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The exponent in the general Randić index

Lane Clark

Department of Mathematics, Southern Illinois University Carbondale, Carbondale IL 62901-4408, USA

Ivan Gutman*

Faculty of Science, University of Kragujevac, 34000 Kragujevac, Serbia
E-mail: gutman@kg.ac.yu

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We determine conditions for the parameters n and δ, for which the general Randić index R_δ is not an acceptable index of branching of n-vertex trees, i.e., for which the n-vertex star and the n-vertex path have not extremal $R_{\delta}-$values among all n-vertex trees. Analogous results are established also in the case of n-vertex chemical trees. Numerous other results for the general Randić index of trees and chemical trees are obtained.

KEY WORDS: Randić index, connectivity index, general Randić index, molecular branching

AMS SUBJECT CLASSIFICATION: 05C07

1. Introduction

There is no general agreement of how to measure "branching" of organic molecules whose molecular graphs are trees [1–7]. Nevertheless, there seems to be a general agreement in mathematical chemistry that, if χ is an acceptable index of branching of trees, then, at the worst,

$$\chi(K_{1,\,n-1}) \leqslant \chi(T_n) \leqslant \chi(P_n) \quad \text{for all trees } T_n \neq K_{1,\,n-1}, P_n, \tag{1}$$

i.e., $\chi(K_{1,n-1})$ and $\chi(P_n)$ are the minimum and maximum values of $\chi(T_n)$ though possibly not uniquely, and more universally,

$$\chi(K_{1,\,n-1}) < \chi(T_n) < \chi(P_n) \quad \text{for all trees } T_n \neq K_{1,n-1}, P_n, \tag{2}$$

i.e., $\chi(K_{1,n-1})$ and $\chi(P_n)$ are the unique minimum and maximum values of $\chi(T_n)$.

*Corresponding author.

Observe that necessary condition (2) implies necessary condition (1). Throughout the paper, $K_{1,n-1}$ is the star of order n and P_n is the path of order n.

Randić [8] introduced the index

$$R_\delta(T) = \sum_{uv \in E(T)} (d_T(u) d_T(v))^\delta$$

of a tree T. To preserve rankings of certain organic molecules, the index had to satisfy seven crucial inequalities. He stated that both $\delta = -0.5$ and $\delta = -1$ satisfied these inequalities and eventually chose $\delta = -0.5$. Since that time, $R_{-0.5}$ has come to be known as the Randić index and R_δ as the general Randić index [9]. The general Randić index with $\delta = -0.5$, and to some extent with $\delta = -1$ and $\delta = +1$, has been extensively used as a measure of branching of trees. Several hundred papers and several books have been written about this index for $\delta = -0.5, -1$, and $+1$; for details (see [9]).

In table 1, we summarize the current state of knowledge regarding the minimum and maximum values of R_δ for $\delta \in | - \{0\}$. From table 1, we see that:

(1) R_δ does not satisfy the bounds in (1), hence not in (2), and therefore is not an acceptable index of branching of trees for $\delta \in (0, \infty)$.

(2) R_δ does not satisfy the upper bound in (1), hence not in (1), and therefore is not an acceptable index of branching of trees for $\delta \in (-\infty, -2]$.

(3) R_δ satisfies (2), hence in (1), and possibly is an acceptable index of branching of trees for $\delta \in [-0.5, 0)$.

Hence, only $\delta \in (-2, -0.5)$ needs to be examined.

In section 2, we give trees $T_n (\forall n \geqslant 24515)$ with $R_{-\delta}(T_n) > R_{-\delta}(P_n)$ for all $-\delta \in [-2, -0.82179]$ (see theorems 7 and 9). Hence, $R_{-\delta}$ is not an acceptable index (1 so 2) of branching of trees for all $-\delta \in (-\infty, -0.82179]$ (see corollary 12).

We also prove the existence of critical values $-0.817268757 \leqslant -\alpha \leqslant -\beta \leqslant -0.5$ where: $R_{-\delta}$ does not satisfy (1 so 2) for all $-\delta \in (-2, -0.817268757)$ and for all $n \geqslant 24515$;

Table 1

δ	$\min R_\delta(T_n)$	$\max R_\delta(T_n)$
$(-\infty, -2]$	$\forall\delta \in (-\infty, 0)$	$w_\delta(T_n) < w_\delta(SS_n), \forall T_n \neq SS_n, n \geqslant 7$[10]
$(-2, -0.5)$	$R_\delta(T_n) > R_\delta(K_{1,n-1})$	unknown; see theorems 7 and 9: $\exists T_n \neq P_n$ with
	$\forall T_n \neq K_{1,n-1}, n \geqslant 5$[11]	$R_\delta(T_n) > R_\delta(P_n), \forall n \geqslant 24515$ and
		$\forall\delta \in (-2, -0.82179)$
$[-0.5, 0)$		$R_\delta(T_n) < R_\delta(P_n), \forall T_n \neq P_n, n \geqslant 7$[10]
$(0, 1]$	$\forall\delta \in (0, \infty)$	$R_\delta(T_n) < R_\delta(K_{1,n-1}), \forall T_n \neq K_{1,n-1}, n \geqslant 2$?[10]
$(1, 2)$	$R_\delta(T_n) > R_\delta(P_n)$	$R_\delta(T_n) < R_\delta(S_n), \forall T_n \neq S_n, n \geqslant 8$?[10]
$[2, \infty)$	$\forall T_n \neq P_n, n \geqslant 5$[11]	$R_\delta(T_n) < R_\delta(BDS_n) \forall T_n \neq BDS_n, n \geqslant 8$[10]

