Kragujevac J. Sci. 24 (2004) 00–00.

FAMILIES OF EQUISEPARABLE TREES AND CHEMICAL TREES

Ivan Gutman, Boris Furtula, Olga Miljković and Marija Rakić

Faculty of Science, P. O. Box 60, 34000 Kragujevac, Serbia & Montenegro

(Received January 27, 2004)

ABSTRACT. Let T be an n-vertex tree and e its edge. By $n_1(e|T)$ and $n_2(e|T)$ are denoted the number of vertices of T lying on the two sides of e; $n_1(e|T) + n_2(e|T) = n$. Conventionally, $n_1(e|T) \leq n_2(e|T)$. If T' and T'' are two trees with the same number n of vertices, and if their edges $e'_1, e'_2, \ldots, e'_{n-1}$ and $e''_1, e''_2, \ldots, e''_{n-1}$ can be labeled so that $n_1(e'_i|T') = n_1(e''_i|T'')$ holds for all $i = 1, 2, \ldots, n-1$, then T' and T'' are said to be equiseparable. There exist large families of equiseparable trees. We report here the results of a systematic study of these families for $7 \leq n \leq 20$.

INTRODUCTION

Let T be an n-vertex tree and $e = (xy)$ its edge. By $n_1(e|T)$ and $n_2(e|T)$ we denote the number of vertices of T, lying on the two sides of the edge e. Then, of course, $n_1(e|T) + n_2(e|T) = n$.

More formally, $n_1(e|T)$ and $n_2(e|T)$ are the number of vertices of T, lying closer to vertex x than to vertex y, and closer to vertex y than to vertex x, respectively. Still more formally, $n_1(e|T)$ and $n_2(e|T)$ are the cardinalities of the sets $\{u \in V(T)\,;\, d(u,x) < d(v,x)\}$ and $\{u \in V(T)\,;\, d(u,x) > d(v,x)\}$, respectively, where $V(T)$ is the vertex set of T and where $d(r,s)$ stands for the distance between the vertices r and s.

In what follows the numbers $n_1(e|T)$ and $n_2(e|T)$ will be selected so that $n_1(e|T) \leq n_2(e|T)$. This convention does not influence the generality of our considerations.

The quantities $n_1(e|T)$ and $n_2(e|T)$ have been encountered already in the 1947 paper by Harold Wiener [1], where he mentions that the sum of distances between all pairs of vertices of a chemical tree:

$$W(T) = \sum_{r<s} d(r,s)$$

can be computed by means of the formula

$$W(T) = \sum_{e} n_1(e|T) \cdot n_2(e|T) \ . \tag{1}$$

Nowadays W is called the *Wiener index*.

The first formal proof of Eq. (1) was given in the book [2]. Eventually, Eq. (1) was much studied; for details see the review [3]. The extension of the right–hand side of (1) to all graphs was named the *Szeged index*; for details see the review [4] and the book [5].

Motivated by Eq. (1), in 2001 the *modified Wiener index* was defined as [6]

$$^{m}W(T) = \sum_{e} [n_1(e|T) \cdot n_2(e|T)]^{-1} \ . \tag{2}$$

Somewhat more recently, also the *variable Wiener index* was put forward [7, 8], viz.:

$$W_\lambda(T) = \sum_{e} [n_1(e|T) \cdot n_2(e|T)]^{\lambda} \tag{3}$$

with λ being an adjustable parameter. For $\lambda = +1$ and $\lambda = -1$, the variable Wiener index reduces, respectively, to the ordinary and to the modified Wiener index.

A further structure–descriptor U, proposed by Zenkevich [9], can be expressed in terms of the numbers $n_1(e|T)$ and $n_2(e|T)$ as [10]:

$$U(T) = \sum_{e} \sqrt{\frac{(C+2H)n + 2H}{[(C+2H)n_1(e|T) + H]\,[(C+2H)n_2(e|T) + H]}} \tag{4}$$

where $C \approx 12.0$ and $H \approx 1.0$ are the relative atomic masses of carbon and hydrogen, respectively.

