communications in mathematical
match
and in computer chemistry

no. 49, September 2003
MATCDY (49) 15- 21 (2003)

ISSN 0340 - 6253

A recursive formula for the Randić index of a tree

Juan Rada and Oswaldo Araujo
Departamento de Matemáticas, Facultad de Ciencias
Universidad de Los Andes, 5101 Mérida, Venezuela
e-mail: juanrada@ciens.ula.ve, araujo@ciens.ula.ve

(Received January 13, 2003)

Abstract

We present a recursive formula for the Randić index $\chi(T)$ of a tree T. As a by-product, we determine χ for trees which are obtained from basic tree operations, such as linking vertices of two different trees by a path.

1 Introduction

Let T be a tree (i.e., an acyclic connected graph) with set of vertices $V(T)$ and set of edges $E(T)$. The Randić index of T is defined as

$$\chi(T) = \sum_{xy \in E(T)} \frac{1}{\sqrt{\delta_x \delta_y}}$$

where δ_x denotes the degree of the vertex x and xy is an edge with terminal vertices x and y.

Randić designed this index with the intention of characterizing branching in chemical species ([12]), and it became one of the most successful graph invariants in applications to physical and chemical properties ([9],[10]). In spite of the numerous practical applications of this index over the last 25 years, only recently results about the mathematical properties of χ have appeared in the literature (see for instance, [1],[2],[3],[4],[5],[6],[7],[8] and [11]).

In this work we present a recursive formula for the Randić index of a tree T. The basic idea is as follows: if T is a tree and $v \in V(T)$ with degree k, then there exists unique subtrees $T_1, \ldots, T_k$ of T which have v as a pendent vertex (i.e. a vertex of degree 1) and are maximal with respect to this property. In Theorem 2.3, we establish a precise relation between $\chi(T)$ and $\sum_{i=1}^{k} \chi(T_i)$. This relation depends strongly on the Randić constant of T at vertex v, which we introduce in Definition 2.2. As a consequence of this result, we determine $\chi(U)$ in Corollary 2.4, for trees U which are obtained from basic tree operations, such as linking vertices of different trees by a path.

2 Recursive formula for the Randić index

Let T be a tree and $v \in V(T)$. Consider the set $\mathcal{P}_v(T)$ of all subtrees of T which have v as a pendent vertex. If P and Q belong to $\mathcal{P}_v(T)$, then the relation $P \subseteq Q$, i.e., P is a subtree of Q, is a partial order over $\mathcal{P}_v(T)$. A subtree $M \in \mathcal{P}_v(T)$ is maximal if $M \subseteq N$ and $N \in \mathcal{P}_v(T)$ implies $M = N$. It is clear that if v is a vertex of degree k, then there are exactly k maximal subtrees $T_1, \ldots, T_k$ in $\mathcal{P}_v(T)$.

Example 2.1 *Consider the tree T shown in Figure 1. The vertex v has degree 3 and T_1, T_2 and T_3 are the maximal subtrees of $\mathcal{P}_v(T)$.*

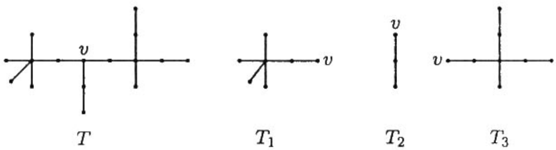

Figure 1

In our next result we express $\chi(T)$ in terms of $\sum_{i=1}^{k} \chi(T_i)$. As we shall see, this relation depends strongly on a constant associated to the vertex v of the tree T, which we next introduce.

Definition 2.2 *Let T be a tree and $v \in V(T)$. The Randić constant of T at v, denoted by $R_T(v)$, is defined as*

$$R_T(v) = \sum_{x \in \mathcal{N}_v} \frac{1}{\sqrt{\delta_x}}$$

where $\mathcal{N}_v$ denotes the set of neighbors of v.

Now we can state and prove the recursive formula for the Randić index of a general tree, in terms of the Randić constant.