$R_{-\delta}$ does not satisfy (1) for a dense set of $-\delta \in (-0.817268757, -\alpha)$ and all $n \geqslant N(\delta)$;
$R_{-\delta}$ satisfies (1) for all $-\delta \in (-\alpha, 0)$ and for all $n \geqslant 7$;
$R_{-\delta}$ does not satisfy (2) for a dense set of $-\delta \in (-0.817268757, -\beta)$ and all $n \geqslant N(\delta)$;
$R_{-\delta}$ satisfies (2) for all $-\delta \in (-\beta, 0)$ and for all $n \geqslant 7$.

Hence, $R_{-\delta}$ changes from, not being to possibly being, an acceptable index (1 or 2) of branching of trees at $-0.817268757 \leqslant -\alpha \leqslant -\beta \leqslant -0.5$ (respectively); see corollaries 3, 6 and theorems 7,9, 11. figure 1 displays much of this information.

Evidently finding the values of $-\alpha, -\beta$ is of interest. We conjecture that -$\alpha = -\beta \approx -0.8$. If the conjecture is true, then the choice of -0.5 by Randić was rather fortuitous. It is likely that $R_{-\delta}$ satisfies the necessary condition (2) to be an acceptable index of branching for all $-\delta \in [-\alpha, -\beta]$, so for all $-\delta \in [-\alpha, 0)$.

We also have analogous results in section 3 for chemical trees (maximum degree at most 4).

It is convenient to write $\delta \in (-\infty, 0)$ as $-\delta$ where $\delta \in (0, \infty)$, so that

$$R_{-\delta}(T) = \sum\nolimits_{uv \in E(T)} \frac{1}{(d_T(u)d_T(v))^{\delta}}$$

with $\delta \in (0, \infty)$. With regard to extreme values of $R_{-\delta}(T)$, only the maximum value of $R_{-\delta}(T)$ for $\delta \in (0.5, 2)$ needs to be examined. We write $\forall$ for "for all", $\exists$ for "there exists" and f_x for the partial derivative of the function f with respect to x.

In table 1, T_n denotes any tree of order n; SS_n denotes the subdivided star of order n of [10]; BDS_n denotes the balanced double star of order n of [10] and S_n denotes the star or balanced double star of order n of [10].

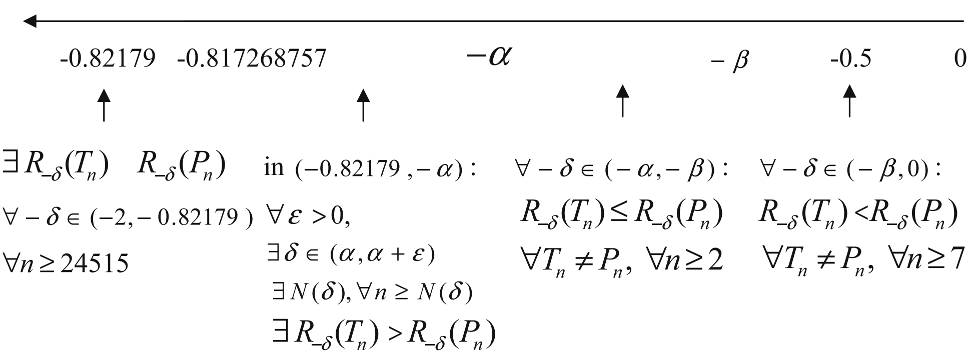

Figure 1.

2. Trees

For $n \geqslant 2$, let

$$A(n) = \{\delta \in (0,\ 2) : \exists\, R_{-\delta}(T_n) > R_{-\delta}(P_n),\ T_n \neq P_n\},$$
$$B(n) = \{\delta \in (0,\ 2) : \exists\, R_{-\delta}(T_n) \geqslant R_{-\delta}(P_n),\ T_n \neq P_n\},$$
$$C(n) = \{\delta \in (0,\ 2) : \exists\, R_{-\delta}(T_n) = R_{-\delta}(P_n),\ T_n \neq P_n\}.$$

By their definition, $A(n)$, $C(n) = B(n) - A(n) \subseteq B(n)$. From [12] (see Remark 8(1)), $1 \in A(n) \subseteq B(n)$ for all $n \geqslant 22$. By Hu et al. [10],

$$A(n), B(n), C(n) \subseteq (0.5,\ 2) \quad \text{for all } n \geqslant 7. \tag{3}$$

By the completeness the real numbers,

$$\alpha(n) = inf\ A(n) \quad \text{and } \beta(n) = \inf B(n)$$

exist for all $n \geqslant 22$. From their definitions, $\alpha(n) \geqslant \beta(n)$.

We first show that $\{A(n)\}_{n \geqslant 22}$ is a non-decreasing sequence of non-empty sets.

