

Characterization of Acyclic Graphs by
Successive Dissection

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(Received: September 24, 1982)

Abstract

A decomposition of acyclic graphs by erasure of a vertex is considered and the process is repeated on the derived subgraphs until only disjoint vertices or edges are obtained. At each stage of the process edges are counted and a sequence $b_0, b_1, b_2, \dots, b_k$ constructed in which b_i represent the number of edges (bonds) at i -th repetition of the decomposition process. Properties of the derived sequences are discussed and several structural regularities outlined. In all cases considered the b -sequence is unique to the graph, thus the approach appears promising in the search for a unique structural characterization of graphs. In particular several isospectral graphs are examined and also isocodal graphs (codes based on enumeration of paths of different length) and no coincidental sequences based on b_i numbers have been detected.

Introduction

One of the most important problems in graph theoretical applications is the question of a unique characterization of graphs, i.e., a unique "name" or "signature." Canonical numbering of vertices results in a unique adjacency matrix which can subsequently be linearized as a binary code.¹ An alternative approach is to select some invariants, proceed with enumeration and thus derive a sequence $i_0, i_1, i_2, \dots, i_k$ with the objective that no two graphs will ever have the same sequence of numbers i_k . The characteristic polynomial was expected to provide such a basis with its coefficients defining the sequence. However, Collatz and Sinogowitz reported on isospectral graphs,² and it was apparent that the construction of the characteristic polynomial is accompanied with a substantial loss of structural information. Coefficients of the characteristic polynomial are simply related to the count of self-returning random walks, and this does not provide a proper basis for a unique characterization of a structure. More recently sequences $p_0, p_1, p_2, \dots, p_k$ where p_i is the count of paths (i.e., self-avoiding walks) on length i have been introduced for discussion of similarity among molecular forms.³ Again it was found that there are structures which have different connectivity yet result in the same sequence of p_i values. This is not surprising, since path numbers count the number of neighbors regardless of their distribution.

The notion that perhaps there is a collection of invariants that will result in unique sequences is certainly attractive. It has an obvious advantage over canonical labels in that it would define a unique name without requiring a labeling of vertices. The search for such invariants remains an attractive proposition even though there is no advance assurances that indeed such invariants exist. It may be difficult to propose such a characterization by way of

illustration; even more difficult may be to provide a proof for the claim on uniqueness. On the other hand a single counterexample would disprove the conjecture of unique characterization.

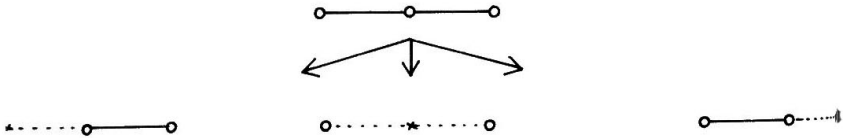
Hence, in view of past experiences, it appears discouraging to make efforts in the search for a unique sequence. However, the problem may be rewarding even if it eventually results in a failure as long as interest is confined to structural invariants and avoids conventional agreements (such as implied in canonical labeling). If a scheme has considerable discriminatory power (a reasonable test of which might be to examine acyclic graphs with 10 or less vertices) then coincidences would signal a special structural condition. For example, failure of unique names via the characteristic polynomial resulted in the concept of isospectral graphs. This opened a new area of interest and resulted in numerous novel insights on the structure, including various constructions of isospectral graphs⁴ and new concepts, such as isospectral points,⁵ and unusual random walks.⁶

