MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **64** (2010) 443-452

ISSN 0340 - 6253

Which Generalized Randić Indices are Suitable Measures of Branching?

Damir Vukičević

Faculty of Natural Sciences and Mathematics, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia

(Received May 11, 2009)

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 $R_p(G) = \sum_{uv \in E(G)} (d_u d_v)^p$. In the paper [1], negative values of p have been analyzed and it has been shown that there is a value μ 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 ϕ 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) $\chi(P_4) < \chi(S_4)$ 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) $\chi(P_4) > \chi(S_4)$ 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:

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

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 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 μ 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 $N \ge 5$ and every tree $T_N \ne S_N$ with N vertices;

and that for every $p>1$, there is a $N \in$ and T_N such that $R_p(T_N) > R_p(S_N)$. In paper [1] it has been shown that $R_p(P_4) < R_p(S_4)$ for every $p \in (0,1]$, and in paper [19] it has been shown that:

$$R_p(P_N) < R_p(T_N) \text{ for every } N \geq 5 \text{ and every tree } T_N \neq P_N \text{ with } N \geq 5 \text{ vertices.}$$

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 $f: E(T) \rightarrow$ be any function, where 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 $f^{ptl(r)} = f^{ptl} : L(T) \rightarrow R$ is called $r-$*pushed to leaves* f and it is defined by:

$$\begin{aligned} f^{ptl}(l) &= f(v_1 l) + \frac{f(v_1 v_2)}{d(v_1)-1} + \frac{f(v_2 v_3)}{(d(v_1)-1)\cdot(d(v_2)-1)} + \\ &+ \ldots + \frac{f(r v_k)}{(d(v_1)-1)\cdot(d(v_2)-1)\cdot \ldots \cdot(d(v_k)-1)} + \frac{f(v_k v_{k-1})}{(d(v_1)-1)(d(v_2)-1)\cdot \ldots \cdot(d(v_{k-1})-1)}, \end{aligned}$$

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

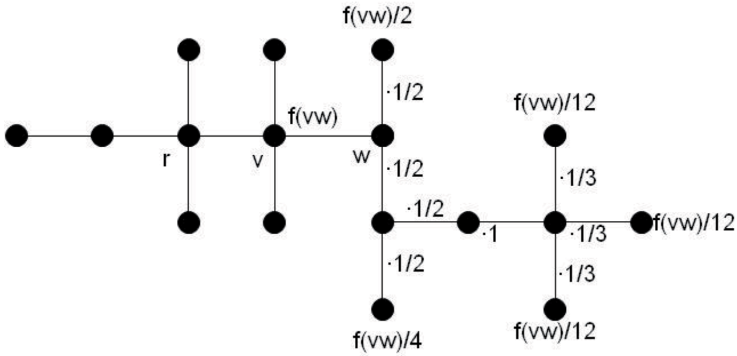

Figure 1. Pushing of $f(vw)$ to the leaves.

It can be easily seen that:

$$\sum_{e \in E(T)} f(e) = \sum_{l \in L(T)} f^{ptl}(l),$$

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 then 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,

$$R_p(T_N) - R_p(P_N) = \sum_{l \in L(T)} F_p^{ptl}(l).$$

Let $x_1,...,x_n \in$ such that $x_n > 1$. Let us define similarly as in [1]:

$$\begin{aligned}\Phi_p(x_1,...,x_n) &= \left[(x_1+1)^p - 4^p\right] + \frac{1}{x_1}\left[(x_1+1)^p(x_2+1)^p - 4^p\right] + \\ &+ \frac{1}{x_1x_2}\left[(x_2+1)^p(x_3+1)^p - 4^p\right] + \ldots + \frac{1}{x_1x_2\ldots x_{n-2}}\left[(x_{n-2}+1)^p \cdot (x_{n-1}+1)^p - 4^p\right] + \\ &+ \frac{1}{x_1x_2\ldots x_{n-2}x_{n-1}}\left[(x_{n-1}+1)^p \cdot (x_n+1)^p - 4^p - \frac{2}{x_n+1}\left(2^p - 4^p\right)\right].\end{aligned}$$