Theorem 1. $1 \in A(n) \subseteq A(n+1)$ for all $n \geqslant 22$.

Proof. Suppose $\delta \in A(n)$ so that $R_{-\delta}(T_n) > R_{-\delta}(P_n)$ for some tree $T_n \neq P_n$ where $n \geqslant 22$. Let $uv \in E(T_n)$ with $d_{T_n}(v) = 1$ and set $T_{n+1} = T_n + vw$ where w is a new vertex. Since $n \geqslant 3$, $d_{T_n}(u) \geqslant 2$. Then

$$\begin{aligned} R_{-\delta}(T_{n+1}) &= R_{-\delta}(T_n) - \frac{1}{(d_{T_n}(u))^\delta} + \frac{1}{(2d_{T_n}(u))^\delta} + \frac{1}{2^\delta} \\ &> R_{-\delta}(P_n) - \frac{1}{(d_{T_n}(u))^\delta} + \frac{1}{(2d_{T_n}(u))^\delta} + \frac{1}{2^\delta} \\ &= \frac{n-3}{4^\delta} + \frac{2}{2^\delta} - \frac{1}{(d_{T_n}(u))^\delta} + \frac{1}{(2d_{T_n}(u))^\delta} + \frac{1}{2^\delta}. \end{aligned}$$

This last quantity is

$$\begin{aligned} &\geqslant \frac{n-2}{4^\delta} + \frac{2}{2^\delta} \\ &\Leftrightarrow \frac{1}{4^\delta} + \frac{1}{(2d_{T_n}(u))^\delta} + \frac{1}{2^\delta} \geqslant \frac{1}{(d_{T_n}(u))^\delta} \\ &\Leftrightarrow (d_{T_n}(u))^\delta + 2^\delta + (2d_{T_n}(u))^\delta \geqslant 4^\delta \end{aligned}$$

which is true since $d_{T_n}(u) \geqslant 2$. Then $\delta \in A(n+1)$ so that $A(n) \subseteq A(n+1)$. □

Corollary 2. $\alpha(n) \geqslant \alpha(n+1)$ for all $n \geqslant 22$.

Proof. For all $n \geqslant 22, \alpha(n) = \inf A(n) \geqslant \inf A(n+1) = \alpha(n+1)$ since $A(n) \subseteq A(n+1)$. □

We next show that the sequence $\{\alpha(n)\}_{n \geqslant 22}$ has a real limit.

Corollary 3. $\mathrm{Lim}_{n\to\infty}\alpha(n) = \alpha$ exists and $\alpha \in [0.5,\ 1]$.

Proof. By Clark and Moon [12] and corollary 2, $\alpha(n)$ is a non-increasing sequence of real numbers in the interval (0.5, 1] for all $n \geqslant 22$. By the completeness of the real numbers, the limit α exists. Consequently, $\alpha \in [0.5, 1]$. □

The proof of theorem 1 with "$>$" replaced with "$\geqslant$" shows that $\{B(n)\}_{n \geqslant 22}$ is a non-decreasing sequence of nonempty sets. corollaries 5 and 6 immediately follow.

Theorem 4. $1 \in B(n) \subseteq B(n+1)$ for $n \geqslant 22$. □

Corollary 5. $\beta(n) \geqslant \beta(n+1)$ for all $n \geqslant 22$. □

Corollary 6. $\lim_{n\to\infty} \beta(n) = \beta$ exists and $\beta \in [0.5,\ 1]$. □

Necessarily, $\beta \leqslant \alpha$. We now improve the upper bound for α.

For each end-vertex v of $K_{1,r} (r \geqslant 1)$, append three disjoint paths P_1, P_2, P_3 of order 3 having end-vertices w_1, w_2, w_3, respectively, by identifying v and w_1, w_2, w_3. Denote the resulting tree by T_r. Then T_r has order $7r+1$ and

$$R_{-\delta}(T_r) = \frac{r}{(4r)^\delta} + \frac{3r}{8^\delta} + \frac{3r}{2^\delta}. \tag{4}$$

For each end-vertex $v_1, \ldots, v_k (1 \leqslant k \leqslant 6)$ of $T_r (r \geqslant 2)$, append vertex disjoint paths $P_1, \ldots, P_k$ of order 2 having end-vertices $w_1, \ldots, w_k$, respectively, by identifying v_1 and $w_1, \ldots, v_k$ and w_k. Denote the resulting tree by $T_{r,k}$. Then $T_{r,k}$ has order $7r+k+1$ and

$$R_{-\delta}(T_{r,k}) = R_{-\delta}(T_r) + \frac{k}{4^\delta}. \tag{5}$$

We write $T_r = T_{r,0}$, which is consistent with (4). These trees were introduced in [12].

Theorem 7. For each $n \geqslant 24515$, there exists a tree T_n with

$$R_{-\delta}(T_n) > R_{-\delta}(P_n)$$

for all $\delta \in [0.82179,\ 1.95]$ where $0.82179 = \delta^*$ is the real solution of $3 + 3 \cdot 4^\delta - 7 \cdot 2^\delta = 0$.

