Available online at www.sciencedirect.com
SCIENCE DIRECT®

ELSEVIER

Discrete Mathematics 271 (2003) 335–342

DISCRETE MATHEMATICS

www.elsevier.com/locate/disc

Note

A note on trees of maximum weight and restricted degrees

Dieter Rautenbach*

Lehrstuhl II für Mathematik, RWTH-Aachen, Aachen 52056, Germany

Received 7 February 2002; received in revised form 21 February 2003; accepted 14 March 2003

Abstract

For a graph G let $w_{-1}(G)$ be the sum of $(d_G(u)d_G(v))^{-1}$ over all edges uv of G. Clark and Moon (Ars Combin. 54 (2000) 223–235) proved an upper bound on w_{-1} for trees and posed the problem to determine a best possible such bound. In the present paper, we do this for trees of maximum degree 3. Furthermore, we prove an asymptotically best possible upper bound on w_{-1} for trees such that all degrees of vertices are either 1, 2 or some fixed $\Delta \geqslant 4$.

Keywords: Randić index; Weight; Tree

1. Introduction

In [11] Randić considered the two parameters

$$w_{-1}(G) = \sum_{uv \in E} (d_G(u)d_G(v))^{-1} \quad \text{and} \quad w_{-1/2}(G) = \sum_{uv \in E} (d_G(u)d_G(v))^{-1/2}$$

as a measure of the branching of the (hydrogen-suppressed) graph $G = (V, E)$ corresponding to a certain molecule (we consider finite and simple graphs and use standard terminology). These parameters—which are nowadays known as *Randić indices*—are classical examples for the numerous *molecular descriptors* [6] that have been defined until today.

In recent years these two parameters originating from chemistry received considerable attention in mathematics cf., e.g. [1,2,8–10].

* Tel.: +49-241-80-94995; fax: +49-241-80-92136.
E-mail address: rauten@math2.rwth-aachen.de (D. Rautenbach).

doi:10.1016/S0012-365X(03)00135-3

Whereas many of the parameters that have been proposed to measure the branching assume their maximum (or minimum) value among all trees of order n for the path P_n (cf., e.g. [3,7] or [12] where this property is established for $w_{-1/2}$), Clark and Moon [5] constructed an infinite sequence $(T_r)_{r\geqslant 1}$ of trees for which

$$\lim_{r\to\infty}\frac{w_{-1}(T_r)}{n(T_r)}=\frac{15}{56}>\frac{1}{4}=\lim_{r\to\infty}\frac{w_{-1}(P_r)}{r},$$

where $n(T)$ denotes the order of T. For all $n\leqslant 19$, Clark et al. [4] determined all trees of order n with maximum value of w_{-1} among all trees of order n.

In [5] Clark and Moon proved $w_{-1}(T)\leqslant(5n+8)/18$ for any tree T of order $n\geqslant 2$ and pose the problem to improve this upper bound such that it is tight for infinitely many values of n (cf. [5, Problem 2]).

In the present paper, we do this for trees of maximum degree 3. In fact, we determine an upper bound that is tight for all values of n. Furthermore, we prove an asymptotically best possible upper bound on w_{-1} for trees such that all degrees of vertices are either 1, 2 or some $\Delta\geqslant 4$.

2. Results

Theorem 2.1. *Let T be a tree of order n and maximum degree 3. Then*

$$w_{-1}(T)\leqslant\begin{cases}0 & \text{if } n=1,\\ 1 & \text{if } n=2,\\ \frac{1}{4}n+\frac{1}{4} & \text{if } 3\leqslant n\leqslant 9,\\ \frac{7}{27}n+\frac{5}{27} & \text{if } n\geqslant 10 \text{ and } n\equiv 1 \bmod 3,\\ \frac{7}{27}n+\frac{19}{108} & \text{if } n\geqslant 11 \text{ and } n\equiv 2 \bmod 3,\\ \frac{7}{27}n+\frac{1}{6} & \text{if } n\geqslant 12 \text{ and } n\equiv 0 \bmod 3.\end{cases}$$

