Iranian Journal of Mathematical Sciences and Informatics
Vol.2, No.1 (2007),pp 15-20

A NOTE ON THE EQUISEPARABLE TREES

ALI REZA ASHRAFI AND SHAHRAM YOUSEFI

DEPARTMENT OF MATHEMATICS, FACULTY OF SCIENCE, UNIVERSITY OF KASHAN, KASHAN, IRAN
CENTER FOR SPACE STUDIES, MALEK-ASHTAR UNIVERSITY OF TECHNOLOGY, TEHRAN, IRAN

EMAIL: ASHRAFI@KASHANU.AC.IR

ABSTRACT. Let T be a tree and $n_1(e|T)$ and $n_2(e|T)$ denote the number of vertices of T, lying on the two sides of the edge e. Suppose T_1 and T_2 are two trees with equal number of vertices, $e \in T_1$ and $f \in T_2$. The edges e and f are said to be equiseparable if either $n_1(e|T_1) = n_1(f|T_2)$ or $n_1(e|T_1) = n_2(f|T_2)$. If there is an one-to-one correspondence between the vertices of T_1 and T_2 such that the corresponding edges are equiseparable, then T_1 and T_2 are called equiseparable trees. Recently, Gutman, Arsic and Furtula investigated some equiseparable alkanes and obtained some useful rules (see J. Serb. Chem. Soc. (68)7 (2003), 549-555). In this paper, we use a combinatorial argument to find an equivalent definition for equiseparability and then prove some results about relation of equiseparability and isomorphism of trees. We also obtain an exact expression for the number of distinct alkanes on n vertices which three of them has degree one.

Keywords: Equiseparable trees, Alkanes, Partitions.

2000 Mathematics subject classification: Primary 05C05, Secondary 92E10.

1. INTRODUCTION

A topological index is a numerical quantity derived in an unambiguous manner from the structural graph of a molecule. These indices are graph invariants, which usually reflect molecular size and shape.

The first nontrivial topological index in chemistry was introduced by H. Wiener[1] in 1947 to study the boiling points of paraffins. Since then, the Wiener index has been used to explain various chemical and physical properties of molecules and to correlate the structure of molecules to their biological activity [2].

Wiener originally defined his index on trees and studied its use for correlations of physicochemical properties of alkanes, alcohols, amines, and other analogous compounds. The original definition was given in terms of edge weights. In an arbitrary tree, every edge is a bridge, that is, after deletion of the edge, the graph is no more connected. The weight of an edge is taken to be the product of numbers of vertices in the two connected components. This number also is equal to the number of all shortest paths in the tree which go through the edge [3]. Thus the usual generalization of the Wiener index on arbitrary graphs is defined to be the sum of all distances in a graph.

Another natural generalization was previously put forward and called the Szeged index, Sz[4,5]. Formulas or special algorithms for Szeged index of several families of graphs were proposed recently [6-9]. We describe first the notation and basic definitions, before stating our results.

First of all, we recall the definition of Szeged index. Suppose G is a graph consisting of an arbitrary set $V = V(G)$ of vertices and a set $E = E(G)$ of unordered pairs $\{x, y\} = xy$ of distinct vertices, called edges. For any edge $e = uv$ of $E(G), N_1(e|G)$ denotes the set of vertices of G that are closer to u than v and $N_2(e|G)$ is the complement of $N_1(e|G)$ in $V(G)$. The Szeged index of G is defined by

$$Sz(G) = \sum_{e \in E(G)} n_1(e|G) n_2(e|G) \tag{1.1}$$

where the sum runs over all edges of G and the numbers $n_1(e|G)$ and $n_2(e|G)$ are cardinalities of the sets $N_1(e|G)$ and $N_2(e|G)$. If G is a tree then we can consider the numbers $n_1(e|G)$ and $n_2(e|G)$ as the count of the vertices of the two fragments, obtained by deleting the edge e from G. In fact, the edge e separates G into two fragments, with $n_1(e|G)$ and $n_2(e|G)$ vertices. According to these observations, Gutman and etal [10] defined the notion of equiseparable trees, as follows:

Definition 1.1. Let T_1 and T_2 be two trees with equal number of vertices, $e \in E(T_1)$ and $f \in E(T_2)$. We say that e and f are equiseparable edges, $e \approx f$, if by deleting e from T_1 and f from T_2 fragments are obtained with equal number of vertices. Moreover, let $e_1, e_2, \cdots, e_m$ be the edges of T_1 and $f_1, f_2, \cdots, f_m$ be the edges of T_2. T_1 and T_2 are said to be equiseparable if one can label the edges of T_1 and T_2 such that for $1 \leq i \leq m$, by deleting e_i from T_1 and f_i from T_2 fragments are obtained with equal number of vertices.