Proof. For $n = 7r + k + 1$ $(0 \leqslant k \leqslant 6)$, let

$$\begin{aligned}
a(r,k,\delta) &= R_{-\delta}(T_{r,k}) - R_{-\delta}(P_n)\\
&= \frac{r}{(4r)^\delta} + \frac{3r}{8^\delta} + \frac{3r}{2^\delta} + \frac{k}{4^\delta} - \frac{7r+k-2}{4^\delta} - \frac{2}{2^\delta}\\
&= \frac{r}{(4r)^\delta} + \frac{3r}{8^\delta} + \frac{3r}{2^\delta} - \frac{7r-2}{4^\delta} - \frac{2}{2^\delta}\\
&= \frac{r2^\delta + r^{\delta+1}(3 + 3\cdot 4^\delta - 7\cdot 2^\delta) + r^\delta(2^{\delta+1} - 2^{2\delta+1})}{(8r)^\delta} = a(r,0,\delta).
\end{aligned}$$

Set $b(r,\delta) = a(r,0,\delta)$. Then b is real-valued and infinitely differentiable as a function of $r \in [0,\infty)$ and as a function of $\delta \in [0,\infty)$. We only consider $r \in \{1,2,\ldots\}$ and $\delta \in [0.5,\ 2]$.
Then

$$\begin{aligned}
b_\delta(r,\delta) &= -\frac{r\ln 4r}{(4r)^\delta} - \frac{9r\ln 2}{8^\delta} - \frac{(3r-2)\ln 2}{2^\delta} + \frac{(14r-4)\ln 2}{4^\delta}\\
&= \frac{\ln 2}{8^\delta}\{2^\delta(14r-4) - 9r - 4^\delta(3r-2)\} - \frac{r\ln 4r}{(4r)^\delta}\\
&= c(r,\delta) - \frac{r\ln 4r}{(4r)^\delta}
\end{aligned}$$

and

$$c_\delta(r,\delta) = \frac{\ln^2 2}{4^\delta}\{(14r-4) - 2^\delta(6r-4)\}.$$

Fix $r \geqslant 2$. Let $\delta_1(r) = log_2\frac{7r-2}{3r-2}$ be the real solution of $(14r-4) - 2^\delta(6r-4) = 0$. We note that $\delta_1(2) = \log_2 3 = 1.5x$ and $\delta_1(r) \downarrow \log_2\frac{7}{3} = 1.22239$ as $r \to \infty$. Then $c_\delta(r,\delta) > 0$ for $\delta \in [0.5, \delta_1(r))$ and $c_\delta(r,\delta) < 0$ for $\delta \in (\delta_1(r), 2]$. Hence, $c(r,\delta)$ increases for $\delta \in [0.5, \delta_1(r))$ and decreases for $\delta \in (\delta_1(r), 2]$.

Note that

$$\begin{aligned}
c(r,\ 0.5) &= \frac{\ln 2}{2\sqrt{2}}\left\{(14\sqrt{2}-15)\,r - (4\sqrt{2}-2)\right\}\\
&= 1.17606\,r - 0.896165 > 0, c(r,\ 1.95)\\
&= 0.00368746\,r + 0.173071 \quad \text{and} \quad c(r,\ 1.97) = -0.00227256\,r\\
&\quad + 0.17321 \ (< 0 \text{ for } r \geqslant xx).
\end{aligned}$$

Consequently,

$$b_\delta(r,\delta) = c(r,\delta) - \frac{r\ln 4r}{(4r)^\delta} \geqslant c(r,\ 1.95) - \frac{r\ln 4r}{(4r)^\delta}, \quad (\forall r \geqslant 2, \forall \delta \in [0.5,\ 1.95])$$

Let $\delta^* = 0.82179\ldots$ be the real solution of $3 + 3\cdot 4^\delta - 7\cdot 2^\delta = 0$. Now

$$\frac{\ln 4r}{16r} \leqslant \frac{r\ln 4r}{(4r)^\delta} \leqslant \frac{r^{0.17821}\ln 4r}{4^{0.82179}} \quad \text{for } \delta \in [0.82179, 2].$$

Hence, $b_\delta(r,\delta) \geqslant c(r, 1.95) - \frac{r^{0.17821}\ln 4r}{4^{0.82179}} = d(r)(\forall r \geqslant 2, \forall\delta \in [0.82179, 1.95])$. Note that $d(r) \geqslant d(3502) = 0.00226825$ for all $r \geqslant 3502$. Then, for each $r \geqslant 3502$, $b(r,\delta)$ increases for $\delta \in [0.82179, 1.95]$, hence, $b(r,\delta) \geqslant b(r, 0.82179) = 0.320061r^{0.17821} - 0.491357 > 0$ for all $\delta \in [0.82179, 1.95]$. Since $a(r,k,\delta) = b(r,\delta)$ $(0 \leqslant k \leqslant 6)$, $a(r,k,\delta) > 0$ for all $\delta \in [0.82179, 1.95]$ and all $n \geqslant 24515$. □

Remark 8.

(1) We note that $a(r,k,1) = a(r, 0, 1) = \frac{r-2}{8} > 0$ for $r \geqslant 3$ and $0 \leqslant k \leqslant 6$.