and

$$\begin{aligned}\Phi_{p,\varepsilon}(x_1,...,x_n) &= \left[(x_1+1)^p - 4^{p+\varepsilon}\right] + \frac{1}{x_1}\left[(x_1+1)^p(x_2+1)^p - 4^{p+\varepsilon}\right] + \\ &+ \frac{1}{x_1x_2}\left[(x_2+1)^p(x_3+1)^p - 4^{p+\varepsilon}\right] + \ldots + \frac{1}{x_1x_2\ldots x_{n-2}}\left[(x_{n-2}+1)^p \cdot (x_{n-1}+1)^p - 4^{p+\varepsilon}\right] + \\ &+ \frac{1}{x_1x_2\ldots x_{n-2}x_{n-1}}\left[(x_{n-1}+1)^p \cdot (x_n+1)^p - 4^{p+\varepsilon} - \frac{2}{x_n+1}\left(2^{p+\varepsilon} - 4^p\right)\right].\end{aligned}$$

Let $lv_1v_2...v_k$, $v_k = r$ be a path from any leaf l to r. Then,

$$F_p^{ptl}(l) = \Phi_p\left(d_{v_1}-1, d_{v_2}-1, ..., d_{v_k}-1\right).$$

Let $x_1,...,x_n \in$, then

$$\begin{aligned}\Phi_p^0(x_1,...,x_n) &= \left[(x_1+1)^p - 4^p\right] + \frac{1}{x_1}\left[(x_1+1)^p(x_2+1)^p - 4^p\right] + \\ &+ \frac{1}{x_1x_2}\left[(x_2+1)^p(x_3+1)^p - 4^p\right] + \ldots + \frac{1}{x_1x_2\ldots x_{n-2}}\left[(x_{n-2}+1)^p \cdot (x_{n-1}+1)^p - 4^p\right] + \\ &+ \frac{1}{x_1x_2\ldots x_{n-2}x_{n-1}}\left[(x_{n-1}+1)^p \cdot (x_n+1)^p - 4^p\right];\end{aligned}$$

$$\Phi^0_{p,\varepsilon}(x_1,\ldots,x_n)=\left[(x_1+1)^{p+\varepsilon}-4^p\right]+\frac{1}{x_1}\left[(x_1+1)^{p+\varepsilon}(x_2+1)^{p+\varepsilon}-4^p\right]+$$
$$+\frac{1}{x_1x_2}\left[(x_2+1)^{p+\varepsilon}(x_3+1)^{p+\varepsilon}-4^p\right]+\ldots+\frac{1}{x_1x_2\ldots x_{n-2}}\left[(x_{n-2}+1)^{p+\varepsilon}\cdot(x_{n-1}+1)^{p+\varepsilon}-4^p\right]+$$
$$+\frac{1}{x_1x_2\ldots x_{n-2}x_{n-1}}\left[(x_{n-1}+1)^{p+\varepsilon}\cdot(x_n+1)^{p+\varepsilon}-4^p\right].$$

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

Theorem 2. Let $p\in$. 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 $n\in$ and every $x_1,\ldots,x_n\in$ such that $x_n>1$. ■

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:

$$\Phi_p(1,2,4,12,187,999970)>\Phi_{p,\varepsilon}(1,2,4,12,187,999970).$$

Hence, it is sufficient to check that $\Phi_{p,\varepsilon}(1,2,4,12,187,999970)>0$ 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. ■

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 $\Phi_p(x_1, \ldots, x_n) < 0$ for every $n \in$ and every $x_1, \ldots, x_n \in$ such that $x_n > 1$. Further, note that:

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

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

Note that for every $p \in [-0.77486, 0.5)$, every $\varepsilon > 0$, every $n \in$ and every $x_1, \ldots, x_n \in$ it holds that:

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

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

1) $\varepsilon = 0.001$ and $p \in \{-0.5, -0.501, \ldots, -0.76\}$;

2) $\varepsilon = 0.0001$ and $p \in \{-0.761, -0.7611, \ldots., -0.7743\}$;

3) $\varepsilon = 0.00001$ and $p \in \{-0.7744, -0.77441, \ldots, -0.77486\}$.