Theorem 2.3 *Let T be a tree and $v \in V(T)$ of degree k. If $T_1, \ldots, T_k$ are the maximal subtrees of $\mathcal{P}_v(T)$ then*

$$\chi(T) = \sum_{i=1}^{k} \chi(T_i) + \left(\frac{1}{\sqrt{k}} - 1\right) R_T(v)$$

Proof. We can express the Randić index of T as

$$\chi(T) = \sum_{\substack{xy \in E(T) \\ x \neq v, y \neq v}} \frac{1}{\sqrt{\delta_x \delta_y}} + \frac{1}{\sqrt{k}} \sum_{x \in \mathcal{N}_v} \frac{1}{\sqrt{\delta_x}}$$

On the other hand, since v is a pendent vertex of each T_i we obtain

$$\chi(T_i) = \sum_{\substack{xy \in E(T_i) \\ x \neq v, y \neq v}} \frac{1}{\sqrt{\delta_x \delta_y}} + \frac{1}{\sqrt{k_i}}$$

where k_i is the degree of the unique neighbor of v in T_i. Hence

$$\sum_{i=1}^{k} \chi(T_i) = \sum_{\substack{xy \in E(T) \\ x \neq v, y \neq v}} \frac{1}{\sqrt{\delta_x \delta_y}} + \sum_{x \in \mathcal{N}_v} \frac{1}{\sqrt{\delta_x}}$$

and consequently

$$\chi(T) - \sum_{i=1}^{k} \chi(T_i) = \left(\frac{1}{\sqrt{k}} - 1\right) R_T(v)$$

■

Consider a tree U which is obtained from the trees S and T, by linking the vertices w of S and v of T by a path τ (see Figure 2).

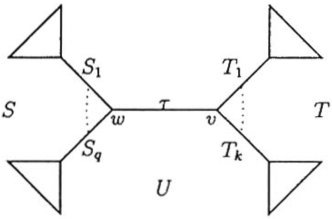

Figure 2

We next determine $\chi(U)$ in terms of $\chi(S)$ and $\chi(T)$.

Corollary 2.4 *Let S and T be trees, $w \in V(S)$ of degree q and $v \in V(T)$ of degree k. If U is the tree obtained from S and T by linking vertices w and v by a path τ of length r, then*

1. *If $r = 0$, that is, if v and w are identified, then*

$$\chi(U) = \chi(S)+\chi(T)+\left(\frac{1}{\sqrt{k+q}} - \frac{1}{\sqrt{q}}\right) R_S(w)+\left(\frac{1}{\sqrt{k+q}} - \frac{1}{\sqrt{k}}\right) R_T(v)$$

2. *If $r = 1$ then*

$$\begin{aligned}\chi(U) &= \chi(S)+\chi(T)+\left(\frac{1}{\sqrt{q+1}} - \frac{1}{\sqrt{q}}\right) R_S(w)+ \\ &\left(\frac{1}{\sqrt{k+1}} - \frac{1}{\sqrt{k}}\right) R_T(v)+\frac{1}{\sqrt{k+1}}\frac{1}{\sqrt{q+1}}\end{aligned}$$

3. *If $r > 1$ then*

$$\begin{aligned}\chi(U) &= \chi(S)+\chi(T)+\left(\frac{1}{\sqrt{q+1}} - \frac{1}{\sqrt{q}}\right) R_S(w)+ \\ &\left(\frac{1}{\sqrt{k+1}} - \frac{1}{\sqrt{k}}\right) R_T(v)+\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{k+1}}+\frac{1}{\sqrt{q+1}}\right)+\frac{r-2}{2}\end{aligned}$$

Proof. Let $S_1, \ldots, S_q$ and $T_1, \ldots, T_k$ be the maximal subtrees of $\mathcal{P}_w(S)$ and $\mathcal{P}_v(T)$, respectively (see Figure 2).

1. If $r = 0$ then by Theorem 2.3 we have

$$\begin{aligned}\chi(U) &= \sum_{i=1}^{q}\chi(S_i)+\sum_{i=1}^{k}\chi(T_i)+\left(\frac{1}{\sqrt{k+q}}-1\right)R_U(v)\\ &= \chi(S)-\left(\frac{1}{\sqrt{q}}-1\right)R_S(w)+\chi(T)-\left(\frac{1}{\sqrt{k}}-1\right)R_T(v)+\\ &\left(\frac{1}{\sqrt{k+q}}-1\right)R_U(v)\end{aligned}$$

The result follows from the fact that

$$R_U(v)=R_S(w)+R_T(v)$$

2. and 3. The maximal subtrees of $\mathcal{P}_v(U)$ are $T_{1,\dots,}T_k, S^*$, where S^* is the tree obtained from S by adjoining the path τ at vertex w. Hence, by Theorem 2.3,

$$\chi(U)=\sum_{i=1}^{k}\chi(T_i)+\chi(S^*)+\left(\frac{1}{\sqrt{k+1}}-1\right)R_U(v) \tag{1}$$