(2) Obviously the trees $T_{r,k}$ and the function $a(r.k,\delta)$ give much more information about the maximum of $R_{-\delta}$ than indicated in theorem 1. We conjecture that the trees $T_{r,k}$ are the maximum trees for some interval of $-\delta$ centered at -1.

(3) Clearly the bound $n \geqslant 24515$ can be improved.

We now cover the gap (1.95, 2) in theorem 7. theorems 7 and 9 together cover the previously unknown range $\delta \in (0.5, 2)$. (See table 1)

Let $n = 3r + s$ where $0 \leqslant s \leqslant 2 \leqslant r$. For each vertex v of the path P_r, append a disjoint path P of order 3 having end-vertex w by identifying v and w. Denote the resulting chemical tree by $T_{r,s}^{\text{chem}}$. Join s new endvertices to any s endvertices of $T_{r,s}^{\text{chem}}$. Denote the resulting chemical tree by T_n^{chem} which has order n.

Theorem 9. For each $n \geqslant 15000$, there exists a chemical tree T_n^{chem} with

$$R_{-\delta}(T_n^{\text{chem}}) > R_{-\delta}(P_n)$$

for all $\delta \in [0.8292, 2]$.

Proof. Let $n = 3r + s$ with $0 \leqslant s \leqslant 2 \leqslant r$ and $T_{r,s}^{\text{chem}}$ and T_n^{chem} be the chemical trees defined before the theorem. Then

$$\begin{aligned} e(r,s,\delta) = R_{-\delta}(T_n^{\text{chem}}) - R_{-\delta}(P_n) &= \frac{r-3}{9^\delta} + \frac{r}{6^\delta} + \frac{r}{2^\delta} - \frac{n-s-5}{4^\delta} - \frac{2}{2^\delta}. \\ &\geqslant \frac{r\{(4/9)^\delta + (2/3)^\delta + 2^\delta - 3 - 2^{\delta+1}/r\}}{4^\delta} = f(r,\delta). \end{aligned}$$

Let $\delta^* = 0.826077\ldots$ be the real solution of $(4/9)^\delta + (2/3)^\delta + 2^\delta - 3 = 0$. For $r \geqslant 5000$, and $\delta \in (0, 2]$,

$$f(r,\delta) \geqslant \frac{r\{(4/9)^\delta + (2/3)^\delta + 2^\delta - 1876/625\}}{4^\delta} = g(r,\delta).$$

Note that $h(\delta) = (4/9)^\delta + (2/3)^\delta + 2^\delta - 1876/625$ is an increasing function of $\delta \in (0, 2]$ and that $h(0.8292) = 0.0000417744$. Then $g(r, \delta) \geqslant g(5000, 0.8292) = 0.066168603$ for all $r \geqslant 5000$, $\delta \in (0.8292, 2]$. Consequently, $e(r, s, \delta) \geqslant f(r, \delta) \geqslant g(5000, 0.8292)$ for all $r \geqslant 5000, 2 \geqslant s \geqslant 0, \delta \in (0.8292, 2]$. This implies our result. □

Remark 10.

(1) We can replace 0.8292 with any $\delta > \delta^*$ and the theorem holds for all sufficiently large n. Our choice struck a balance between small δ and the resulting large n.

(2) Clearly the bound $n \geqslant 15,000$ can be lowered.

(3) Appending two disjoint paths of order 3 at each vertex of the path P_r gives the real solution $\delta^{**} = 0.83251\ldots$ of $1 + 2^{\delta+1} + 2^{3\delta+1} - 5 \cdot 2^{2\delta} = 0$ which is larger than δ^*, i.e., this class of trees is worse than the class of trees considered in theorem 9.

We further improve the upper bound for α.

Theorem 11. $0.5 \leqslant \beta \leqslant \alpha \leqslant 0.817268757$.

Proof. With the trees $T_{r,k}$ and function $g(r,\delta) = f(r, 0, \delta)$ of Theorem 7, we have $g(30, 0.817268757) = 5.08062 \times 10^{-7}$ which gives the optimal value $\bar{\delta} = 0.817268757$ for the class of trees $T_{r,k}$. Then $\bar{\delta} \in A(211) \subseteq B(211)$, hence, $\beta(211) \leqslant \alpha(211) \leqslant \bar{\delta}$. Since the sequences $\{\alpha(n)\}_{n \geqslant 22}$, $\{\beta(n)\}_{n \geqslant 22}$ are non-increasing, $\beta \leqslant \alpha \leqslant \bar{\delta}$. □

