Which Generalized Randić Indices are Suitable Measures of Branching?

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Abstract

Molecular branching is very important notion, because it influences many physicochemical properties of chemical compounds. However, there is no consensus how to measure branching. Never the less two requirements seem to be obvious: star is the most branched graph and path is the least branched graph. Hence, every measure of branching should have these two graphs as extremal graphs. In the paper we analyze general Randić index defined by

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

In the paper [1], negative values of $p$ have been analyzed and it has been shown that there is a value $\mu$ such that $R_p$, $p < \mu$ is not suitable measure for branching and that $R_p$ for $p \in (\mu, 0)$ may be a suitable measure of branching. In [1], it was shown that $\mu \in [-0.826077, -0.5]$ and it has been conjectured that $\mu \approx -0.8$. In this paper it is shown that $\mu \approx -0.7749$, more precisely that $\mu \in (-0.77492, -0.77486)$. Also, positive values of $p$ are analyzed here and it has been shown that $R_p$ is suitable measure for branching if and only if
$p \in (0,1]$. These results further results of paper [2] where only chemical graphs have been considered.

1. Introduction

It is well known that many chemical and physical properties of chemical compounds depend on their branching. Hence, it would be interesting to find a numerical value of branching. Unfortunately, so far there is no consensus how to measure branching, because it is not always easy to say which of two given trees is more branched. However, in some cases this is not difficult. Obviously path with $N$ vertices $P_N$ is the least branched among all trees with $N$ vertices. Similarly it is easy to see that star $S_N$ with $N$ vertices is more branched then any of the vertices with $N$ vertices. Moreover, sometimes authors give more rules for determination of more branched tree [3-5]. In this paper, we shall restrict only on this basic (the least restrictive) condition that observed function $\phi$ may be suitable measure of branching if it has path $P_N$ and star $S_N$ as only extremal graphs (one attaining minimum and other attaining maximum), i.e. if it holds one of the following:

1) $\chi(P_3) < \chi(S_3)$ and $\chi(P_N) < \chi(T_N) < \chi(S_N)$ for every tree $T_N \neq P_N, K_{1,N-1}$ with $N \geq 5$ vertices;
2) $\chi(P_3) > \chi(S_3)$ and $\chi(P_N) > \chi(T_N) > \chi(S_N)$ for every tree $T_N \neq P_N, K_{1,N-1}$ with $N \geq 5$ vertices.

Randić index [6] in of the most famous molecular descriptors and it is defined by

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

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. It satisfies condition 2) and hence it is suitable measure of branching. This index is generalized to:
Note that this can be rewritten as:

\[ R_p(G) = \sum_{uv \in E(G)} (d_ud_v)^p. \]

where \( \Delta \) is 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 [7-17]. Hence, it is of interest to find which of these indices suitable measures of branching are. In paper [1], negative values of \( p \) have been analyzed, because authors restricted their attention on the condition 2) and condition 2) is not met for any positive number \( p \). It has been shown that there is a value \( \mu \) such that \( R_p, p < \mu \) is not suitable measure for branching and that \( R_p \) for \( p \in (\mu, 0) \) satisfies condition 2) and hence it can be considered as suitable measure of branching. Moreover, in paper [1], it has been shown that \( \mu \in [-0.826077, 0.5] \) and it has been shown that conjectured that \( \mu \approx -0.8 \).

In this paper it is shown that \( \mu \approx -0.7749 \), more precisely that \( \mu \in (-0.77492, 0.77486) \). Also, positive values of \( p \) are analyzed here and it is shown that \( R_p, p > 0 \), is suitable measure of branching if and only if \( p \in (0, 1] \).

2. Positive values of \( p \)

In paper [1], it has been shown that 2) is not satisfied for any positive value of \( p \). In paper [18], it has been shown that for every \( p \in (0, 1] \) it holds that:

\[ R_p(T_N) < R_p(S_N) \] for every \( N \geq 5 \) and every tree \( T_N \neq S_N \) with \( N \) vertices;
and that for every $p > 1$, there is a $N \in \mathbb{N}$ and $T_N$ such that $R_p(T_N) > R_p(S_N)$. In paper [1] it has been shown that $R_p(P_n) < R_p(S_n)$ for every $p \in (0,1]$, and in paper [19] it has been shown that:

$$R_p(P_N) < R_p(T_N)$$

for every $N \geq 5$ and every tree $T_N \neq P_N$ with $N \geq 5$ vertices.

