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ISOSPECTRAL MULTITREES[†,★]

M. RANDIĆ[★] and B. BAKER

Department of Mathematics and Computer Science, Drake University, Des Moines, Iowa 50311, USA

[★]and *Ames Laboratory – DOE*[☆], *Iowa State University, Ames, Iowa 50011, USA*

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Abstract

We examined trees with one multiple edge (of multiplicity k) and report all isospectral graphs found when the number of vertices was $n \leqslant 9$. The search for isospectral multitrees was carried out systematically by constructing the characteristic polynomials of all trees having one weighted edge. For all multitrees having $n \leqslant 7$ vertices, we tabulated the coefficients of the characteristic polynomial. We restricted the analysis to trees with the maximal valency $d = 4$. The number of graphs considered exceeds 300. The smallest pair of isospectral multitrees (i.e. trees with a multiple edge) has $n = 6$ vertices. There is a pair of trees when $n = 7$, three pairs when $n = 8$, and five pairs when $n = 9$. In all cases, when $k = 1$ is assumed, isospectral multitrees reduce to the *same* tree. When $k = 0$ is assumed, isospectral trees produce either the same disconnected graph, or an isospectral forest.

[†]Dedicated to Basil E. Gillam, Professor Emeritus of the Department of Mathematics and Computer Science at Drake University.
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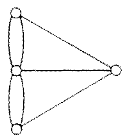
1. Introduction

While isospectral (or cospectral) graphs, i.e. nonisomorphic graphs with the same set of eigenvalues, have received considerable attention, one cannot escape noticing a lack a results on isospectral multigraphs. Multigraphs are graphs in which at least one pair of vertices is connected with two or more lines. A simple multigraph is a graph associated with the well-known problem of Königsberg bridges [1]:



Before 1970, isospectral graphs were considered rare, the exception rather than the rule. Later, it became apparent that they are rather common. In the case of trees, reported by Schwenk [3], as the number of vertices increases, the ratio of the number of isospectral trees to the number of all trees approaches 1. Hence, the somewhat provocative title of the article by Schwenk: *Almost all trees are cospectral.* Despite their abundance and much past interest, there are a number of unresolved questions concerning isospectral graphs. For example, are isospectral trees having a single branching vertex possible? So far, not one single case has been reported. Are isospectral *trees* having no vertices of degree 2 (the so-called "proper" graphs) possible? Isospectral graphs having no vertices of degree 2 are known [3]. No case of isospectral trees in which at least one partner has no vertices of degree $d = 2$ has yet been reported.

It is surprising to find no mention of isospectral multitrees in the literature. A single illustration of isospectral multitrees [4] was constructed from isospectral trees by connecting "isospectral" points by a multiple link, as shown in fig. 1. Such

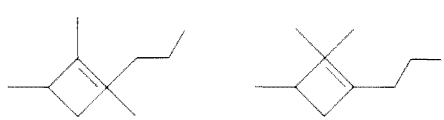


Fig. 1. Trivially constructed isospectral multitrees obtained by connecting isospectral points of isospectral trees.

constructions do not reveal structural novelties and represent a trivial extension of trees to multitrees. We report here on a systematic search for isospectral multitrees. We also briefly consider constructions of families of isospectral multitrees. Graphs such as those in figs. 1 and 2, which can be obtained using known properties of isospectral graphs without multiple bonds, are excluded from consideration. The isospectral graphs of fig. 2 can be constructed by attaching a fragment having a multiple

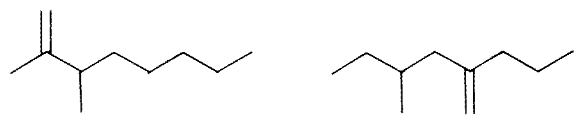


Fig. 2. Trivially constructed isospectral multitrees obtained by attaching a fragment having multibond to isospectral points of isospectral trees.

bond to the parent endospectral graph. Such constructions, which hold for *any* fragment (hence also for a fragment with a multiple link), can therefore be viewed as trivial, and the corresponding isospectral graphs as uninteresting.

