}\right).$$

The paper [12] contains 8 theorems, 2 propositions, 2 corollaries and 1 lemma, in which many results were mentioned. Two theorems were stated as follows:

Theorem 2.1 (*Hansen and Mélot [12, Theorem 8]*). *Let T be a chemical tree of order n with $n_1 \geqslant 5$ pendent vertices. Then*

$$R(T) \geqslant \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2} \tag{2.1}$$

with equality if and only if n_1 is even and T is isomorphic to $L_e(n, n_1)$.

Theorem 2.2 (*Theorem 10 of [12]*). *Let T be a chemical tree of order n with $n_1 \geqslant 3$ pendent vertices. Then*

$$R(T) \leqslant \frac{n}{2} - a_0' n_1,$$

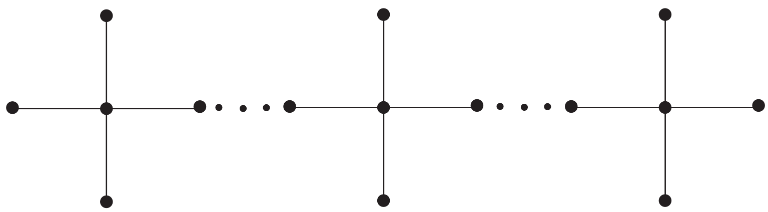

Fig. 1. Structure of $L_e(n, n_1)$.

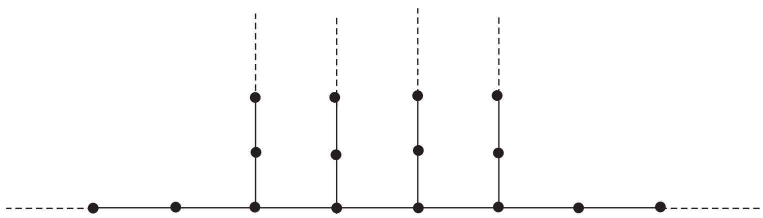

Fig. 2. Structure of $U(n, n_1)$.

where

$$a_0' = \frac{7}{6} - \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{6}} \approx 0.0513$$

with equality if and only if T is isomorphic to $U(n, n_1)$.

In the proof of [12, Theorem 8], expression (21):

$$R(T - v_1v_2) \geqslant \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2} + \frac{1}{2} - \frac{1}{\sqrt{2}}$$

was mis-calculated and should be

$$R(T - v_1v_2) \geqslant \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2} - \frac{1}{2\sqrt{2}}.$$

Then combining expressions (21) and (22) there

$$R(T) - R(T - v_1v_2) \geqslant \frac{3}{2} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} + \frac{1}{\sqrt{8}},$$

we get

$$R(T) \geqslant \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2} + \frac{3}{2} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}}.$$

But, this time we have $\frac{3}{2} - \frac{2}{\sqrt{3}} - \frac{1}{\sqrt{6}} < 0$, which does not lead to the proof of the theorem.

In the proof of Theorem 10 of [12], one cannot obtain expression (58): $x_{23} - x_{13} = n_1$, since by (54): $x_{22} = n - \frac{1}{2}(5n_1 + x_{23} - x_{13}) + 2 + n_4$, we only have that $5n_1 + x_{23} - x_{13}$ is even for all n_1, i.e., $x_{23} - x_{13}$ has the same parity as n_1, or $x_{23} - x_{13} = n_1 + 2k$, but not $x_{23} - x_{13} = (2k + 1)n_1$. Note that the last two expressions are not equivalent.

Although we find mistakes in their proofs, we still believe that the two theorems are true and the results of [12] remains correct. In the following sections, we will give their corrected proofs.

3. Corrected Proof of Theorem 2.1

Our proof is shorter, and uses linear programming approach, which was introduced in the paper [8] and is widely used in chemical graph theory.