In Eqs. (1)–(4) the summation goes over all edges of the tree T.

Studies of the above mentioned structure–descriptors lead to the concept of *equiseparable trees* [11]. Two trees T' and T'' of equal number n of vertices are said to be equiseparable if their edges $e'_1, e'_2, \ldots, e'_{n-1}$ and $e''_1, e''_2, \ldots, e''_{n-1}$ can be labeled so that the equality $n_1(e'_i|T') = n_1(e''_i|T'')$ holds for all $i = 1, 2, \ldots, n-1$. From the inspection of Eqs. (1)–(4) we see that equiseparable trees have equal Wiener indices, W_λ-values (for all λ), as well as Zenkevich indices U.

It is known [12] that the Wiener index measures the van der Waals surface area of an alkane molecule, which explains the correlations found between W and a great variety of physico–chemical properties of alkanes (for details see the review [13] and the book [14]). The Zenkevich index provides a measure of the internal (vibrational) energy of the underlying alkane molecule [10, 15]. Consequently, the molecules represented by equiseparable chemical trees are expected to have many similar physico–chemical properties.

General procedures for constructing pairs of equiseparable trees were developed [11, 16], and it gradually became evident [17] that equiseparable trees and chemical trees occur in large families. In order to gain information on the frequency of the occurrence of equiseparable trees, we examined all trees with up to 20 vertices. A preliminary account of our findings was reported in [17]. Here we give a more detailed account.

SEPARATION SEQUENCE AND SEPARATION NUMBER

Let T be an n-vertex tree and $e_1, e_2, \ldots, e_{n-1}$ its edges. We are interested in the sequence of numbers

$$\{n_1(e_1|T)\, ,\, n_1(e_2|T)\, ,\, \ldots\, ,\, n_1(e_{n-1}|T)\} \ . \tag{5}$$

Because the form of the sequence (5) depends on the labeling of the edges of T, we have to find another labeling–independent representation. This is achieved by means of the *separation sequence*.

Because of $n_1(e_i|T) + n_2(e_i|T) = n$ and $n_1(e_i|T) \leq n_2(e_i|T)$, each of the numbers $n_1(e_i|T)$, $i = 1, 2, \ldots, n-1$, is an integer satisfying the inequality

$$1 \leq n_1(e_i|T) \leq \lfloor n/2 \rfloor \ .$$

Let $k_i(T)$ among the numbers $n_1(e_i|T)$, $i = 1, 2, \ldots, n-1$, be equal to i . Then the ordered ($\lfloor n/2 \rfloor$)-tuple

$$\sigma(T) = \Big\{ k_1(T) \, , \, k_2(T) \, , \, \ldots \, , \, k_{\lfloor n/2 \rfloor}(T) \Big\} \tag{6}$$

is independent of the labeling of the edges of T . We refer to $\sigma(T)$ as to the *separation sequence* of the tree T . Clearly, two trees are equiseparable if and only if their separation sequences coincide.

It is worth noting that

$$\sum_{i=1}^{\lfloor n/2 \rfloor} k_i(T) = n - 1 \ . \tag{7}$$

Consequently, only trees with equal number of vertices can have coinciding separation sequences.

Our initial idea was to compute the separation sequence of all n-vertex trees and to find among them those which coincide. This task can, however, be made somewhat simpler.

First, because of the relation (7), if n is fixed and known, we don't need to compute all $\lfloor n/2 \rfloor$ distinct $k_i(T)$-values. Namely, if we know $\lfloor n/2 \rfloor - 1$ distinct $k_i(T)$'s, then the missing one can be determined from the relation (7). In particular, it is sufficient to compute $k_i(T)$, $i = 2, 3, \ldots, \lfloor n/2 \rfloor$.

Second, it can be shown that for $i > 1$, the maximum possible $k_i(T)$-value is equal to $\lfloor (n-1)/2 \rfloor$. This maximum value is achieved for $i = 2$, for the tree $T_n^\dagger$ whose structure is the following. If n is odd, then $T_n^\dagger$ is obtained by joining a vertex with the end vertices of $(n-1)/2$ disjoint copies of P_2 . If n is even, then $T_n^\dagger$ is obtained by joining a vertex of P_2 with the end vertices of $(n-2)/2$ disjoint copies of P_2 .