2. Characteristic polynomials via ultimate pruning

Our systematic search for isospectral multitrees is based on the construction of the characteristic polynomials of all trees of a certain size, having a pair of multi-connected vertices. As will be seen, the assumed multiplicity k for the multiple edge, when the $k = 0$ and $k = 1$ cases are excluded, does not influence the property of isospectrality. Therefore, without loss of generality, we may assume for the trees considered that $k = 2$, i.e. they have one double bond.

The construction of the characteristic polynomial for graphs of arbitrary size was considered to be extremely tedious [5]. The difficulty arises from the exponential growth of the number of terms arising in the construction of the polynomial [6]. This is evident from the pictorial approach to the characteristic polynomial of Spialter [7] or the combinatorial approach of Sachs [8], who expressed individual coefficients of the characteristic polynomial by a collection of qualified subgraphs. Their work was preceded by an early contribution of Coulson [9], who derived coefficients of a secular determinant $|A - xI|$ by counting selected subgraphs contributing to the expansion. We may also mention the pioneering work of Denes König, the author of the first book on Graph Theory [10], who interpreted a determinant of the adjacency matrix of the graph as a linear combination of selected subgraphs. A number of known techniques in numerical analysis for deriving the characteristic polynomial, such as the method of Krylov [11], Le Verrier's method [12], and others [13], have only recently attracted attention for graph-theoretical applications [14]. In addition, some novel approaches for the construction of the characteristic polynomial of graphs have been developed [15], although their practical value remains to be seen. Computer programs for deriving the coefficients of the characteristic polynomial also became available [16,17].

Of particular interest for the present study of isospectral multitrees are the following developments: Firstly, Balasubramanian [18] outlined an elegant scheme for a construction of the characteristic polynomial of *trees*. In this approach, one considers a determinant for a reduced tree, obtained by pruning terminal vertices. Instead of an initial $n \times n$ determinant, we thus obtain a smaller $n' \times n'$ determinant, where n' is the number of vertices that remain after eliminating the terminal vertices. Trees can be pruned repeatedly, until ultimately 2×2 determinants are obtained. Reduced determinants are constructed so that their expansion gives the correct characteristic polynomial of the initial graph. Secondly, the use of Chebyshev polynomials as the basis for the construction of the characteristic polynomials simplifies expressions for the polynomials and makes comparisons simpler [20]. Chebyshev polynomials form a more "natural" basis for expressing characteristic polynomials of graphs, in particular for trees, because they themselves *are* the characteristic polynomials of linear graphs on n vertices. The multiplication table for Chebyshev polynomials has a simple structure [20,21]:

$$L(m) \times L(n) = L(m+n) + L(m+n-2) + L(m+n-4) + \ldots + L(m-n),$$

which allows expressing products of the polynomials as a linear combination of $L(k)$ terms of a same parity (i.e. L having all even or all odd subscripts). Instead of the gradual pruning of terminal vertices in a tree, one can alternatively, in a single step, prune arbitrary end groups. In this way, one can immediately consider a 2×2 determinant, constructed by selecting a bond and its ends as terminals [21]. Let a and b represent the end vertices of an "ultimate" edge, and let A and B represent fragments attached to vertices a and b, respectively, and also let A and B represent the characteristic polynomials of the mentioned fragments. Let $A - a$ represent the subgraph of A, obtained by erasure of the vertex a (which implies also erasure of its incident edges). Analogously, let $B - b$ represent the subgraph of B, obtained by erasure of the vertex b. Again, the same symbols $A - a$ and $B - b$ will represent also the characteristic polynomials of the corresponding subgraphs. Then the 2×2 determinant is:

$$\begin{vmatrix} A & A-a \\ B-b & B \end{vmatrix} .$$

3. An illustration

Consider a pair of isospectral graphs from fig. 3, in which the fragments A, B are linear chains. The characteristic polynomials of the two graphs can, therefore, be

Fig. 3. A pair of isospectral trees.

expressed directly by $L(k)$, where k indicates the number of vertices in the corresponding chains. We selected as "ultimate" the bond between the unique branching vertices. Therefore, for the two isospectral trees we obtain:

$$\begin{vmatrix} L(5) & L(1)\,L(3) \\ L(1)\,L(3) & L(5) \end{vmatrix} \qquad \begin{vmatrix} L(3) & L(1)\,L(1) \\ L(2)\,L(4) & L(7) \end{vmatrix}.$$