Let *T* be a chemical tree with *n* vertices and n_1 pendent vertices. Denote by x_{ij} the number of edges joining the vertices of degrees *i* and *j*, and n_i the number of vertices of degree *i* in *G*. Then, we have another description for the Randić index of *T*,

$$R(T) = \sum_{1 \leqslant i \leqslant j \leqslant 4} \frac{x_{ij}}{\sqrt{ij}}. \tag{3.1}$$

Note that $x_{11} = 0$ whenever $n \geqslant 3$, and therefore the case $i = j = 1$ need not be considered any further. Consequently, the right-hand side of (3.1) is a linear function of the following nine variables $x_{12}, x_{13}, x_{14}, x_{22}, x_{23}, x_{24}, x_{33}, x_{34}, x_{44}$. Then

$$n_1 + n_2 + n_3 + n_4 = n. \tag{3.2}$$

Counting the edges terminating at vertices of degree *i*, we obtain for $i = 1, 2, 3, 4$

$$x_{12} + x_{13} + x_{14} = n_1, \tag{3.3}$$

$$x_{12} + 2x_{22} + x_{23} + x_{24} = 2n_2, \tag{3.4}$$

$$x_{13} + x_{23} + 2x_{33} + x_{34} = 3n_3, \tag{3.5}$$

$$x_{14} + x_{24} + x_{34} + 2x_{44} = 4n_4. \tag{3.6}$$

Another linearly independent relation of this kind is

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2m = 2(n-1). \tag{3.7}$$

Now we will solve the linear programming

$$\min R(T) = \sum_{1 \leqslant i \leqslant j \leqslant 4} \frac{x_{ij}}{\sqrt{ij}}$$

with constraints (3.3)–(3.8).

By calculations, we have

$$x_{22} = \frac{2n - 5n_1 + 6}{2} - \frac{1}{2}x_{12} + \frac{1}{6}x_{13} + \frac{1}{2}x_{14} - \frac{1}{3}x_{23} + \frac{1}{3}x_{33} + \frac{2}{3}x_{34} + x_{44}, \tag{3.8}$$

$$x_{24} = 2n_1 - 4 - \tfrac{2}{3}x_{13} - x_{14} - \tfrac{2}{3}x_{23} - \tfrac{4}{3}x_{33} - \tfrac{5}{3}x_{34} - 2x_{44}. \tag{3.9}$$

Substituting (3.8) and (3.9) into (3.2), we have

$$\begin{aligned} R(G) = {} & \frac{2n + (2\sqrt{2} - 5)n_1 + 6 - 4\sqrt{2}}{4} + c_{12}x_{12} + c_{13}x_{13} + c_{14}x_{14} \\ & + c_{23}x_{23} + c_{33}x_{33} + c_{34}x_{34} + c_{44}x_{44}, \end{aligned} \tag{3.10}$$

where

$$\begin{aligned} c_{12} &= 1/\sqrt{2} - 1/4 \approx 0.45711, \\ c_{13} &= 1/\sqrt{3} + 1/12 - \sqrt{2}/6 \approx 0.42498, \\ c_{14} &= 3/4 - 1/\sqrt{8} \approx 0.39645, \\ c_{23} &= 1/\sqrt{6} - 1/6 - \sqrt{2}/6 \approx 0.00588, \\ c_{33} &= 1/2 - \sqrt{2}/3 \approx 0.02860, \\ c_{34} &= 1/\sqrt{12} + 1/3 - 5\sqrt{2}/12 \approx 0.03275, \\ c_{44} &= 3/4 - 1/\sqrt{2} \approx 0.04289. \end{aligned}$$

Because all coefficients c_{ij} on the right-hand side of (3.10) are positive-valued, it is clear that for fixed n and n_1, $R(T)$ will be minimum if the parameters x_{12}, x_{13}, x_{14}, x_{23}, x_{33}, x_{34} and x_{44} are all equal to zero (provided this is possible). However, a tree must have at least two pendent vertices, and so we have

$$x_{12} + x_{13} + x_{14} > 0. \tag{3.11}$$

Since $c_{14} < c_{13} < c_{12}$, considering the minimum of $R(T)$, the best solution of (3.11) is that all pendent vertices are adjacent to vertices with degree 4, i.e., $x_{14} = n_1$.

Thus, we get

$$\begin{aligned} R(T) &\geqslant \frac{2n + (2\sqrt{2} - 5)n_1 + 6 - 4\sqrt{2}}{4} + \left(\frac{3}{4} - \frac{1}{\sqrt{8}}\right) n_1 \\ &= \frac{n}{2} + \frac{n_1}{2}\left(\frac{1}{\sqrt{2}} - 1\right) + \frac{3}{2} - \sqrt{2}, \end{aligned}$$

equality holds if and only if $x_{12} = x_{13} = x_{23} = x_{33} = x_{34} = x_{44} = 0$, $x_{14} = n_1$ and $n_3 = 0$. The proof is complete. □

4. Corrected and shorter Proof of Theorem 2.2

As one of the referees suggested to us, Mélot [20] in his PhD thesis, already found the erroneous in the proof of the result, and gave a correct one. But, we did not know the existence of the thesis before we were suggested. However, our next two lemmas Lemmas 4.1 and 4.2 allow a significant shorter proof than the proof of [20].