In order to calculate $\chi(S^*)$, we note that the maximal subtrees of $\mathcal{P}_w(S^*)$ are $S_1,\dots,S_q,\tau$. So, again by Theorem 2.3,

$$\chi(S^*)=\sum_{i=1}^{q}\chi(S_i)+\chi(\tau)+\left(\frac{1}{\sqrt{q+1}}-1\right)R_{S^*}(w)$$

Since

$$R_{S^*}(w)-R_S(w)=\begin{cases}1 & \text{if } r=1\\ \frac{1}{\sqrt{2}} & \text{if } r>1\end{cases}$$

and

$$\chi(\tau)=\begin{cases}1 & \text{if } r=1\\ \sqrt{2}+\frac{r-2}{2} & \text{if } r>1\end{cases}$$

we deduce

$$\chi(S^*)=\begin{cases}\chi(S)+\left(\frac{1}{\sqrt{q+1}}-\frac{1}{\sqrt{q}}\right)R_S(w)+\frac{1}{\sqrt{q+1}} & \text{if } r=1\\ \chi(S)+\left(\frac{1}{\sqrt{q+1}}-\frac{1}{\sqrt{q}}\right)R_S(w)+\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{q+1}}+1\right)+\frac{r-2}{2} & \text{if } r>1\end{cases} \tag{2}$$

Finally, it can be easily seen that

$$R_U(v)-R_T(v)=\begin{cases}\frac{1}{\sqrt{q+1}} & \text{if } r=1\\ \frac{1}{\sqrt{2}} & \text{if } r>1\end{cases} \tag{3}$$

and so the result follows by substituting (2) and (3) in (1). ∎

In particular, equation (2) in the proof of Corollary 2.4, gives the variation of the Randić index when we adjoint a path to a tree.

Example 2.5 *Let S^* be the tree obtained from S by adjoining the path τ of length 2 at vertex w, as shown in Figure 3*

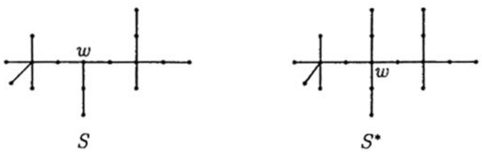

Figure 3

Then

$$\chi(S^*) - \chi(S) = \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{3}}\right)\left(\frac{3}{\sqrt{2}}\right) + \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{4}} + 1\right)$$

ACKNOWLEDGMENTS

Partial financial support was received by the authors from Consejo de Desarrollo Científico, Humanístico y Tecnológico de la Universidad de Los Andes (CDCHT-ULA).

References

[1] O. Araujo and J. A. de la Peña, The connectivity index of a weighted graph, Lin. Alg. Appl. 283 (1998), 171-177.

[2] B. Bollobás and P. Erdös, Graphs of extremal weights, Ars Combinatoria 50 (1998), 225-233.

[3] G. Caporossi, I. Gutman and P. Hansen, Variable neighborhood search for extremal graphs IV: Chemical trees with extremal connectivity index, Comput. Chem. 23 (1999) 469-477.

[4] G. Caporossi, I. Gutman, P. Hansen and L. Pavlovic, Graphs with maximum connectivity index, Comput. Biol. Chem. 27 (2003) 85-90.

[5] L.H. Clark and J.W. Moon, On the general Randić index for certain families of trees, Ars Combinatoria 54 (2000) 223-235.

[6] I. Gutman, O. Miljkovic, G. Caporossi and P. Hansen, Alkanes with small and large Randić connectivity index, Chem. Phys. Lett. 306 (1999), 366-372.

[7] I. Gutman, O. Araujo and J. Rada, An identity for Randić's connectivity index and its applications, ACH Models in Chem. 137 (2000) 653-658.

[8] I. Gutman and O. Miljkovic, Molecules with smallest connectivity indices, MATCH - Commun. Math. Comput. Chem. 41 (2000) 57-70.

[9] L. B. Kier and L. H. Hall, Molecular connectivity in chemistry and drug research, Academic Press, New York, 1976.

[10] L. B. Kier and L. H. Hall, Molecular connectivity in structure-activity analysis, Wiley, New York, 1986.

[11] J. Rada and C. Uzcátegui, Randić structure of a graph, to appear in Discr. Appl. Math.

[12] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97 (1975), 6609-6615.