One can immediately write for the characteristic polynomials:

$$L(5)\,L(5) - L(3)\,L(3)\,L(1)\,L(1) \quad \text{and} \quad L(7)\,L(3) - L(4)\,L(2)\,L(1),$$

respectively. Use of the multiplication rule for $L(k)$ allows one to simplify the above expressions. For example, the diagonal elements of the two determinants lead to the following results:

$$L(5)\,L(5) = L(10) + L(8) + L(6) + L(4) + L(2) + 1$$

$$L(3)\,L(7) = L(10) + L(8) + L(6) + L(4).$$

The products in the off-diagonal elements similarly give:

$$L(1)\,L(3) = L(4) + L(2)$$

$$L(2)\,L(4) = L(6) + L(4) + L(2)$$

$$L(1)\,L(1) = L(2) + 1\,,$$

where $L(0) = 1$. These have to be multiplied in the expansion of the determinant, giving:

$$[L(4) + L(2)]\;[L(4) + L(2)] = L(8) + 2\,L(6) + 2\,L(4) + 3\,L(2) + 3$$

$$[L(6) + L(4) + L(2)]\;[L(2) + 1] = L(8) + 3\,L(6) + 4\,L(4) + 3\,L(2) + 1.$$

By combining the above results accordingly, we finally obtain for the characteristic polynomial of both graphs the same polynomial:

$$L(10) - 2\,L(6) - 3\,L(3) - 3\,L(2) - 1.$$

4. Characteristic polynomials for multitrees with $n = 6$ and $n = 7$

To derive the characteristic polynomials of multitrees with a single multibond of weight $k^{1/2}$, the outlined approach will now be used. Use of $k^{1/2}$, rather than k, makes the expressions for the coefficients of the characteristic polynomials simpler. As will be seen, k need not be specified; the coefficients of the characteristic polynomials are directly expressed in terms of k. In applications, the coefficients can be found by inserting the proper value of $k^{1/2}$. For example, $k = 4$ describes the presence of doubly connected vertices, $k = 9$ describes the case of triply connected vertices.

We start by selecting as the "ultimate" edge for the construction of the 2×2 determinant, from which the characteristic polynomial will be computed with an edge of multiplicity k. Consider the simplest case, a chain having three vertices, two of which are linked by a multibond:

The 2×2 determinant becomes:

$$\begin{vmatrix} L(2) & \sqrt{k}\, L(1) \\ \sqrt{k} & L(1) \end{vmatrix} .$$

That this is the correct form for the determinant can be verified by a direct expansion of the 3×3 determinant for the graph. From the above determinant, we immediately obtain for the characteristic polynomial in a Chebyshev expansion:

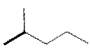
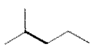
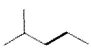
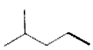
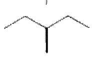
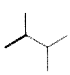
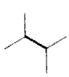
$$\begin{aligned} Ch(L(k), G) &= L(2)\, L(1) - k\, L(1) \\ &= L(3) + L(1) - k\, L(1) \\ &= L(3) + (1 - k)\, L(1). \end{aligned}$$

The coefficients of the $L(3)$ and $L(1)$ functions are 1 and $(1 - k)$, respectively. If we set $k = 1$, the above reduces to $L(3)$, the correct form of the characteristic polynomial of a linear chain having three vertices. In table 1, we list the coefficients of the characteristic polynomials, in a Chebyshev expansion, for all multitrees having $n = 6, 7$ vertices. The coefficients of the characteristic polynomial for larger multitrees will be reported elsewhere [22].

Some regularities of the coefficients shown in table 1 are apparent. The leading coefficient of the characteristic polynomials is 1 which, for brevity, has not been included in the tabulation. The coefficient of the next $L(k)$ term appears always as $(1 - k)$. Observe also that for many multitrees some coefficients are independent of k. The constant term (i.e. the last term when n is even) gives the value of the determinant of the adjacency matrix. As we see from table 1, there are trees (shown in fig. 4) whose determinant does not depend on k. In the case of linear chains, all non-zero coefficients are always $(1 - k)$, while the number of non-zero coefficients depends, in a straightforward way, on the location of the multibond.