Combining all these results, we get:

**Theorem 1.** Let $p > 0$. $R_p$ is suitable measure of branching if and only if $p \in (0,1]$.

### 3. Negative values of $p$

In paper [1], it has been shown that 1) is not satisfied for any positive value of $p$. Hence, we only need to analyze requirement 2). Let us denote by $G(d_1, d_2, \ldots, d_n)$ graph that has vertex $u$ such that all leaves are on distance $n$ from $u$ and that for every path from leaf $l$ to $u$ $lu_1u_2\ldots u_n \ (u_n = u)$, it holds that degree of vertex $u_i$ is equal to $d_i$.

In paper [20], the concept of the push-to leaves function is introduced and it has been applied in papers [2,21,22]. For the sake of the completeness, we shall repeat its definition.

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

$$f^{ptl}(l) = f(v_l) + \frac{f(v_1v_2)}{d(v_1)-1} + \frac{f(v_2v_3)}{(d(v_1)-1)(d(v_2)-1)} + \cdots + \frac{f(v_kv_{k-1})}{(d(v_1)-1)(d(v_2)-1)\cdots (d(v_{k-1})-1)}$$

where $v_1, v_2, \ldots, v_k$ are vertices on the path from $v_l$ to $r$ in $T$. The push-to leaves function is useful in measuring the degree of branching at a particular vertex in a tree.
where \( l_{v_1v_2...v_k} \) is a path from \( r \) to \( l \) (specially, if \( rl \in E(T) \), then \( f_{ptl}^m(l) = f(rl) \)). On the following figure is presented „pushing to the leaves“ of just one single value \( f(vw) \).

![Figure 1. Pushing of \( f(vw) \) to the leaves.](image)

It can be easily seen that:

\[
\sum_{e \in E(T)} f(e) = \sum_{l \in L(T)} f_{ptl}^m(l),
\]

because all the values \( f(e) \) are „pushed to the leaves“. Analogously as in paper [2], we define: Let \( T_N \neq P_N \) be chemical tree with \( N \) vertices and let \( r \) be any vertex of degree greater than 2. Let us define function \( F_p \) by: \( F_p(uv) = (d_u d_v)^p - 4^p \) for \( u, v \neq r \) and by \( F_p(rv) = (d_r d_v)^p - 4^p - \frac{2}{d_r} (2^p - 4^p) \). It can be easily seen that:

\[
R_p(T_N) - R_p(P_N) = \sum_{e \in E(T_N)} F_p(e),
\]

Hence,

\[
R_p(T_N) - R_p(P_N) = \sum_{l \in L(T_N)} F_{ptl}^m(l).
\]
Let \( x_1, \ldots, x_n \in \mathbb{R} \) such that \( x_n > 1 \). Let us define similarly as in [1]:

\[
\Phi_p(x_1, \ldots, x_n) = \left( x_1 + 1 \right)^p \left( x_2 + 1 \right)^p - 4^p + \frac{1}{x_1} \left( x_1 + 1 \right)^p \left( x_2 + 1 \right)^p - 4^p + \frac{1}{x_1 x_2} \left( x_2 + 1 \right)^p \left( x_3 + 1 \right)^p - 4^p + \cdots + \frac{1}{x_1 x_2 \cdots x_{n-2}} \left( x_{n-2} + 1 \right)^p \left( x_{n-1} + 1 \right)^p - 4^p + \frac{1}{x_1 x_2 \cdots x_{n-2} x_{n-1}} \left( x_{n-1} + 1 \right)^p \left( x_n + 1 \right)^p - 4^p - \frac{2}{x_n + 1} \left( 2^p - 4^p \right).
\]

and

\[
\Phi_{p,v}(x_1, \ldots, x_n) = \left( x_1 + 1 \right)^p \left( x_2 + 1 \right)^p - 4^{p+v} + \frac{1}{x_1} \left( x_1 + 1 \right)^p \left( x_2 + 1 \right)^p - 4^{p+v} + \frac{1}{x_1 x_2} \left( x_2 + 1 \right)^p \left( x_3 + 1 \right)^p - 4^{p+v} + \cdots + \frac{1}{x_1 x_2 \cdots x_{n-2}} \left( x_{n-2} + 1 \right)^p \left( x_{n-1} + 1 \right)^p - 4^{p+v} + \frac{1}{x_1 x_2 \cdots x_{n-2} x_{n-1}} \left( x_{n-1} + 1 \right)^p \left( x_n + 1 \right)^p - 4^{p+v} - \frac{2}{x_n + 1} \left( 2^{p+v} - 4^p \right).
\]