Suppose G is a graph. A 1-1 and onto function $f : V(G) \longrightarrow V(G)$ is called an automorphism of G if f preserves adjacency and non-adjacency. It is an easy fact that the set of all automorphisms of G, which is denoted by $Aut(G)$, is a group under composition of functions . Suppose x and y are vertices of G. We say that x and y are similar if there is an automorphism of G which takes x to y. Equivalence classes of the similarity relation are called orbits of G.

Let T be a tree with n vertices and $[n/2]$ denotes the greatest integers less than or equal to $n/2$. For $1 \leq r \leq [n/2]$, we define:

$$A_r(T) = \{e \in E(T)|n_1(e|T) = r \text{ or } n - r\},$$
$$X(T) = \{A_r(T)|1 \leq r \leq [n/2], A_r(T) \neq \emptyset\}.$$

A partition[11] of a set X, is a family of pairwise disjoint, non-empty subsets whose union is X. Let n and k be positive integers with $n \leq k$. Set $\alpha_r(T) = |A_r(T)|, 1 \leq r \leq [n/2]$. In the next section, we find a relation between equiseparable trees and the numbers $\alpha_r(T) = |Ar(T)|, 1 \leq r \leq [n/2]$.

Throughout this paper, all graphs and groups considered are assumed to be finite. Our notation is standard and taken mainly from Refs. [11-13]. The topics of interest in this paper are the following theorems:

Theorem 1.2. *For every tree T, $X(T)$ is a partition of T. Moreover, trees T_1 and T_2 with equal number of vertices are equiseparable if and only if for every $1 \leq r \leq [n/2]$, $\alpha_r(T_1) = \alpha_r(T_2)$.*

Theorem 1.3. *Let T be a tree. Then every non-empty subset $A_r(T)$ of $V(T)$ is a union of orbits of T. In particular, the number of orbits of T is at least $|X(T)|$.*

Theorem 1.4. *The exact number of distinct alkanes with n vertices and $\alpha_1(T) = 3$ is equal to*

$$n_3 = \sum_{i=0}^{k} \left[\frac{n - (2 + 3i)}{2}\right] \qquad , \qquad k = \left[\frac{n-4}{3}\right].$$

Also, all of these alkanes are mutually non-equiseparable.

2. PROOF OF THE THEOREMS

Proof of Theorem 1.2. Obviously, if the tree T has n vertices, then for all of its edges, $n_1(e|T) + n_2(e|T) = n$. This shows that $A_r(T) = A_{n-r}(T)$ and we can assume that $1 \leq r \leq [n/2]$. We first prove that $X(T)$ is a partition of $V(T)$. By definition of $X(T)$, every element of $X(T)$ is non-empty. Suppose for $1 \leq r, sleq[n/2], A_r(T) \cap A_s(T) \neq \emptyset$ and $e \in A_r(T) \cap A_s(T)$. Then By definition of $A_r(T)$ and $A_s(T)$, $n_1(e|T) = r$ or $n - r$ and $n_1(e|T) = s$ or $n - s$. This implies that $r = s$ or $r + s = n$. Hence $A_r(T) = A_s(T)$. Finally, we prove that $\cap A_r(T) = E(T)$. Since for every r, $A_r(T) \subseteq E(T)$, we have $\cap A_r(T) \subseteq E(T)$. Suppose $f \in E(T)$ is arbitrary and $n_1(f|T) = s$. Then $f \in A_s(T) \subseteq \cap A_r(T)$, as desired.

We now prove the "Moreover" part of the theorem. In order to do this, we assume that T_1 and T_2 are equiseparable trees with n vertices such that $e_r \approx f_r$, for $1 \leq r \leq n$. Define $\mu_r : A_r(T_1) \longrightarrow A_r(T_2)$ by $\mu_r(e_t) = f_t$. Suppose $e_t \in A_r(T_1)$ and $n_1(e_t|T_1) = u$. Then $n_1(f_t|T_1) = u$ or $n-u$ and so $f_t \in A_r(T_2)$. Thus μ_r is well-defined and since T_1 and T_2 are equiseparable, μ_r is bijective. Therefore, for any $1 \leq r \leq [n/2]$, $\alpha_r(T_1) = \alpha_r(T_2)$. Conversely, we assume that $\alpha_r(T_1) = \alpha_r(T_2)$, for $1 \leq r \leq [n/2]$. Hence for every $1 \leq r \leq [n/2]$, we can consider a bijective function $\beta_r : A_r(T_1) \longrightarrow A_r(T_2)$. Then $e \approx \beta_r(e)$, $1 \leq r \leq [n/2]$. This completes the theorem.