Table 1

The coefficients of the characteristic polynomials in a Chebyshev expansion for all multitrees having $n = 6$ and $n = 7$ vertices and maximal valency of $d = 4$

Graph	L_4	L_2	L_0
	$1 - k$		
	$1 - k$	$1 - k$	
	$1 - k$	$1 - k$	$1 - k$
	$1 - k$	$-k$	
	$1 - k$	$1 - 2k$	$1 - k$
	$1 - k$	$-k$	
	$1 - k$	-1	$-1 + k$
	$1 - k$	-1	-1
	$1 - k$	$1 - 2k$	$-k$
	$1 - k$	$-k$	$-k$
	$1 - k$	$-1 - k$	-1
	$1 - k$	$1 - 3k$	$1 - 2k$
	$1 - k$	$-1 - 2k$	$-1 - k$
	$1 - k$	$-3k$	$-2k$
	$1 - k$	-3	$-3 + k$

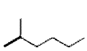
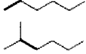
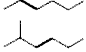
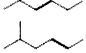
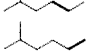
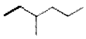
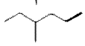
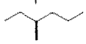
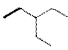
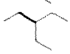
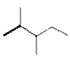
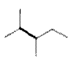
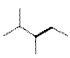
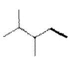
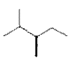
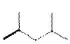
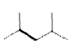
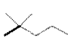
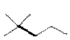
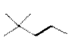
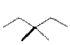
Graph	L_5	L_3	L_1
	$1 - k$		
	$1 - k$	$1 - k$	
	$1 - k$	$1 - k$	$1 - k$
	$1 - k$	$-k$	
	$1 - k$	$1 - 2k$	$1 - k$
	$1 - k$	$-k$	$1 - k$
	$1 - k$	$-k$	$-1 + k$
	$1 - k$	-1	$-1 + k$

Table 1 (continued)

Graph	L_5	L_3	L_1
	$1 - k$	-1	-1
	$1 - k$	$1 - 2k$	$-k$
	$1 - k$	$1 - 2k$	$1 - 2k$
	$1 - k$	$-k$	-1
	$1 - k$	$1 - 2k$	$-k$
	$1 - k$	$-k$	$-k$
	$1 - k$	-1	-2
	$1 - k$	$1 - 2k$	$-2k$
	$1 - k$	$-1 - k$	-2
	$1 - k$	$1 - 3k$	$1 - 3k$
	$1 - k$	$-2k$	$-1 - k$
	$1 - k$	-2	$-3 + k$
	$1 - k$	$-1 - k$	$-1 - k$
	$1 - k$	$-1 - k$	$-1 + k$
	$1 - k$	$-2k$	$1 - k$
	$1 - k$	$-1 - 2k$	$-1 - k$
	$1 - k$	$-3k$	$1 - 3k$
	$1 - k$	$-2 - k$	$3 + k$
	$1 - k$	-3	$-5 + 3k$
	$1 - k$	-3	$-5 + k$
	$1 - k$	$-3k$	$-1 - 3k$
	$1 - k$	$-1 - 2k$	$2 - 2k$
	$1 - k$	$-2 - 2k$	$-3 - k$
	$1 - k$	$-4k$	$1 - 5k$
	$1 - k$	$-1 - 3k$	$-1 - 3k$

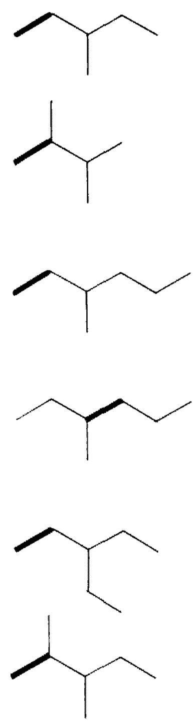


Fig. 4. Multitrees having the constant term of the characteristic polynomial independent of k (the multibond weight).