Therefore, if we restrict our considerations to trees with 20 or fewer vertices, then it will be $k_i(T) \leq 9$ for all $i > 1$ and all T .

In view of this, we define the *separation number* as

$$SN(T) = \sum_{i=2}^{\lfloor n/2 \rfloor} k_i(T) \, 10^{\lfloor n/2 \rfloor - i}$$

which is an integer whose decade form is be written with at most $\lfloor n/2 \rfloor - 1$ digits. Thus, if $n \leq 20$, then, in the worst case, $SN(T)$ is a 9-digit integer.

Two trees with equal number of vertices are equiseparable if and only if their SN-values are equal. (Note that trees with different number of vertices may have equal separation numbers. For instance, for the star S_n we have $SN(S_n) = 0$, irrespective of the number n of vertices.)

As an illustration, consider the tree T^* depicted in Fig. 1. This is the molecular graph of 2,4-dimethyl-4-etyl-6-isopropylnonane. Its edges are (deliberately) labeled by $e_1, e_2, \ldots, e_{15}$ in an unorderly manner. By direct calculation (or simply, by inspection) we obtain: $n_1(e_1|T^*) = 3$, $n_1(e_2|T^*) = 3$, $n_1(e_3|T^*) = 6$, $n_1(e_4|T^*) = 1$, $n_1(e_5|T^*) = 1$, $n_1(e_6|T^*) = 2$, $n_1(e_7|T^*) = 1$, $n_1(e_8|T^*) = 2$, $n_1(e_9|T^*) = 1$, $n_1(e_{10}|T^*) = 1$, $n_1(e_{11}|T^*) = 1$, $n_1(e_{12}|T^*) = 3$, $n_1(e_{13}|T^*) = 1$, $n_1(e_{14}|T^*) = 4$, and $n_1(e_{15}|T^*) = 8$. Therefore, $k_1(T^*) = 7$, $k_2(T^*) = 2$, $k_3(T^*) = 3$, $k_4(T^*) = 1$, $k_5(T^*) = 0$, $k_6(T^*) = 1$, $k_7(T^*) = 0$, and $k_8(T^*) = 1$, Consequently, the separation sequence and the separation number of T^* are equal to $\sigma(T^*) = (7, 2, 3, 1, 0, 1, 0, 1)$ and $SN = 2310101$.

Figure 1. The molecular graph of 2,4-dimethyl-4-etyl-6-isopropylnonane. Its separation sequence is $(7, 2, 3, 1, 0, 1, 0, 1)$ and its separation number is 2310101.

NUMERICAL WORK

Calculations were performed on all trees with $7 \leq n \leq 20$ vertices. For each particular value of n, the structures of all n-vertex trees were available in appropriate coded forms. From these codes the adjacency matrix was reconstructed, and the numbers $n_1(e_i|T)$, the separation sequences, and the separation numbers determined. This was sequentially done for all n-vertex trees, and a list of SN-number was created. From this list the recognition of families of equiseparable trees is achieved by comparing and ordering integers.

Chemical trees were detected by computing the vertex degrees (i. e., summing the rows of the adjacency matrix). Whenever, a computed vertex degree exceeded 4, the respective tree was discarded. If no vertex was found to have degree greater than 4, the respective tree was recognized as a chemical tree. Its SN-value was recorded in a separate list, which eventually was processed in the same manner as the list of SN-values of all n-vertex trees.

RESULTS

Our main results are summarized in the Tables 1 & 3 (for trees) and 2 & 4 (for chemical trees).

From Tables 1–4 we see that there exist very large families of equiseparable trees and chemical trees, and that only a relatively small number of trees have no equiseparable mate. A typical family of equiseparable chemical trees is depicted in Fig. 2.