Suppose that T_1 and T_2 are trees with equal number of vertices. The previous theorem gives an algorithm for determining whether or not T_1 and T_2 are equiseparable?

We now obtain a lower bound for the number of orbits in a finite tree T. To do this, we prove the theorem 2:

Proof of Theorem 1.3. It is obvious that, if $\alpha \in Aut(T)$ and $e \in E(T)$ then $e \approx \alpha(e)$ and α induces a labeling on $V(T)$ such that the corresponding edges are equiseparable. We now assume that A is an orbit of T and $e \in A$. By Theorem 1, there exists $1 \leq r \leq [n/2]$ such that $e \in A_r(T)$. Also, by the mentioned property of automorphisms, for all $\alpha \in Aut(T)$, $\alpha(e) \approx e$. This shows that $A \subseteq A_r(T)$. Thus every orbit of T containing an element of $A_r(T)$ is contained in $A_r(T)$, i.e., $A_r(T)$ is a union of orbits of T. Now since $V(T)$ is the union of both $A_r(T)$'s and its orbits, the number of orbits of T is at least $|X(T)|$.

The following examples show that the number of orbits of T can be equal or less than $|X(T)|$.

Example 2.1. Consider the star-like tree T of Figure 1 with n vertices. This tree has exactly one orbit and $A_1(T) = E(T)$. Hence $|X(T)| = 1$ and the number of orbits of T is equal to $|X(T)|$.

Example 2.2. Consider the star-like tree F of Figure 2 with n vertices. Define e_r to be the edge $\{1, r\} = 1r$, $1 \leq r \leq n-1$, and $e_n = \{n-1, n\}$. Then this tree has exactly three orbits $\{e_1, e_2, \cdots, e_{n-2}\}$, $\{e_{n-1}\}$, $\{e_n\}$ and $|A_1(T)| = |E(T)| - 1$. Hence $|X(T)| = 2$ and the number of orbits of F is greater than $|X(T)|$.

It is an easy fact that for any tree T with $|E(T)| > 0$, $\alpha_1(T) \geq 2$ with equality if and only if T is the tree of Figure 3. Therefore, there is exactly one tree with $\alpha_1(T) = 2$. Now it is natural to ask about T, when $\alpha_1(T) \geq 3$. In theorem 3, we obtain the exact number of trees with $\alpha_1(T) = 3$.

Proof of Theorem 1.4. Let T be a tree with exactly n vertices and $A_1(T) = \{v_1, v_2, v_3\}$. It is obvious that T has a unique vertex v of degree 3. Suppose d is the minimum distance of the unique paths between v_1, v_2, v_3 and v. We first claim that $d \leq [(n-1)/3]$. Suppose the contrary, i.e. $d \geq [(n-1)/3] + 1$. If m denotes the number of edges of T then $n - 1 = m \geq 3d \geq 3[(n-1)/3] + 3 \geq n$, which is impossible. Suppose $d = 1$. Then the number of distinct alkanes with $\alpha_1(T) = 3$ is equal to $[(n-2)/2]$. For $d = 2$, this number is equal to $[((n-2)-3)/2]$ and so on. Thus if we define $I = d - 1$ and $k = [(n-1)/3] - 1 = [(n-4)/3]$ then we have:

$$n_3 = \sum_{i=0}^{k} \left[\frac{n - (2 + 3i)}{2} \right] \qquad , \qquad k = \left[\frac{n-4}{3} \right].$$

On the other hand, our constructions of distinct alkanes show that all of these alkanes are mutually non-equiseparable.

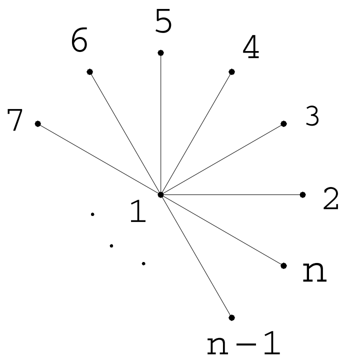

FIGURE 1

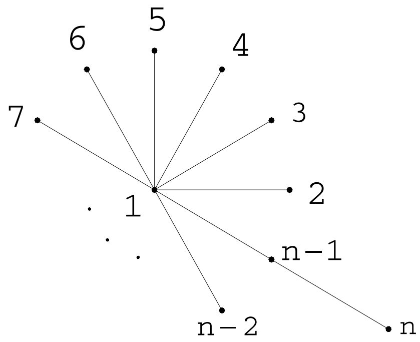

FIGURE 2

FIGURE 3
Some trees with exactly n vertices

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