5. Isospectral multigraphs

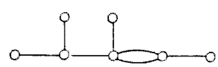
Our interest is in multitrees for which all the coefficients of the characteristic polynomial are equal. The first case, the smallest isospectral multitree, occurs when n = 6. In table 2, we show the corresponding eigenvalues and the characteristic polynomials, assuming as multibond a double bond. Numerical results were obtained using the MATLAB routine available for VAX computers [17]. Among sixteen multitrees on six vertices, this is the only pair of isospectral graphs. When n = 7, we again found a pair of isospectral multitrees, one pair among thirty-two possible multitrees. As the size of the graphs increases, so does the number of isospectral multitrees. When n = 8, there are eighty-two multitrees (with maximal valency of d = 4 or $d = 3 + k^{1/2}$) and we found three isospectral pairs among them. Finally, when n = 9, we have examined all 109 possible multitrees and found five isospectral pairs. In all, we found ten pairs of isospectral multitrees, i.e. twenty trees among some 330 trees, which is fewer than the number of isospectral trees for the corresponding sample size of simple trees.

In fig. 5, we illustrate all the isospectral multitrees found. We considered only trees with the maximal valency of 4, because of a chemical bias, where graphs having

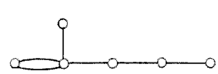
Table 2

The coefficients of the characteristic polynomial and the associated eigenvalues for the smallest pair of isospectral multitrees (as output of MATLAB routine)

```
0.   1.   0.   0.   0.   0.
1.   0.   1.   0.   0.   1.
0.   1.   0.   2.   0.   0.
0.   0.   2.   0.   1.   0.
0.   0.   0.   1.   0.   0.
0.   1.   0.   0.   0.   0.

<>
poly (c)

ANS =

      1.0000
      0.0000
    - 8.0000
      0.0000
     11.0000
      0.0000
      0.0000

<>
eig (c)

ANS =

      2.4972
    - 1.3281
      0.0000
      0.0000
      1.3281
      2.4972
```



```
0.   2.   0.   0.   0.   0.
2.   0.   1.   0.   0.   1.
0.   1.   0.   1.   0.   0.
0.   0.   1.   0.   1.   0.
0.   0.   0.   1.   0.   0.
0.   1.   0.   0.   0.   0.

<>
poly (a)

ANS =

      1.0000
      0.0000
    - 8.0000
      0.0000
     11.0000
      0.0000
      0.0000

<>
eig (a)

ANS =

    - 2.4972
    - 1.3281
      0.0000
      0.0000
      1.3281
      2.4972
```



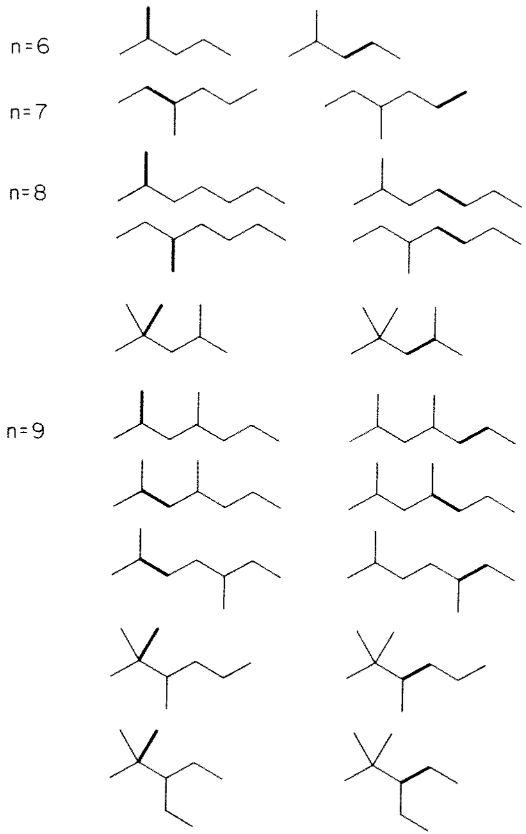


Fig. 5. All the isospectral multitrees with $n \leqslant 9$ vertices.