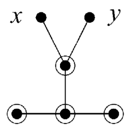
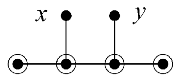
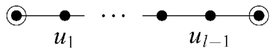
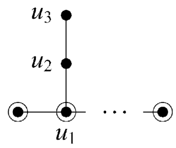
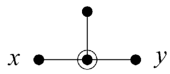
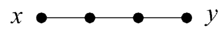
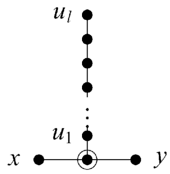
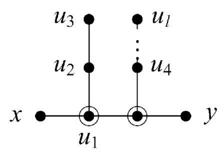
The given bounds are best possible.

Proof. Let the tree T be such that it has maximum w_{-1}-value among all trees of order n and maximum degree 3.

The idea of the proof is to determine the structure of T as far as necessary to calculate $w_{-1}(T)$. We will do this using Tables 1 and 2 that contain information about the contribution to w_{-1} of the edges in specific substructures. Each line of the two tables compares two such substructures. We adopt the following conventions. All vertices have exactly the same degree in the given picture of the substructure as in the tree T with two exceptions. The encircled vertices (⦿) are assumed to have degree 3 in T and the vertices denoted by x and y in Lines 1, 3 and 4 of Table 1 may have an arbitrary degree in $\{1,2,3\}$.

Line 1 (in Table 1) claims that the contribution to w_{-1} of the five depicted edges is the same ('=') for the left and the right substructure. To verify this line we have to calculate this contribution which is $1/3d_T(x)+1/3d_T(y)+\frac{3}{9}$.

Table 1

1		$=$	
2		$<\ (l \geq 4)$	
3		$<$	
4		$<\ (l \geq 5)$	

In the lines of Table 2 we compare pairs of substructures. Line 5 (in Table 2) claims that the contribution to w_{-1} of the four depicted edges is smaller ('$<$') for the left substructure than for the right substructure. Again, to verify this line we have to calculate the contributions which is $\frac{4}{6}$ for the left substructure and $\frac{1}{9}+\frac{2}{6}+\frac{1}{4}$ for the right substructure. Note that we do not assume the two substructures forming one of the considered pairs to be vertex-disjoint. From these two examples it should be obvious how to read and verify all lines in the two tables and we leave this task to the reader. We shall now consider the structure of T.