Lemma 4.1 (*Caporossi et al. [9]*). *Let G be a connected graph with n vertices. Then*

$$R(G) = \frac{n}{2} - \sum_{e \in E(G)} \omega^*(e),$$

where $\omega^*(e) = \frac{1}{2}(1/\sqrt{d(u)} - 1/\sqrt{d(v)})^2$ *for* $e = uv$.

Lemma 4.2. *Let T be a chemical tree with n vertices and* n_1 $(n_1 \geqslant 3)$ *pendent vertices and with maximum Randić index. For each* $v \in V(T)$, *if* $d(v) = 2$, *then v must be on a pendent path.*

Proof. By contradiction. Let $v \in V(T)$ and $d(v) = 2$. Suppose v is not on any pendent path. There must be a path $v_1 v_2 \cdots v_s v w_t \cdots w_2 w_1$ ($s \geqslant 1$ and $t \geqslant 1$) such that $d(v_1) = p \geqslant 3$, $d(w_1) = q \geqslant 3$ and $d(v_2) = \cdots = d(v_s) = d(w_t) = \cdots = d(w_2) = 2$. Let x be a pendent vertex of T and y its neighbor with $d(y) = l \geqslant 2$. Let $T' = T - v_1 v_2 - w_2 w_1 + v_1 w_1 + x v_2$. Then T' is also a tree with n vertices and n_1 pendent vertices. We have

$$\begin{aligned} R(T) - R(T') &= \frac{1}{\sqrt{2p}} + \frac{1}{\sqrt{2q}} + \frac{1}{\sqrt{l}} - \frac{1}{\sqrt{pq}} - \frac{1}{\sqrt{2l}} - \frac{1}{\sqrt{2}} \\ &= \left(\frac{1}{\sqrt{p}} - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{q}}\right) + \left(\frac{1}{\sqrt{2}} - 1\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{l}}\right) < 0, \end{aligned}$$

a contradiction. □

Now we are at the point to give a corrected proof to Theorem 2.2.

Proof. Let T be a chemical tree with n vertices and n_1 $(n_1 \geqslant 3)$ pendent vertices. By Lemma 4.2, we assume that all vertices of T with degree two are on pendent paths, then $x_{12} = x_{23} + x_{24}$. Note that $x_{12} + x_{13} + x_{14} = n_1$, and by Lemma 4.1,

$$\begin{aligned} R(T) &= \frac{n}{2} - \sum_{e \in E(T)} \omega^*(e) \\ &= \frac{n}{2} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)^2 x_{12} - \frac{1}{2}\left[\left(1 - \frac{1}{\sqrt{3}}\right)^2 x_{13} + \left(1 - \frac{1}{2}\right)^2 x_{14}\right] \\ &\quad - \frac{1}{2}\left[\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 x_{23} + \left(\frac{1}{\sqrt{2}} - \frac{1}{2}\right)^2 x_{24}\right] - \frac{1}{2}\left(\frac{1}{\sqrt{3}} - \frac{1}{2}\right)^2 x_{34} \\ &\leqslant \frac{n}{2} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)^2 x_{12} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)^2 (x_{13} + x_{14}) - \frac{1}{2}\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 (x_{23} + x_{24}) \\ &= \frac{n}{2} - \frac{1}{2}\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2\right] x_{12} - \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)^2 (x_{13} + x_{14}) \\ &= \frac{n}{2} - \frac{1}{2}\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2\right] n_1 \\ &\quad + \frac{1}{2}\left[\left(1 - \frac{1}{\sqrt{2}}\right)^2 + \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)^2 - \left(1 - \frac{1}{\sqrt{3}}\right)^2\right] (x_{13} + x_{14}) \\ &= \frac{n}{2} + \frac{(3\sqrt{2} + \sqrt{6} - 7)n_1}{6} - \left(1 - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}}\right)(x_{13} + x_{14}) \\ &\leqslant \frac{n}{2} + \frac{(3\sqrt{2} + \sqrt{6} - 7)n_1}{6}. \end{aligned}$$

The equality holds if all the equalities in the above inequalities hold. Thus $x_{13} = x_{14} = x_{24} = x_{34} = 0$. Then $x_{44} = 0$ since T is a tree. The proof is complete. □

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