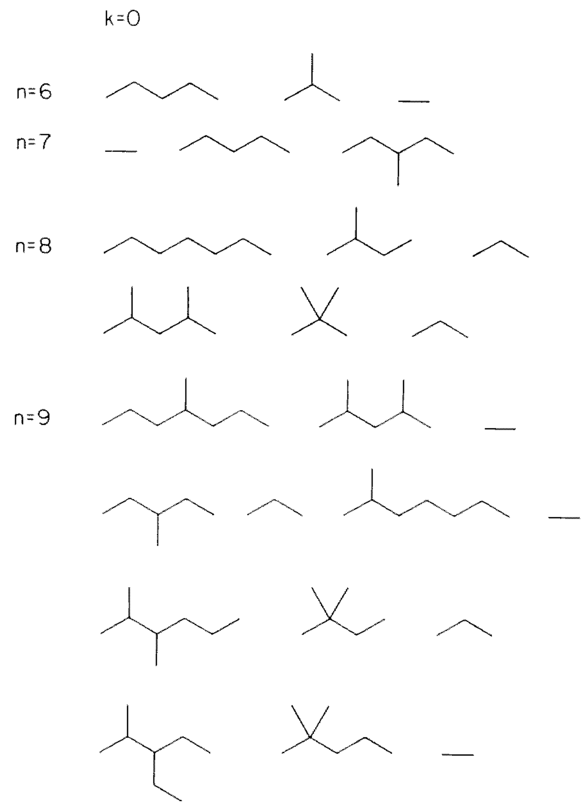


Fig. 6. Isospectral forests obtained from isospectral multitrees when $k = 0$ is assumed.

vertices of higher valency have fewer applications. Observe that in all the cases of fig. 6, when $k = 1$ is assumed, isospectral multitrees reduce to the same graph. This need not necessarily be the case because multitrees could also, when $k = 1$, reduce to nonisomorphic isospectral trees. However, we have not yet found any such case. Because there was no restriction on the value of k when deriving the polynomials, we can consider the $k = 0$ cases. These cases correspond, pictorially speaking, to an erasure of a multibond and, unless a multibond is terminal, will produce disconnected graphs. An erasure of multibonds in isospectral pairs may produce different or identical, connected or disconnected, trees. In the former case, we arrive as isospectral forests (fig. 6). While the cases are probably not new, clearly it was not previously perceived that isospectral forests can be related to isospectral multitrees. However, not every pair of isospectral multitrees found, when $k = 0$, produces a novel isospectral forest. When $n = 8$, there are two pairs of isospectral multitrees which reduce to the same isospectral forest, while when $n = 9$, there is an additional pair of isospectral multitrees which reduces to the same tree.

Because powers of Chebyshev polynomials of a low index appear frequently in computations of the characteristic polynomials, a table of powers of $L(k)$ was constructed to expedite the search. In the case of powers of $L(1)$, the coefficients of the corresponding $L(k)$ can be conveniently displayed in a triangular form (table 3). The

Table 3

The pattern made by the coefficients of powers of $L(1)$ when expanded in terms of Chebyshev polynomials $L(k)$

Coefficients											L_1^n	Expansion
									1		L_1	L_1
								1		1	L_1^2	$L_2 + 1$
							1		2		L_1^3	$L_3 + 2L_1$
						1		3		2	L_1^4	$L_4 + 3L_2 + 2$
					1		4		5		L_1^5	$L_5 + 4L_3 + 5L_1$
				1		5		9		5	L_1^6	$L_6 + 5L_4 + 9L_2 + 5$
			1		6		14		14		L_1^7	$L_7 + 6L_5 + 14L_3 + 14$
		1		7		20		28		14	L_1^8	$L_8 + 7L_6 + 20L_4 + 28L_2 + 14$
	1		8		27		48		42		L_1^9	$L_9 + 8L_7 + 27L_5 + 48L_3 + 42L_1$
1		9		35		75		90		42	L_1^{10}	$L_{10} + 9L_8 + 35L_6 + 75L_4 + 90L_2 + 42$

pattern made by the coefficients is reminiscent of the Pascal triangle. The coefficients can be obtained, like in the Pascal triangle, by adding numbers in a preceding row. The last column is constructed by interpreting the "missing" entries of the rows above as zero, giving for the last two columns the same entries: 1, 2, 5, 14, 42, 132, ... These are the well-known Catalan numbers:

$$C(n) = \frac{(2n)!}{n!\,(n+1)!}$$

emerging in numerous mathematical and chemical applications [23]. For example, the number of canonical "excited" valence structures for a conjugated polycyclic hydrocarbon having $n + 1$ double bonds is given by $C(n)$ [24]. The triangle of table 3 appeared also in a biological context.