Summary

We summarize the results of this section regarding necessary conditions (1) and (2). We have

$$[0.82179,\ 2) \subseteq A(n) \subseteq A(n+1) \subseteq \bigcup_{n \geqslant 24515} A(n) \subseteq [\alpha,\ 2) \subseteq [0.5, 2) \quad \text{for all } n \geqslant 24515,$$

$$[0.82179,\ 2) \subseteq B(n) \subseteq B(n+1) \subseteq \bigcup_{n \geqslant 24515} B(n) \subseteq [\beta,\ 2) \subseteq [0.5, 2) \quad \text{for all } n \geqslant 24515,$$

where

$$0.5 \leqslant \beta \leqslant \alpha \leqslant 0.817268757.$$

For all $n \geqslant 24515$ there exists a tree T_n (theorem 7) with

$$R_{-\delta}(T_n) > R_{-\delta}(P_n) \tag{6}$$

for all $-\delta \in [-1.95, -0.82179]$, and, for all $n \geqslant 15000$ there exists a chemical tree T_n^{chem} (theorem 9) with

$$R_{-\delta}(T_n^{\text{chem}}) > R_{-\delta}(P_n) \tag{7}$$

for all $-\delta \in [-2, -0.8292]$. From the definition of $A(n)$, $B(n)$,

$$R_{-\delta}(T_n) \leqslant R_{-\delta}(P_n), \quad \forall T_n \neq P_n \tag{8}$$

for all $n \geqslant 2$ and all $-\delta \in (-\alpha, -0.5)$, and, more importantly,

$$R_{-\delta}(T_n) < R_{-\delta}(P_n), \quad \forall T_n \neq P_n \tag{9}$$

for all $n \geqslant 2$ and all $-\delta \in (-\beta, -0.5)$. The **mere existence** of β gives result (8). Both $(-\beta, -0.5) \subseteq (-\alpha, -0.5)$ may be empty, however.

Corollary 12. (1) $R_{-\delta}$ is not an acceptable index (not 1 so not 2) of branching of trees for all $-\delta \in (-\infty, -0.82179]$ and (2) $R_{-\delta}$ satisfies necessary condition (2) so (1) to be an acceptable index of branching of trees for all $-\delta \in (-\beta, 0)$.

The values of $-\alpha$ and $-\beta$ are important, since they are measures of when $R_{-\delta}$ ceases to be an acceptable index (1 or 2) of branching for trees. We have some evidence for the following conjecture.

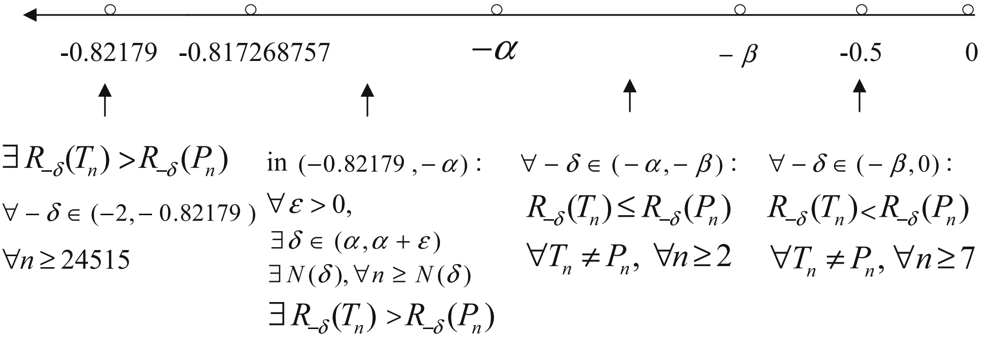

Figure 2.

Conjecture 13. $-\alpha = -\beta \approx -0.8$.
If this conjecture is true, then the choice of –0.5 by Randić was rather fortuitous. We next show that $C(n) \neq \phi$ for all $n \geqslant 1303$.

Theorem 14. For all $n \geqslant 1303$, there exists $\lambda(n) \in C(n) \cap [0.75,\ 0.82179]$.

Proof. We use the trees and functions from theorem 7. For $n = 7r + k + 1 (0 \leqslant k \leqslant 6)$,

$$\begin{aligned} f(r,k,\delta) &= R_{-\delta}(T_{r,k}) - R_{-\delta}(P_n) \\ &= \frac{r}{(4r)^\delta} + \frac{3r}{8^\delta} + \frac{3r}{2^\delta} - \frac{7r-2}{4^\delta} - \frac{2}{2^\delta} \\ &= \frac{r2^\delta + r^{\delta+1}(3 + 3\cdot 4^\delta - 7\cdot 2^\delta) + r^\delta(2^{\delta+1} - 2^{2\delta+1})}{(8r)^\delta} = f(r,0,\delta). \end{aligned}$$

Set $g(r,\delta) = f(r,0,\delta)$. Recall that $\delta^* = 0.82179$ is the real solution of $3 + 3\cdot 4^\delta - 7\cdot 2^\delta = 0$. Then $g(r,\ 0.82179) = 0.320061 r^{0.17821} - 0.491357 > 0$ for all $r \geqslant 186$. Now,

$$g(r, 0.75) = (3\cdot 2^{-2.25} + 3\cdot 2^{-0.75} - 7\cdot 2^{-1.5})\, r + 2^{-1.5} r^{0.25} + 2^{-0.5} - 2^{0.25}$$

so that,

$$\begin{aligned} \frac{d}{dr} g(r, 0.75) &= 3\cdot 2^{-2.25} + 3\cdot 2^{-0.75} - 7\cdot 2^{-1.5} + 0.25\cdot 2^{-1.5} r^{-0.75} < 0. \\ &\Leftrightarrow r > 1.66175. \end{aligned}$$