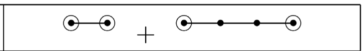
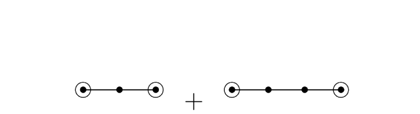
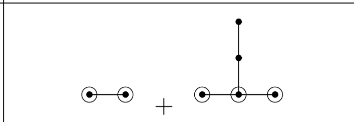
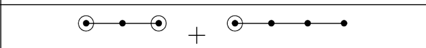
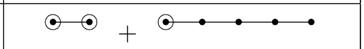
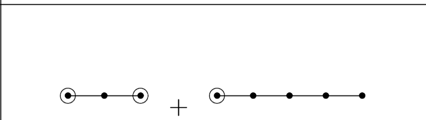
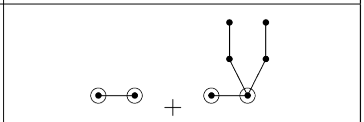
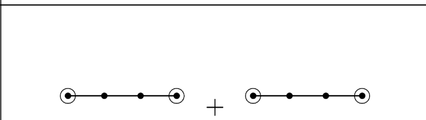
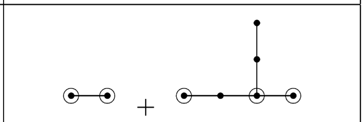
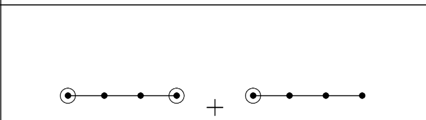
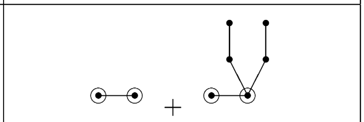
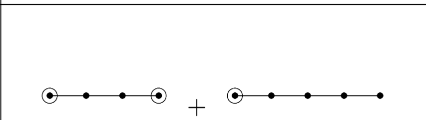
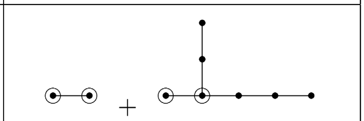
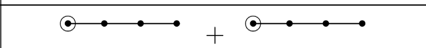
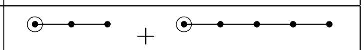
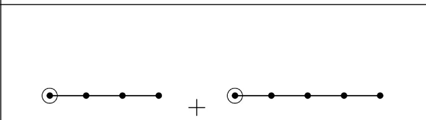
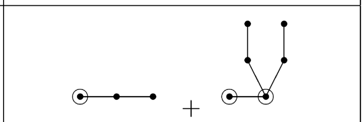
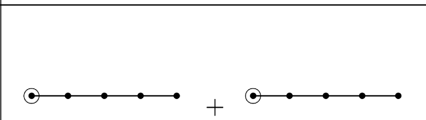
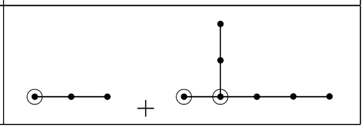
By repeatedly applying the transformation corresponding to Line 1, we can assume w.l.o.g. that no vertex of degree 3 in T has three neighbours of degree 3. This implies that the vertices of degree 3 in T induce a collection of paths.

If $u_0u_1u_2\dots u_l$ is a path in T for $l \geqslant 0$ such that $d_T(u_0)=d_T(u_l)=3$ and $d_T(u_1)=\cdots=d_T(u_{l-1})=2$, then Line 2 implies that $l \in \{0,1,2,3\}$. Such a path will be called a *path of type 1 and length l*.

If $u_0u_1u_2\dots u_l$ is a path in T for $l \geqslant 1$ such that $d_T(u_0)=3$, $d_T(u_1)=\cdots=d_T(u_{l-1})=2$ and $d_T(u_l)=1$, then the Lines 3 and 4 imply that $l \in \{2,3,4\}$. Such a path will be called a *path of type 2 and length l*.

Lines 5–14 of Table 2 imply that we can assume w.l.o.g. that T does not contain two of the following four substructures: A path of type 1 and length 2 or 3 or a path of type 2 and length 3 or 4. At this point we can start to calculate $w_{-1}(T)$.

Table 2

5		$<$	
6		$<$	
7		$<$	
8		$<$	
9		$<$	
10		$<$	
11		$<$	
12		$=$	
13		$<$	
14		$<$	

Let n_3 denote the number of vertices of degree 3 in T. If $n_3 = 0$, then T is a path and $w_{-1}(T) = 0$, if $n = 1$, $w_{-1}(T) = 1$, if $n = 2$ and $w_{-1}(T) = (n+1)/4$, if $n \geqslant 3$. Now let $n_3 \geqslant 1$. If T does not contain either a path of type 1 and length 2 or 3 or a path of type 2 and length 3 or 4, then the vertices of degree 3 induce a path, $n = 3n_3 + 4 \geqslant 7$ and $w_{-1}(T) = \frac{7}{9}n_3 + \frac{11}{9} = \frac{7}{27}n + \frac{5}{27}$. If T contains a path of type 1 and length 2 (and hence no path of type 1 and length 3 and no path of type 2 and length 3 or 4), then the vertices of degree 3 induce two disjoint paths, $n = 3n_3 + 5 \geqslant 11$ and $w_{-1}(T) = \frac{7}{9}n_3 + \frac{13}{9} = \frac{7}{27}n + \frac{4}{27}$. The remaining cases are verified analogously, by straightforward calculation. The results obtained are summarized in Table 3.