Let \( l_1 v_2 \ldots v_k, v_k = r \) be a path from any leaf \( l \) to \( r \). Then,

\[
F_p^{\mu l}(l) = \Phi_p(d_{l_1} - 1, d_{v_2} - 1, \ldots, d_{v_k} - 1).
\]

Let \( x_1, \ldots, x_n \in \mathbb{R} \) , then

\[
\Phi_p(x_1, \ldots, x_n) = \left( x_1 + 1 \right)^p \left( x_2 + 1 \right)^p - 4^p + \frac{1}{x_1} \left( x_1 + 1 \right)^p \left( x_2 + 1 \right)^p - 4^p + \frac{1}{x_1 x_2} \left( x_2 + 1 \right)^p \left( x_3 + 1 \right)^p - 4^p + \cdots + \frac{1}{x_1 x_2 \cdots x_{n-2}} \left( x_{n-2} + 1 \right)^p \left( x_{n-1} + 1 \right)^p - 4^p + \frac{1}{x_1 x_2 \cdots x_{n-2} x_{n-1}} \left( x_{n-1} + 1 \right)^p \left( x_n + 1 \right)^p - 4^p.
\]
\[
\Phi_{p,c}^0(x_1, \ldots, x_n) = \left[ (x_1 + 1)^{p+\varepsilon} - 4^p \right] + \frac{1}{x_1} \left[ (x_1 + 1)^{p+\varepsilon} (x_2 + 1)^{p+\varepsilon} - 4^p \right] + \frac{1}{x_1 x_2} \left[ (x_2 + 1)^{p+\varepsilon} (x_3 + 1)^{p+\varepsilon} - 4^p \right] + \ldots + \frac{1}{x_1 x_2 \ldots x_{n-2}} \left[ (x_{n-2} + 1)^{p+\varepsilon} (x_{n-1} + 1)^{p+\varepsilon} - 4^p \right] + \frac{1}{x_1 x_2 \ldots x_{n-2} x_{n-1}} \left[ (x_{n-1} + 1)^{p+\varepsilon} (x_n + 1)^{p+\varepsilon} - 4^p \right].
\]

Completely analogously as in paper [2], it can be proved that:

**Theorem 2.** Let \( p \in \mathbb{R} \). Then, \( R_p(T_N) < R_p(P_N) \) for every \( N \geq 4 \) and for every tree \( T_N \) with \( N \geq 4 \) vertices if and only if \( \Phi_p(x_1, \ldots, x_n) < 0 \) for every \( n \in \mathbb{N} \) and every \( x_1, \ldots, x_n \in \mathbb{R} \) such that \( x_n > 1 \). \( \blacksquare \)

Let us prove:

**Theorem 3.** Let \( p \in [-0.827, -0.77492] \), then \( \Phi_p(1,2,4,12,187,999970) > 0 \).

**Proof:** First note that for every \( p \in [-0.827, -0.77492] \) and \( \varepsilon > 0 \), it holds:

\[
\Phi_p(1,2,4,12,187,999970) > \Phi_{p,c}(1,2,4,12,187,999970).
\]

Hence, it is sufficient to check that \( \Phi_{p,c}(1,2,4,12,187,999970) > 0 \) for:

1) \( \varepsilon = 0.001 \) and \( p \in \{-0.827, -0.826, \ldots, 0.782\} \);
2) \( \varepsilon = 0.0001 \) and \( p \in \{-0.781, -0.7809, \ldots, -0.7756\} \);
3) \( \varepsilon = 0.00001 \) and \( p \in \{-0.7755, -0.77549, \ldots, -0.77498\} \);
4) \( \varepsilon = 0.000001 \) and \( p \in \{-0.77497, -0.774969, -0.77492\} \).