Hence, $g(r, 0.75) \leqslant g(2, 0.75) = -0.182434$ for all $r \geqslant 2$. By the Intermediate Value Theorem, there exists $\lambda = \lambda(r) \in (0.75, \delta^*)$ with $g(r,\lambda) = 0$ for all $r \geqslant 186$. Since $f(r,k,\delta) = g(r,\delta) (0 \leqslant k \leqslant 6)$, there exists $\lambda = \lambda(r) \in (0.75, \delta^*)$ with $g(r,\lambda) = 0$ for all $n \geqslant 1303$. Consequently, $C(n) \neq \phi$ for all $n \geqslant 1303$. □

By the completeness of the reals,

$$\gamma(n) = \inf C(n)$$

exists for all $n \geqslant 1303$. Since $C(n) \subseteq B(n)$,

$$\gamma(n) \in [\beta(n),\ 0.82179] \subseteq [\beta, 0.82179] \tag{10}$$

for all $n \geqslant 1303$.

In [13], $\gamma(n)$ was determined for $10 \leqslant n \leqslant 20$. Its existence for $n \geqslant 21$ was not established. We found that $0.85096 = \gamma(19) \leqslant \gamma(n) \leqslant \gamma(n) \leqslant \gamma(12) = 0.918330$ for $10 \leqslant n \leqslant 20$; several of the trees were chemical trees. We conjectured that $\gamma(n) \approx 0.9$. From (9), we see that this conjecture was incorrect: $\gamma(n)$ exists and $\gamma(n) \leqslant 0.82179$ for at least all $n \geqslant 1303$.

Unfortunately, our methods do not show that $\lim_{n\to\infty} \gamma(n)$ exists. We conjecture that the limit does exist.

3. Chemical trees

For $n \geqslant 2$, let

$$\begin{aligned} A^{\text{chem}}(n) &= \{\delta \in (0,\ 2) : \exists\, R_{-\delta}(T_n) > R_{-\delta}(P_n),\ \text{chemical tree } T_n \neq P_n\},\\ B^{\text{chem}}(n) &= \{\delta \in (0,\ 2) : \exists\, R_{-\delta}(T_n) \geqslant R_{-\delta}(P_n),\ \text{chemical tree } T_n \neq P_n\},\\ C^{\text{chem}}(n) &= \{\delta \in (0,\ 2) : \exists\, R_{-\delta}(T_n) = R_{-\delta}(P_n),\ \text{chemical tree } T_n \neq P_n\}. \end{aligned}$$

By their definition, $A^{\text{chem}}(n), C^{\text{chem}}(n) = B^{\text{chem}}(n) - A^{\text{chem}}(n) \subseteq B^{\text{chem}}(n)$. We note that $T_{3,k} (1 \leqslant k \leqslant 6)$ of theorem 7 is a chemical tree of order $21 + k$ with $R_{-1}(T_{3,k}) > R_{-1}(P_{21+k})$. Hence, $1 \in A^{\text{chem}}(n) \subseteq B^{\text{chem}}(n)$ for all $n \geqslant 22$. From theorem 9,

$$[0.8292, 2) \subseteq A^{\text{chem}}(n) \subseteq B^{\text{chem}}(n)$$

for all $n \geqslant 15000$. By Hu et al. [10],

$$A^{\text{chem}}(n), B^{\text{chem}}(n), C^{\text{chem}}(n) \subseteq (0.5, 2) \quad \text{for all } n \geqslant 7. \tag{11}$$

By the completeness the real numbers,

$$\alpha^{\text{chem}}(n) = \inf A^{\text{chem}}(n) \text{ and } \beta^{\text{chem}}(n) = \inf B^{\text{chem}}(n)$$

exist for all $n \geqslant 22$. From their definitions, $\alpha^{\text{chem}}(n) \geqslant \max\{\alpha(n), \beta^{\text{chem}}(n)\} \geqslant \min\{\alpha(n), \beta^{\text{chem}}(n)\} \geqslant \beta(n)$.

As noted above, $T_{3,k} \in (1 \leqslant k \leqslant 6)$ is a chemical tree of order $21 + k$ with $R_{-1}(T_{3,k}) R_{-1}(P_{21+k})$. Since, the tree $T_{n+1} = T_n + vw$ in the proof of theorem 1 is a chemical tree if the tree T_n is a chemical tree, the analogs of theorems 1 and 4 and corollaries 2, 3, 5, and 6 for chemical trees immediately follow. We merely state the results below noting that we have used remark 10(1) in corollaries 17 and 20.

Theorem 15. $1 \in A^{\text{chem}}(n) \subseteq A^{\text{chem}}(n+1)$ for all $n \geqslant 22$. □

Corollary 16. $\alpha^{\text{chem}}(n) \geqslant \alpha^{\text{chem}}(n+1)$ for all $n \geqslant 22$. □

Corollary 17. $\lim_{n\to\infty} \alpha^{\text{chem}}(n) = \alpha^{\text{chem}}$ exists and $\alpha^{\text{chem}} \in [0.5, 0.826077]$. □

Theorem 18. $1 \in B^{\text{chem}}(n) \subseteq B^{\text{chem}}(n+1)$ for $n \geqslant 22$. □

Corollary 19. $\beta^{\text{chem}}(n) \geqslant \beta^{\text{chem}}(n+1)$ for all $n \geqslant 22$. □

Corollary 20. $\lim_{n\to\infty} \beta^{\text{chem}}(n) = \beta^{\text{chem}}$ exists and $\beta^{\text{chem}} \in [0.5,\ 0.826077]$. □

Necessarily, $\beta^{\text{chem}} \leqslant \alpha^{\text{chem}}$.