We suggest here a procedure for arriving at a collection of graph invariants which have a "natural" ordinal number and thus provide the basis for construction of a sequence for a graph. We will confine our attention here to acyclic graphs (trees) and will demonstrate that the resulting sequences are unique for all graphs with 8 vertices. Within the same collection of graphs neither the characteristic polynomial nor path codes are unique, so the present approach demonstrates a better discrimination. It is, however, premature to conjecture on the unique aspect of the proposed codes. Work is in progress to derive a computer program for verification of the codes for larger acyclic structures.⁷ As will be seen later the construction of the proposed sequences involves an iterative scheme, and the work involved grows with

the size of graphs. This makes it impractical to extend the application to larger graphs unless all smaller graphs have already been catalogued. We confine our interest here to acyclic graphs in order to illustrate the approach and to point to some regularities in the derived codes. In a separate paper⁸ we consider polycyclic structures and regularities observed there. Finally, we will complete the search for new codes with regular graphs as the candidate structures which may be expected to be most prone to lead to a common code for non-isomorphic structures.

Outline of the Approach

The present work is an outgrowth of our earlier suggestion of dissection of graphs by successively deleting its vertices.⁹ Consider the simple graph shown below and erase each time one of the vertices:



One derives three subgraphs (one of which has no edge) referred to as Ulam's subgraphs in view of its introduction by Ulam in the famous conjecture on reconstruction.¹⁰ We count bonds (edges) at the initial stage and at the end. At each stage we have two bonds, and using symbols b_0 and b_1 respectively for the count of bonds at the start and after the first erasure of a vertex we obtain $b_0 = 2$ and $b_1 = 2$. Thus, we can construct a sequence b_0, b_1 as 2, 2 to represent the linear graph having two bonds. The process can be

applied to any graph and after deriving numbers b_0 and b_1 one is left with a collection of subgraphs, each having $n-1$ vertices if the initial graph had n vertices. The number of edges in Ulam subgraphs is, in the case of acyclic graphs, at most $n-2$ (when a terminal vertex has been deleted) or less if an inner vertex is erased. Hence, the process can continue for all those subgraphs having more than a single edge. In fact, the process can be continued successively until eventually all subgraphs have been broken down into isolated vertices or isolated edges.

In Table 1 we illustrate the process on simple graphs representing smaller alkanes: butane and pentane isomers. This table can be compared with a similar table in ref. 9, but instead of counting the total of atoms and bonds we record the number of bonds at each successive step and ignore the count of vertices (or atoms). Because isolated vertices are of no interest here we have not represented them in the table. Dissection of hexane isomers is shown in Table 2.

One sees that the process is cumulative; each larger structure generates subgraphs of a smaller size and requires information on such smaller structures. The number of components to be considered grows, but because at each step only the total is recorded, one cannot in advance be assured that different graphs will generate different sequences. We therefore undertook to examine a fair sample of acyclic graphs in order to see how different sequences emerge. We hope to recognize some regularities in the sequences and to see if they offer a promising basis for a unique characterization. In Table 3 we list the results for nine isomers of heptane C_7H_{16} , and in Table 4 the sequences for the 18 isomers of octane C_8H_{18} are given:

Table 1: Construction of Bond-Sequences for Butane and Pentane Isomers




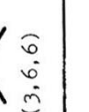

	$2 \text{ } \diagup \text{ } \diagdown$ $2 (2,2) + 2 (1)$		3, 6, 4
	$3 \text{ } \diagup \text{ } \diagdown$ $3 (2,2)$		3, 6, 6
	$2 \text{ } \diagup \text{ } \diagdown$ $2 (3,6,4) + 2 (2,2) + 2 (1)$		4, 12, 16, 8
	$2 \text{ } \diagup \text{ } \diagdown$ $2 (3,6,4) + (2) + (2,2) + (3,6,6)$		4, 12, 20, 14
	$4 \text{ } \diagup \text{ } \diagdown$ $4 (3,6,6)$		4, 12, 24, 24