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

$$\Phi_{p,\varepsilon}(x_1, \ldots, x_n) < \Phi^0_{p,\varepsilon}(x_1, \ldots, x_n);$$

$$\Phi^0_{p,\varepsilon}\left(x_1,\ldots,x_n,x_{n+1}\right) < \Phi^0_{p,\varepsilon}\left(x_1,\ldots,x_n\right);$$
$$\Phi^0_{p,\varepsilon}\left(x_1,\ldots,x_{n-1},x_n+1\right) < \Phi^0_{p,\varepsilon}\left(x_1,\ldots,x_{n-1},x_n\right);$$

Pseudo-code of this function is given below:

$\mathrm{Rec}\left(x_1,\ldots,x_n\right)$

  If $\Phi^0_{p,\varepsilon}\left(x_1,\ldots,x_n\right)$ then

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

      print "Claim does not hold for observed p and ε"

      exit program

    If $x_n = 1$ then

      $\mathrm{Rec}\left(x_1,\ldots,x_n,2\right)$

    Else

      $\mathrm{Rec}\left(x_1,\ldots,x_n,1\right)$

    $\mathrm{Rec}\left(x_1,\ldots,x_n+1\right)$

This function is called with $\mathrm{Rec}(1)$. If it does not display message "Claim does not hold for observed p and ε", then it holds $\Phi_{p,\varepsilon}\left(x_1,\ldots,x_n\right) > 0$ for every $x_1,\ldots,x_n \in$ 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 $\mu \in \left(-0.77492,-0.77486\right)$ 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 μ rounded to four decimal places is -0.7749. This kind of precession is sufficient for almost all practical chemical purposes. Never the less, it would be nice to find the exact solution of μ which remains an open problem.

Acknowledgment. The partial support of Croatian Ministry of Science, Education and Sport (grants no. 177-0000000-0884 and 037-0000000-2779) is gratefully acknowledged.

References

1. L. Clark, I. Gutman, *J. Math. Chem*. **43** (2008) 32-44.
2. D. Vukičević, Which generalized Randić indices are suitable measures of molecular branching, preprint.
3. I. Gutman, D. Vukičević, J. Žerovnik, *Croat. Chem. Acta* **77** (2004) 103-109.
4. D. Vukičević, J. Žerovnik, *MATCH Commun. Math. Comput. Chem*. **53** (2005) 385-402.
5. D. Vukičević, J. Žerovnik, *Acta Chim. Slov*. **52** (2005) 272-281.
6. M. Randić, *J. Am. Chem. Soc*. **97** (1975) 6609-6615.
7. G. Caporossi, I. Gutman, P. Hansen, *MATCH Commun. Math. Comput. Chem*. **23** (1999) 469-477.
8. M. Fischermann, A. Hoffman, D. Rautenbach, L. Volkmann, *Discr. Appl. Mat.* **128** (2003) 375-385.
9. Lj. Pavlović, *Discr. Appl. Math.* **127** (2003) 615-626.
10. G. Caporossi, I. Gutman, P. Hansen, Lj. Pavlović, *Comput. Biol. Chem,* **27** (2003) 85-90.
11. D. Vukičević, A. Graovac, *Croat. Chem. Acta* **77** (2004) 313-319.
12. D. Vukičević, A. Graovac, *Croat. Chem. Acta* **77** (2004) 481-490.
13. D. Vukičević, A. Graovac, *Croat. Chem. Acta* **77** (2004) 501-508.
14. D. Vukičević, N. Trinajstić, *Croat. Chem. Acta* **76** (2003) 183-187.
15. D. Vukičević, N. Trinajstić, *MATCH Commun. Math. Comput. Chem*. **53** (2005) 111-138.
16. D. Veljan, D. Vukičević, *J. Math. Chem*. **40** (2006) 155-178.
17. D. Vukičević, On the Edge Degrees of Trees, *Glas. Mat. Ser. III*, to appear.
18. Y. Hu, X. Li, Y. Yuan, *MATCH Commun. Math. Comput. Chem*. **52** (2004) 129-146.
19. Y. Hu, X. Li, and Y. Yuan, *MATCH Commun. Math. Comput. Chem*. **52** (2004) 119-128.
20. D. Vukičević, Upper Bound of Randić Index in Terms of Numbers of Vertices of Degree 1 and 2; published in *Recent Results in the Theory of Randić index* (Eds. I. Gutman, B. Furtula) 83-90.
21. D. Vukičević, T. Pisanski, On the extremal values of ratios of number of paths, preprint.
22. D. Vukičević, A. Graovac, On the extremal values of ratios of number of walks, preprint.