6. Construction of isospectral multitrees

In fig. 7, we collected isospectral multitrees of different sizes showing apparent structural similarities. The trees having $n = 6$ and $n = 8$ vertices, shown at the top of

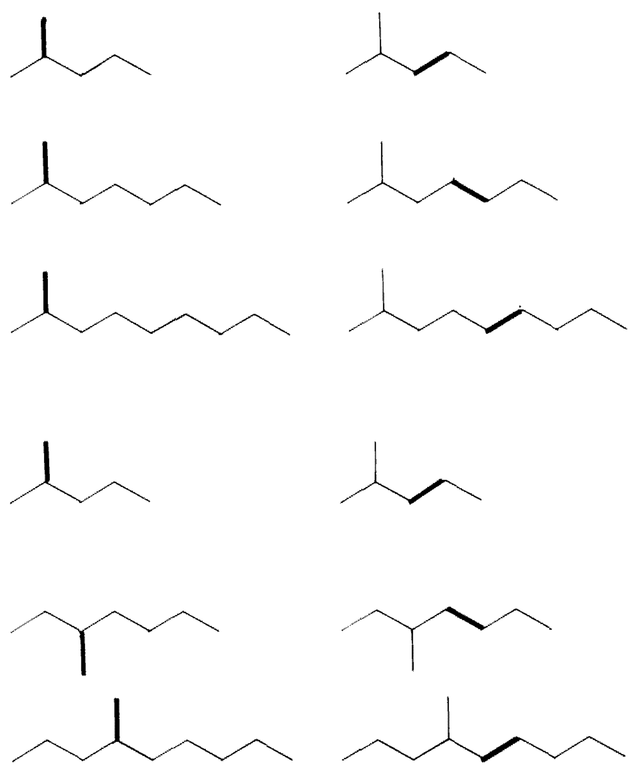


Fig. 7. Isospectral multitrees of different sizes showing apparent structural similarity.

fig. 7, have the same coefficients in their characteristic polynomials: 1, $(1 - k)$, and $-k$ although, due to their sizes, the coefficients correspond to different powers of x.

The larger graphs can be viewed as obtained from the smaller ones by increasing the length of the "backbone" chain. The lengths of the "chains" are increased by adding or inserting edges, at one side or both sides of the unique multiedge. Are such "operations" legitimate? Is this a valid "augmentation" process which will always yield larger isospectral multitrees? We have verified the "process" for the $n = 10$ case and found that the corresponding multitrees possess the same characteristic polynomial: $L(10) + (1 - k)\, L(8) - kL(6)$. Hence, not only are multitrees derived in this way isospectral, but their characteristic polynomial has the same simple structure already observed. One many conjecture the same to be true for the family of graphs of which the above are the initial members.

Similarly, the isospectral trees of the lower part of fig. 7 suggest another family of isospectral multitrees. The higher members of this family are constructed by adding, at each end of the "long" chain, an edge. Again, upon verification, we find that our guess was correct; the $n = 10$ multitrees of fig. 9 have the same characteristic polynomial: $L(10) + (1 - k)\, L(8) - kL(6) - kL(4) - kL(2)$, i.e. are isospectral.

7. Multigraphs with several multiple edges

The isospectral multitrees found (fig. 5) can formally be viewed as derived from a single graph by *interchanging* a pair of weights k and 1 between the unique edges defining the isospectral pair. For example, the smallest isospectral multitrees can be viewed as obtained from a parent simple tree by *switching* the weight factors k and 1 from the terminal bond in one tree to the central bonds in another (fig. 8). If

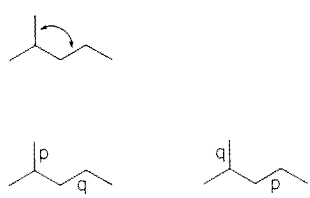
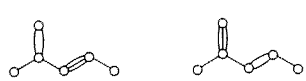


Fig. 8. Isospectral multitrees viewed as obtained from a parent tree by "switching" the weights for a pair of edges.

