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Which generalized Randić indices are suitable measures of molecular branching?

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ABSTRACT

Molecular branching is a very important notion, because it influences many physicochemical properties of chemical compounds. However, there is no consensus on how to measure branching. Nevertheless two requirements seem to be obvious: star is the most branched graph and path is the least branched graph. Every measure of branching should have these two graphs as extremal graphs. In this paper we restrict our attention to chemical trees (i.e. simple connected graphs with maximal degree at most 4), hence we have only one requirement that the path be an extremal graph. Here, we show that the generalized Randić index $R_p(G) = \sum_{uv \in E(G)} (d_u d_v)^p$ is a suitable measure for branching if and only if $p \in [\lambda, 0) \cup (0, \lambda')$ where λ is the solution of the equation $2^x + 6^x + \frac{1}{2} \cdot 12^x + \frac{1}{4} \cdot 16^x - \frac{11}{4} \cdot 4^x = 0$ in the interval $(-0.793, -0.792)$ and λ' is the positive solution of the equation $3 \cdot 3^x - 2 \cdot 2^x - 4^x = 0$. These results include the solution of the problem proposed by Clark and Gutman.

1. Introduction

Randić index [12] is one of the most famous molecular descriptors whose chemical and mathematical properties have been extensively studied [5,10,13]. It is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u \cdot d_v}},$$

where $E(G)$ is the set of edges of graph G and d_u and d_v are degrees of vertices u and v, respectively. This index is generalized to

$$R_p(G) = \sum_{uv \in E(G)} (d_u d_v)^p .$$

Note that this can be rewritten as

$$R_p(G) = \sum_{1 \le i \le j \le \Delta} (i \cdot j)^p \cdot m_{ij},$$

where Δ is the maximal degree of graph G and m_{ij} is the number of the edges connecting vertices of degrees i and j. Numbers m_{ij} have been extensively studied [1,2,4,11,14,15,17,19,20,22,23].

Branching [6] of molecules is very important, but there is no unique measure of this property. However every molecular descriptor used as a branching descriptor should have a path and a star graph as two opposing extremal graphs (it is readily

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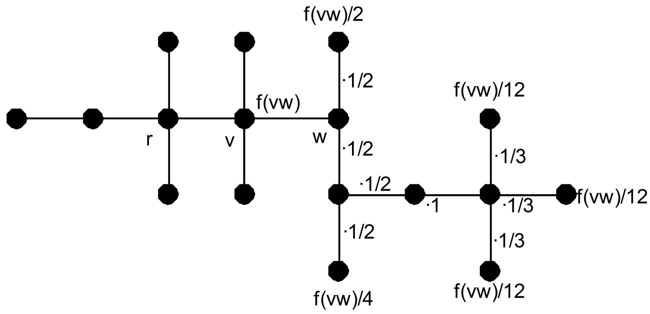

Fig. 1. Pushing of $f(vw)$ to the leaves.

seen that star $S_N = K_{1,N-1}$ is the most branched graph and path P_N is the least branched graph among all trees with $N \geq 4$ vertices). More precisely we are interested in descriptors χ such that one of the following holds:

(1) $\chi\left(K_{1,3}\right) < \chi\left(P_4\right)$ and $\chi\left(K_{1,N-1}\right) < \chi\left(T_N\right) < \chi\left(P_N\right)$ for every tree $T_N \neq P_N, K_{1,N-1}$ with $N \geq 5$ vertices;
(2) $\chi\left(P_4\right) < \chi\left(K_{1,3}\right)$ and $\chi\left(P_N\right) < \chi\left(T_N\right) < \chi\left(K_{1,N-1}\right)$ for every tree $T_N \neq P_N, K_{1,N-1}$ with $N \geq 5$ vertices.

Sometimes authors require some more restrictive conditions [7,24,25], but here, similarly as is done in paper [3], we restrict ourselves to the above requirements. Moreover, since we restrict our attention to chemical graphs our requirements are even less restrictive. Namely, we just require that

(1′) $\chi\left(T_N\right) < \chi\left(P_N\right)$ for every tree $T_N \neq P_N$ with $N \geq 4$ vertices;
(2′) $\chi\left(P_N\right) < \chi\left(T_N\right)$ for every tree $T_N \neq P_N$ with $N \geq 4$ vertices.

In papers [8,9], it has been shown that requirement (1) for $p < 0$ implies that it is sufficient to take $p \in [-0.5, 0)$ and necessary to take $p \in (-2, 0)$. These results have been furthered in [3], where it is shown that $R_p\left(T_N\right) < R_p\left(P_N\right)$ for $p < 0$ implies that it is necessary to take $p \in (-0.826077, 0)$. Moreover, it is shown that there is a value such that it is necessary and sufficient to take $p \in [\mu, 0)$ and it is conjectured that $\mu \approx -0.8$.

Here, we further these results by finding μ. Namely, by showing that μ is the solution λ of the equation

$$2^x + 6^x + \frac{1}{2} \cdot 12^x + \frac{1}{4} \cdot 16^x - \frac{11}{4} \cdot 4^x = 0,$$

in the interval $(-0.793, -0.792)$. Hence, $\mu = \lambda \approx -0.79263$. Moreover, we show that for $p \in \left(0, \lambda'\right)$ it holds that

$$R_p\left(T_N\right) > R_p\left(P_N\right) \quad \text{for every } N \in \mathbb{N} \text{ and every tree } T_N \neq P_N \text{ with } N \geq 4 \text{ vertices}$$

where λ' is the positive solution of the equation

$$3 \cdot 3^x - 2 \cdot 2^x - 4^x = 0.$$

Hence, $\lambda' \approx 3.08164$.

2. Analysis of R_p for $p < 0$

First, let us note that there is no $p < 0$ such that requirement (2′) holds. It is sufficient to note that

$$R_p\left(P_5\right) = 2 \cdot 2^p + 2 \cdot 4^p > 4 \cdot 4^p = R_p\left(K_{1,4}\right).$$

Hence, we just need to analyze requirement (1′). In these analyses, we shall need the concept of push-to-leaves function defined in paper [16] and used in papers [18,21]. The definition is repeated here for the sake of the completeness of the results.

Let T be any tree with at least three vertices and $f : E(T) \to \mathbb{R}$ be any function, where $\mathbb{R}$ is the set of real numbers. Let r be any vertex of degree greater than 1 in T. Denote by $L(T)$ the set of leaves (or pendant vertices) in T. The function $f^{ptl(r)} = f^{ptl} : L(T) \to R$ is called *r-pushed to leaves f* and it is defined by

$$f^{ptl}(l) = f(lv_1) + \frac{f(v_1v_2)}{d(v_1) - 1} + \frac{f(v_2v_3)}{(d(v_1) - 1) \cdot (d(v_2) - 1)} + \cdots + \frac{f(v_kv_{k-1})}{(d(v_1) - 1)(d(v_2) - 1) \cdot \ldots \cdot (d(v_{k-1}) - 1)} + \frac{f(v_kr)}{(d(v_1) - 1) \cdot (d(v_2) - 1) \cdot \ldots \cdot (d(v_k) - 1)},$$

where $lv_1v_2 \cdots v_kr$ is a path from r to l (specially, if $rl \in E(T)$, then $f^{ptl}(l) = f(rl)$). In the following figure "pushing to the leaves" (Fig. 1) of just one single value $f(vw)$ is presented.