Table 3

Structure	Order n	$n \bmod 3$	Weight w_{-1}
—	1	1	0
—	2	2	1
T is a path, i.e. $n_3 = 0$	$\geqslant 3$	–	$\frac{1}{4}n + \frac{1}{4}$
T contains no path of type 1 and length 2 or 3 and no a path of type 2 and length 3 or 4	$\geqslant 7$	1	$\frac{7}{27}n + \frac{5}{27}$
T contains a path of type 1 and length 2	$\geqslant 11$	2	$\frac{7}{27}n + \frac{4}{27}$
T contains a path of type 1 and length 3	$\geqslant 12$	0	$\frac{7}{27}n + \frac{5}{36}$
T contains a path of type 2 and length 3	$\geqslant 8$	2	$\frac{7}{27}n + \frac{19}{108}$
T contains a path of type 2 and length 4	$\geqslant 9$	0	$\frac{7}{27}n + \frac{1}{6}$

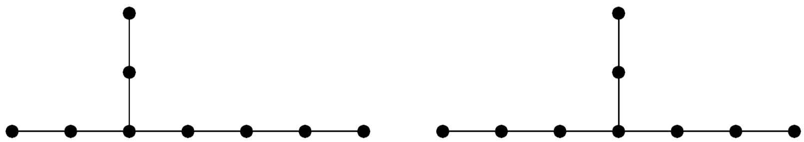


Fig. 1.

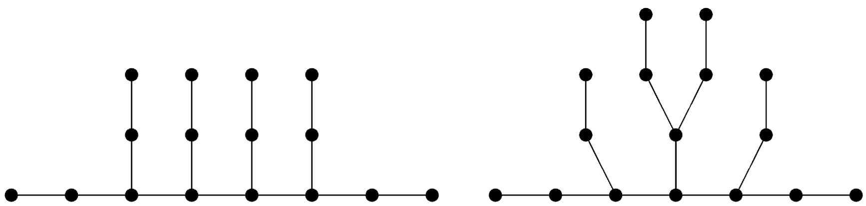


Fig. 2.

Comparing the entries of Table 3 for the different parities of n yields the desired result. Since we actually calculated w_{-1} for specific trees, the given bounds are best possible. □

Remark 2.2. The extremal trees for Theorem 2.1 are not unique. Actually, it follows easily from the above proof that all extremal trees arise from the trees that we considered to determine the entries of Table 3 by a sequence of local changes corresponding to Line 1 of Table 1 and Line 12 of Table 2.

The smallest order n for which the extremal trees are not unique is $n = 9$. In this case there are exactly the two extremal trees shown in Fig. 1 which arise from each other by a local change corresponding to Line 12 of Table 2.

The two trees in Fig. 2 are both extremal for $n = 16$ and arise from each other by a local change corresponding to Line 1 of Table 1.

Remark 2.3. It is quite obvious that there is only little hope to extend the method of the proof of Theorem 2.1 to larger maximum degrees.

The next result extends Theorem 2.1 in an asymptotically best possible way.

Theorem 2.4. *Let T be a tree of order n such that $d_T(u)\in\{1,2,\Delta\}$ for all vertices u of T and some $\Delta\geqslant 4$. Then*

$$w_{-1}(T)\leqslant \frac{(\Delta-1)(\Delta^2-2)}{2\Delta^2(2\Delta-3)}n+\mathcal{O}(\Delta).$$

Proof. We may assume $n\geqslant 3$. For $i,j\in\{1,2,\Delta\}$ let n_i denote the number of vertices of T of degree i and $m_{i,j}$ denote the number of edges uv of T such that $\{d_T(u),d_T(v)\}=\{i,j\}$. We may assume w.l.o.g. that the tree T is chosen among all trees of order n with $d_T(u)\in\{1,2,\Delta\}$ for all vertices u of T such that

(i) it has maximum w_{-1}-value and
(ii) subject to condition (i), $m_{2,2}$ is minimal.