The large number and the increasing size of the families of equiseparable trees and chemical trees suggests that *almost all trees have an equiseparable mate*. More precisely: the ratio of the number of n-vertex trees having no equiseparable mate, and the total number of n-vertex trees tends to zero as $n \to \infty$. A formal proof of this result will be communicated separately [18].

F		$n=7$	$n=8$	$n=9$	$n=10$	$n=11$	$n=12$	
1		9	17	22	47	57	106	
2		1	3	9	18	35	73	
3		–	–	1	3	9	20	
4		–	–	1	1	7	12	
5		–	–	–	2	6	16	
6		–	–	–	–	1	8	
7		–	–	–	–	–	1	
8		–	–	–	–	1	3	
9		–	–	–	–	1	1	
10		–	–	–	–	–	–	
11		–	–	–	–	–	1	
12		–	–	–	–	–	1	
13		–	–	–	–	–	–	
F	$n=13$	$n=14$	$n=15$	$n=16$	$n=17$	$n=18$	$n=19$	$n=20$
1	147	275	316	670	805	1539	1923	3695
2	108	215	329	625	892	1752	2466	4783
3	50	98	149	339	501	961	1385	2747
4	34	66	136	259	466	896	1508	2904
5	23	62	97	205	309	688	940	1896
6	17	44	83	192	335	660	1127	2262
7	6	18	48	76	142	302	492	1036
8	7	21	64	106	234	481	904	1801
9	11	22	34	104	152	317	501	955
10	5	9	30	79	169	333	618	1284
11	1	6	18	31	81	171	283	552
12	4	8	26	71	142	340	601	1327
13	1	3	17	26	44	115	182	413
14	2	6	12	40	116	252	454	1036
15	1	7	12	42	71	132	278	488
16	1	3	7	24	66	144	348	693
17	1	2	14	20	48	121	183	407
18	–	1	11	26	72	159	320	674
19	–	2	3	16	27	78	148	303
20	2	3	11	23	60	137	266	618

Table 1. Number of families of equiseparable n-vertex trees of small size (F). The case $F = 1$ pertains to trees having no equiseparable mate.

F	$n=7$	$n=8$	$n=9$	$n=10$	$n=11$	$n=12$
1	7	14	19	44	54	105
2	1	2	5	6	20	39
3	–	–	2	5	9	22
4	–	–	–	1	5	11
5	–	–	–	–	1	2
6	–	–	–	–	1	5
7	–	–	–	–	1	2
8	–	–	–	–	–	1
9	–	–	–	–	–	–

F	$n=13$	$n=14$	$n=15$	$n=16$	$n=17$	$n=18$	$n=19$	$n=20$
1	145	287	347	768	943	1876	2396	4783
2	81	157	269	502	823	1653	2495	4991
3	37	75	126	285	439	861	1347	2727
4	23	52	97	218	377	777	1393	2689
5	9	28	64	123	235	488	723	1542
6	9	29	61	131	256	533	942	1961
7	8	13	28	67	128	268	458	952
8	5	11	35	70	159	350	703	1381
9	2	6	14	40	89	175	368	716
10	2	6	25	49	106	256	468	1074
11	4	5	18	36	76	168	267	558
12	–	3	9	26	80	185	416	935
13	–	3	7	21	42	91	169	340
14	–	1	9	24	63	163	314	691
15	1	1	6	11	34	71	145	338
16	–	–	4	13	33	97	229	499
17	–	–	3	5	19	46	100	218
18	–	1	4	11	34	81	195	437
19	–	–	1	8	20	45	104	216
20	–	2	2	10	25	58	173	408

Table 2. Number of families of equiseparable n-vertex chemical trees of small size (F). The case $F = 1$ pertains to chemical trees having no equiseparable mate.