We next show that $C^{\text{chem}}(n) \neq \phi$ for all $n \geqslant 15000$.

Theorem 21. For all $n \geqslant 15,000$, there exists $\lambda(n) \in C^{\text{chem}}(n) \cap [0.75,\ 0.8292]$.

Proof. Let $n = 3r + s$ with $0 \leqslant s \leqslant 2 \leqslant r$. With the chemical trees and functions of theorem 9,

$$e(r,s,\delta) \leqslant \frac{r}{9^\delta} + \frac{r}{6^\delta} + \frac{r}{2^\delta} - \frac{3r-5}{4^\delta} = \frac{r\{(4/9)^\delta + (2/3)^\delta + 2^\delta - 3 + 5/r\}}{4^\delta} = h(r,\delta).$$

Let $i(r) = (4/9)^{0.75} + (2/3)^{0.75} + 2^{0.75} - 3 + 5/r$. Then $i(r)$ is a decreasing function of r and I(192) $= -0.0100465\ldots$ Hence, $e(r,\ s,\ 0.75) < 0$ for all $r \geqslant 192$. From the proof of Theorem 9, $e(r,\ s,\ 0.8292) > 0$ for all $r \geqslant 5000$, $2 \geqslant s \geqslant 0$, $\delta \in (0.8292,\ 2]$. By the Intermediate Value Theorem, there exists $\lambda = \lambda(r) \in (0.75,\ 0.8292)$ with $e(r,\ s, \lambda) = 0$ for all $r \geqslant 5000$, $2 \geqslant s \geqslant 0$. Consequently, $C^{\text{chem}}(n) \neq \phi$ for all $n \geqslant 15000$. □

By the completeness of the reals,

$$\gamma^{\text{chem}}(n) = inf\, C^{\text{chem}}(n)$$

exists for all $n \geqslant 15,000$. Since $C^{\text{chem}}(n) \subseteq B^{\text{chem}}(n) \subseteq B(n)$,

$$\gamma^{\text{chem}}(n) \in [\beta^{\text{chem}}(n), 0.8292] \subseteq [\beta^{\text{chem}},\ 0.8292] \subseteq [0.5,\ 0.8292]$$

for all $n \geqslant 15000$.

In [13], $\gamma^{\text{chem}}(n)$ was found for $10 \leqslant n \leqslant 17$. Its existence for $n \geqslant 18$ was not established. We found that $0.86594 = \gamma^{\text{chem}}(16) \leqslant \gamma^{\text{chem}}(n) \leqslant \gamma^{\text{chem}}(12) = 0.918330$ for $10 \leqslant n \leqslant 17$ and conjectured that $\gamma^{\text{chem}}(n) \approx 0.9$. From (6), we see that this conjecture was incorrect: $\gamma^{\text{chem}}(n)$ exists for at least all $n \geqslant 15000$ and $\gamma^{\text{chem}}(n) \leqslant 0.826077 + \varepsilon$.

The values of $-\alpha^{\text{chem}}$ and $-\beta^{\text{chem}}$ are important, since they are measures of when $R_{-\delta}$ ceases to be an acceptable index (1 or 2) of branching of chemical trees. We have some confidence in the following conjecture.

Conjecture 22. $-\alpha_{\text{chem}} = -\beta_{\text{chem}} \approx -0.8$.

If this conjecture is true, then the natural choice of -0.5 by Randić was rather fortuitous.

Again, our methods do not show that $\lim_{n\to\infty}\gamma^{\text{chem}}(n)$ exists. We conjecture that the limit does exist however.

4. Conclusion

We list several questions that we find interesting as follows:

(1) Prove or disprove the conjectures $-\alpha = -\beta$ and $-\alpha^{\mathrm{chem}} = -\beta^{\mathrm{chem}}$.

(2) Find any of the values of $-\alpha$, $-\beta$, $-\alpha^{\mathrm{chem}}$ or $-\beta^{\mathrm{chem}}$.

(3) Improve the bounds $-\alpha, -\beta \in [-0.82179, -0.5]$ and $-\alpha^{\mathrm{chem}}, -\beta^{\mathrm{chem}} \in [-0.826077, -0.5]$; slight improvements of the lower bounds might be made.

(4) Prove or disprove that $\lim_{n\to\infty} \gamma(n)$ and $\lim_{n\to\infty} \gamma^{\mathrm{chem}}(n)$ exist.

[1] If either $\lim_{n\to\inf t} \gamma(n)$ or $\lim_{n\to\infty} \gamma^{\mathrm{chem}}(n)$ exist, find the value of the limit.

[2] Improve the bounds $\gamma(n) \in [0.5, 0.82179]$ and $\gamma^{\mathrm{chem}}(n) \in [0.5, 0.826077]$ ($n \geqslant 5000$).

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