We will bound $m_{2,2}$ and $m_{1,\Delta}$ from above. Furthermore, we will bound from above the number of vertices of degree 2 that are adjacent to two vertices of degree Δ.

Claim 1. $m_{2,2}\leqslant 2\Delta-3$.

Proof. We assume that there are $2\Delta-2$ edges $u_1v_1,u_2v_2,\ldots,u_{2\Delta-2}v_{2\Delta-2}$ of T such that $d_T(u_i)=d_T(v_i)=2$ for $1\leqslant i\leqslant 2\Delta-2$. Let x be a vertex of T such that $d_T(x)=1$ and let y be the unique neighbour of x. Clearly, $d_T(y)\in\{2,\Delta\}$.

The tree T' arises from T and $\Delta-1$ disjoint copies of the path P_2 on two vertices by contracting all edges u_iv_i for $1\leqslant i\leqslant 2\Delta-2$ and joining x to one vertex in each of the $\Delta-1$ paths. We have

$$w_{-1}(T')-w_{-1}(T)=\frac{1}{d_T(y)\Delta}+\frac{\Delta-1}{2\Delta}+\frac{\Delta-1}{2}-\frac{2\Delta-2}{4}-\frac{1}{d_T(y)}\geqslant 0,$$

where we leave the simple task to verify the last inequality to the reader. We obtain a contradiction either to condition (i) or to condition (ii) and the proof of the claim is complete. □

Claim 2. $m_{1,\Delta}\leqslant \Delta-2$.

Proof. We assume that $m_{1,\Delta}\geqslant\Delta-1$.

First, we assume that there are two vertices x and y of T of degree Δ such that y has a neighbour z of degree 1 and x has a neighbour u of degree different from 1 that does not lie on the path in T from x to y. The tree T' arises from T by deleting the edges yz and xu and adding the new edges xz and yu. We have $w_{-1}(T')=w_{-1}(T)$.

Possibly iterating this construction we can assume w.l.o.g. that T contains a vertex x of degree Δ that has exactly $\Delta-1$ neighbours $y_1, y_2, \ldots, y_{\Delta-1}$ of degree 1 and one neighbour z of degree 2 or Δ. The tree T'' arises from T and a path $P_{\Delta-1}$ on $\Delta-1$ vertices by deleting the vertices $y_1, y_2, \ldots, y_{\Delta-1}$ and joining x to a vertex of degree 1 in the path $P_{\Delta-1}$. We have

$$w_{-1}(T') - w_{-1}(T) = \frac{1}{2d_T(z)} + \frac{\Delta-2}{4} + \frac{1}{2} - \frac{1}{d_T(z)\Delta} - \frac{\Delta-1}{\Delta} > 0$$

where we leave the simple task to verify the last inequality to the reader. We obtain a contradiction to condition (i) and the proof of the claim is complete. □

Claim 3. *There are at most $2\Delta-3$ vertices of degree 2 that are adjacent to two vertices of degree Δ.*

Proof. We assume that there are $2\Delta-2$ such vertices $x_1, x_2, \ldots, x_{2\Delta-2}$. Let y be a vertex of T of degree 1 and let z be the unique neighbour of y. Clearly, $d_T(z) \in \{2, \Delta\}$.