such a viewpoint is correct, it ought to hold also if we interchange weights p and q instead of k and 1. Hence, trees shown in fig. 8 with $p \neq q \neq 1$ may represent a general case of isospectral multitrees. In the case $p = 2$ and $q = 3$, we have:



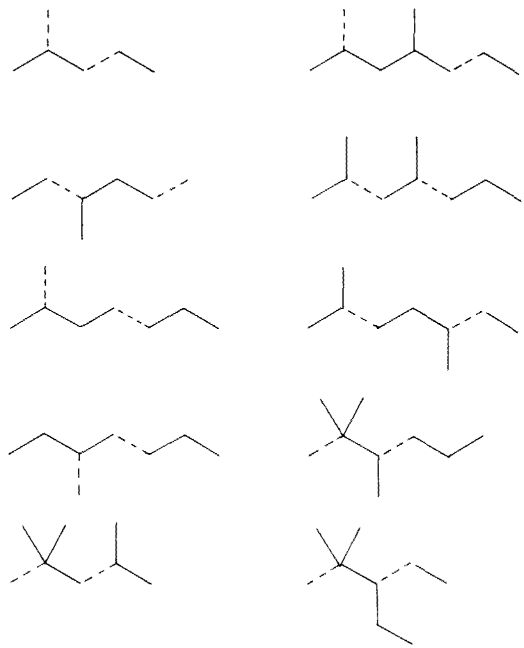


Fig. 9. Parent trees for obtaining isospectral multitrees by exchanging the weights p and q between the two unique edges.

By constructing the corresponding characteristic polynomials, we verified that the two multitrees are indeed isospectral. We examined all the multitrees of table 2 and tested whether they remain isospectral when assuming special weights $p = 2$ and $q = 3$ instead of k and 1. We always found that isospectrality was preserved. Hence, isospectral multitrees can be represented by a single graph having two *unique* edges associated with distinct weight, as illustrated in fig. 9. When either p or q is assumed to be zero, we obtain isospectral forests involving multitrees as illustrated in fig. 10 for assumed unspecified multiple bond weights.

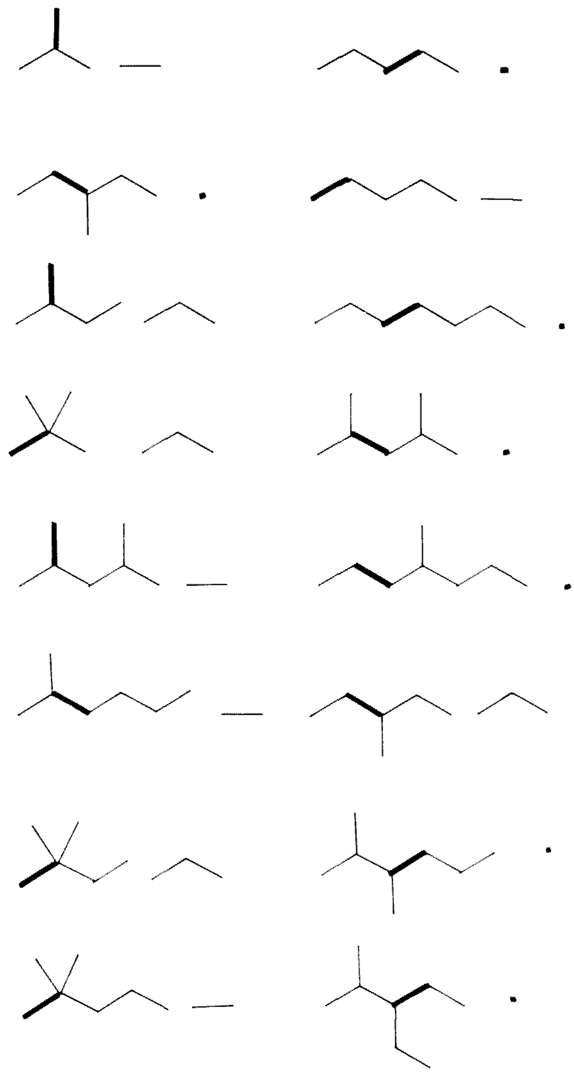


Fig. 10. Isospectral forests involving multitrees.

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