This is verified by computer. \( \blacksquare \)

Combining the last Theorem and results of [1], we get:

**Theorem 4.** Let \( p \leq -0.77492 \), then \( R_p \) is not suitable measure of branching.
In paper [19], it has been proved that $R_p(S_N) < R_p(T_N)$ for every $N \geq 4$ and every tree $T_N \neq S_N$ with $N$ vertices for every $p < 0$. In paper [18], it has been proved that $R_p(T_N) < R_p(P_N)$ for $p \in [-0.5, 0)$. Hence, it remains to prove that:

**Theorem 5.** Let $p \in [-0.77486, -0.5)$, then $R_p(T_N) < R_p(P_N)$ for every $N \geq 4$ and every $T_N \neq P_N$.

**Proof:** From Theorem [2], it follows that it is sufficient to prove that $\Phi_p(x_1, ..., x_n) < 0$ for every $n \in \mathbb{N}$ and every $x_1, ..., x_n \in \mathbb{R}$ such that $x_n > 1$. Further, note that:

$$\Phi_p(x_1, ..., x, 1, 1, x_{i+3}, ..., x_n) = \Phi_p(x_1, ..., x, 1, x_{i+3}, ..., x_n),$$

Hence it is sufficient to prove that $\Phi_p(x_1, ..., x_n) < 0$ for every $n \in \mathbb{N}$ and every $x_1, ..., x_n \in \mathbb{R}$ such that $x_n > 1$ and that there are no two consecutive ones in the sequence $x_1, ..., x_n$.

Note that for every $p \in [-0.77486, 0.5)$, every $\varepsilon > 0$, every $n \in \mathbb{N}$ and every $x_1, ..., x_n \in \mathbb{R}$ it holds that:

$$\Phi_p(x_1, ..., x_n) < \Phi_{p, \varepsilon}(x_1, ..., x_n).$$

Hence, it is sufficient to check that $\Phi_{p, \varepsilon}(x_1, ..., x_n) > 0$ every $x_1, ..., x_n \in \mathbb{R}$ such that $x_n > 1$ and that there are no two consecutive ones in the sequence $x_1, ..., x_n$ when

1) $\varepsilon = 0.001$ and $p \in \{-0.5, -0.501, ..., -0.76\}$;
2) $\varepsilon = 0.0001$ and $p \in \{-0.761, -0.7611, ..., -0.7743\}$;
3) $\varepsilon = 0.00001$ and $p \in \{-0.7744, -0.77441, ..., -0.77486\}$.

We shall do this by applying recursive function based on the following three observations:

$$\Phi_{p, \varepsilon}(x_1, ..., x_n) < \Phi^0_{p, \varepsilon}(x_1, ..., x_n);$$
\[
\Phi_{p,\varepsilon}^0(x_1, \ldots, x_n, x_{n+1}) < \Phi_{p,\varepsilon}^0(x_1, \ldots, x_n);
\]
\[
\Phi_{p,\varepsilon}^0(x_1, \ldots, x_{n-1}, x_n + 1) < \Phi_{p,\varepsilon}^0(x_1, \ldots, x_{n-1}, x_n);
\]

Pseudo-code of this function is given below:

Rec\((x_1, \ldots, x_n)\)

If \(\Phi_{p,\varepsilon}^0(x_1, \ldots, x_n)\) then

If \(x_n > 2\) and \(\Phi_{p,\varepsilon}(x_1, \ldots, x_n) > 0\) then

print “Claim does not hold for observed \(p\) and \(\varepsilon\)”

exit program

If \(x_n = 1\) then

Rec\((x_1, \ldots, x_n, 2)\)

Else

Rec\((x_1, \ldots, x_n, 1)\)

Rec\((x_1, \ldots, x_n + 1)\)

This function is called with Rec\((1)\). If it does not display message “Claim does not hold for observed \(p\) and \(\varepsilon\)” then it holds \(\Phi_{p,\varepsilon}(x_1, \ldots, x_n) > 0\) for every \(x_1, \ldots, x_n \in \mathbb{R}\) such that \(x_n > 1\) and that there are no two consecutive ones in the sequence \(x_1, \ldots, x_n\) for the observed \(p\) and \(r\). All pairs of \(p\) and \(r\) listed in 1)-3) have been checked by computer and that proved the theorem.

Collecting all the results, we get:

**Theorem 6.** Let \(p < 0\). There is real number \(\mu \in (-0.77492, -0.77486)\) such that \(R_p\) is suitable measure of branching if and only if \(p > \mu\).

Although we did not find the exact solution, it is found that \(\mu\) rounded to four decimal places is \(-0.7749\). This kind of precession is sufficient for almost all practical chemical purposes. Nevertheless, it would be nice to find the exact solution of \(\mu\) which remains an open problem.
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