The tree T' arises from T and $\Delta-1$ disjoint copies of the path P_2 on two vertices by deleting the vertices $x_1, x_2, \ldots, x_{2\Delta-2}$, joining the two neighbours of x_i by a new edge for $1 \leqslant i \leqslant 2\Delta-2$ and joining y to one vertex in each of the $\Delta-1$ paths. We have

$$w_{-1}(T') - w_{-1}(T) = \frac{2\Delta-2}{\Delta^2} + \frac{1}{d_T(z)\Delta} + \frac{\Delta-1}{2\Delta} + \frac{\Delta-1}{2} - \frac{2(2\Delta-2)}{2\Delta} - \frac{1}{d_T(z)} > 0,$$

where we leave the simple task to verify the last inequality to the reader. We obtain a contradiction to condition (i) and the proof of the claim is complete. □

The above claims easily imply the following relations:

$$m_{2,2} = \mathcal{O}(\Delta),$$

$$m_{1,\Delta} = \mathcal{O}(\Delta),$$

$$m_{1,2} = n_1 + \mathcal{O}(\Delta),$$

$$m_{2,\Delta} = n_1 + \mathcal{O}(\Delta),$$

$$2m_{\Delta,\Delta} = \Delta n_\Delta - n_1 + \mathcal{O}(\Delta),$$

$$n_1 = (\Delta-2)n_\Delta + \mathcal{O}(\Delta),$$

$$n_2 = (\Delta-2)n_\Delta + \mathcal{O}(\Delta),$$

$$n = (2\Delta-3)n_\Delta + \mathcal{O}(\Delta).$$

From these we deduce

$$\begin{aligned} w_{-1}(T) &= \frac{m_{1,2}}{2} + \frac{m_{1,\Delta}}{\Delta} + \frac{m_{2,2}}{4} + \frac{m_{2,\Delta}}{2\Delta} + \frac{m_{\Delta,\Delta}}{\Delta^2} \\ &\leqslant \frac{n_1}{2} + \frac{n_1}{2\Delta} + \frac{\Delta n_\Delta - n_1}{2\Delta^2} + \mathcal{O}(\Delta) \\ &= \frac{(\Delta-1)(\Delta^2-2)}{2\Delta^2(2\Delta-3)} n + \mathcal{O}(\Delta) \end{aligned}$$

and the proof is complete. □

Remark 2.5. In order to see that Theorem 2.4 is asymptotically best possible, consider trees that arise from a path P_l and $\Delta l - 2(l-1)$ paths P_2 by joining each vertex in P_l with exactly one vertex in an appropriate number of the paths P_2.

References

[1] B. Bollobás, P. Erdős, Graphs of extremal weights, Ars Combin. 50 (1998) 225–233.
[2] B. Bollobás, P. Erdős, A. Sakar, Extremal graphs for weights, Discrete Math. 200 (1999) 5–19.
[3] G. Caporossi, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs IV: chemical trees with extremal connectivity index, Comput. Chem. 23 (1999) 469–477.
[4] L.H. Clark, I. Gutman, M. Lepovic, D. Vidovic, Exponent-dependent properties of the connectivity index, Indian J. Chem. 41 A (2002) 457–461.
[5] L.H. Clark, J.W. Moon, On the general Randić index for certain families of trees, Ars Combin. 54 (2000) 223–235.
[6] V. Consonni, R. Todeschini, Handbook of Molecular Descriptors, Wiley-VCH, Weinheim, 2000.
[7] C. Delorme, O. Favaron, D. Rautenbach, On the Randić index, Research Report 1214, LRI, Université Paris-Sud, 1999.
[8] C. Delorme, O. Favaron, D. Rautenbach, On the Randić index, Discrete Math. 257 (2002) 29–38.
[9] M. Fischermann, A. Hoffmann, D. Rautenbach, L. Volkmann, A linear-programming approach to the generalized Randić index, Discrete Appl. Math., to be published.
[10] I. Gutman, O. Miljković, L. Pavlović, On graphs with extremal connectivity indices, Bull. Acad. Serbe Sci. Arts 121 (2000) 1–14.
[11] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97 (1975) 6609–6615.
[12] P. Yu, An upper bound for the Randić of trees, J. Math. Studies 31 (1998) 225–230 (in Chinese).