n												
7	2	1	1	1	1	1	1	1	1	1	–	–
8	2	2	2	1	1	1	1	1	1	1	1	1
9	4	3	2	2	2	2	2	2	2	2	2	1
10	5	5	4	3	3	3	2	2	2	2	2	2
11	9	8	6	5	5	5	5	5	5	4	4	4
12	12	11	9	8	8	8	7	6	6	6	6	6
13	20	20	17	16	15	14	14	13	12	12	12	12
14	34	27	25	23	22	21	20	20	20	19	19	18
15	54	47	45	44	40	37	35	35	34	33	33	33
16	84	70	70	67	63	62	61	58	58	56	56	54
17	138	135	126	109	108	107	105	102	96	95	94	93
18	227	206	198	196	177	174	172	171	167	157	154	153
19	370	365	330	328	317	316	313	300	292	284	282	277
20	603	597	564	563	543	541	534	494	486	476	467	466

Table 3. Sizes of the twelve largest families of equiseparable n-vertex trees.

n												
7	2	1	1	1	1	1	1	1	–	–	–	–
8	2	2	1	1	1	1	1	1	1	1	1	1
9	3	3	2	2	2	2	2	1	1	1	1	1
10	4	3	3	3	3	3	2	2	2	2	2	2
11	7	6	5	4	4	4	4	4	3	3	3	3
12	8	7	7	6	6	6	6	6	5	5	4	4
13	15	11	11	11	11	10	10	9	9	8	8	8
14	20	20	18	15	14	13	13	13	12	12	12	11
15	35	31	27	27	25	24	23	22	22	21	21	21
16	49	42	40	40	37	35	35	33	31	30	30	30
17	80	75	69	68	67	63	61	56	56	55	55	54
18	123	116	112	104	93	91	91	87	87	83	80	79
19	203	181	180	170	162	161	154	151	147	146	146	138
20	314	295	291	286	252	251	244	228	222	218	211	203

Table 4. Sizes of the twelve largest families of equiseparable n-vertex chemical trees.

Figure 2. A characteristic 12-membered family of equiseparable trees. These have $n = 12$ vertices. Among them the first 8 are chemical trees whereas the remaining 4 are not.

References

[1] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[2] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.

[3] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[4] I. Gutman, A. A. Dobrynin, The Szeged index – a success story, *Graph Theory Notes New York* **34** (1998) 37–44.

[5] M. V. Diudea, I. Gutman, L. Jäntchi, *Molecular Topology*, Nova, Huntington, 2001.

[6] S. Nikolić, N. Trinajstić, M. Randić, Wiener index revisited, *Chem. Phys. Lett.* **333** (2001) 319–321.

[7] I. Gutman, D. Vukičević, J. Žerovnik, A class of modified Wiener indices, *Croat. Chem. Acta*, in press.

[8] B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, On variable Wiener index, *Indian J. Chem.* **42A** (2003) 1279–1282.

[9] I. G. Zenkevich, Dependence of chromatographic retention indices on the dynamic characteristics of molecules, *Russ. J. Phys. Chem.* **73** (1999) 797–801.

[10] I. Gutman, I. G. Zenkevich, Wiener index and vibrational energy, *Z. Naturforsch.* **57a** (2002) 824–828.

[11] I. Gutman, B. Arsić, B. Furtula, Equiseparable chemical trees, *J. Serb. Chem. Soc.* **68** (2003) 549–555.

[12] I. Gutman, T. Körtvélyesi, Wiener indices and molecular surfaces, *Z. Naturforsch.* **50a** (1995) 669–671.

[13] D. H. Rouvray, The rich legacy of half century of the Wiener index, in: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry — Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 16–37.

[14] I. Gutman, *Hemijska teorija grafova*, PMF Kragujevac, Kragujevac, 2003.

[15] I. Gutman, D. Vidović, B. Furtula, I. G. Zenkevich, Wiener–type indices and internal molecular energy, *J. Serb. Chem. Soc.* **68** (2003) 401–408.

[16] I. Gutman, B. Furtula, D. Vukičević, B. Arsić, Equiseparable molecules and molecular graphs, *Indian J. Chem.* **43A** (2004) 7–10.

[17] O. Miljković, B. Furtula, I. Gutman, Statistics of equiseparable trees and chemical trees, MATCH Commun. Math. Comput. Chem. **51** (2004) 179–184.

[18] D. Vukičević, I. Gutman, Almost all trees have an equiseparable mate, in preparation.