Table 2: Construction of Bond-Sequences for Hexane Isomers


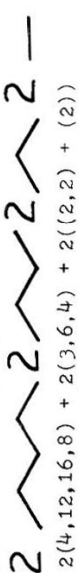

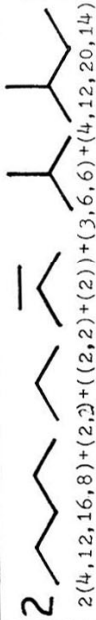
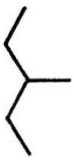
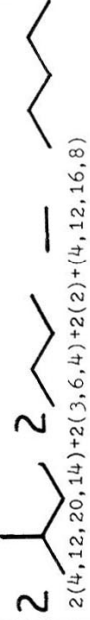
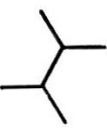
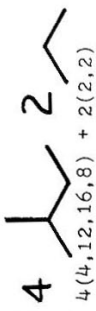

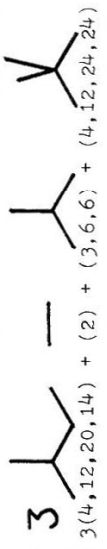
	 2(4,12,16,8) + 2(3,6,4) + 2((2,2) + (2))	5, 20, 40, 40, 16
	 2(4,12,16,8)+(2,2)+((2,2)+(2))+(3,6,6)+(4,12,20,14)	5, 20, 46, 58, 30
	 2(4,12,20,14)+2(3,6,4)+2(2)+(4,12,16,8)	5, 20, 48, 64, 36
	 4(4,12,16,8) + 2((2,2))	5, 20, 52, 80, 56
	 3(4,12,20,14) + (2) + (3,6,6) + (4,12,24,24)	5, 20, 54, 90, 66

Table 3: Bond-Sequences for Heptane Isomers

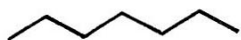
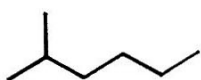
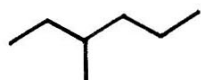
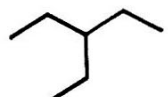
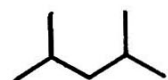
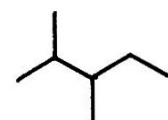
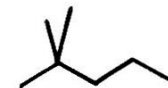

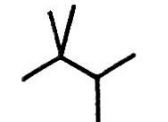
	6, 30, 80, 120, 96, 32
	6, 30, 88, 156, 152, 62
	6, 30, 92, 174, 184, 82
	6, 30, 96, 192, 216, 108
	6, 30, 96, 196, 232, 120
	6, 30, 100, 218, 280, 158
	6, 30, 100, 222, 288, 156
	6, 30, 104, 244, 336, 204
	6, 30, 108, 270, 420, 300

Table 4: Bond-Sequences for Octane Isomers

n-octane	7, 42, 140, 280, 336, 224, 64
2-methylheptane	7, 42, 150, 340, 476, 374, 126
3-methylheptane	7, 42, 156, 376, 568, 484, 176
4-methylheptane	7, 42, 158, 388, 600, 524, 196
2,5-dimethylhexane	7, 42, 160, 404, 652, 608, 248
3-ethylhexane	7, 42, 164, 424, 629, 652, 272
2,4-dimethylhexane	7, 42, 166, 444, 772, 782, 346
2,2-dimethylhexane	7, 42, 166, 452, 804, 810, 342
2,3-dimethylhexane	7, 42, 168, 460, 824, 856, 384
3,4-dimethylhexane	7, 42, 172, 488, 912, 1000, 480
2-methyl-3-ethylpentane	7, 42, 174, 500, 944, 1052, 532
3,3-dimethylhexane	7, 42, 174, 508, 976, 1088, 524
2,2,4-trimethylpentane	7, 42, 176, 524, 1056, 1272, 672
2,3,4-trimethylpentane	7, 42, 178, 536, 1096, 1352, 752
3-methyl-3-ethylpentane	7, 42, 180, 552, 1116, 1332, 720
2,2,3-trimethylpentane	7, 42, 182, 572, 1236, 1614, 930
2,3,3-trimethylpentane	7, 42, 184, 588, 1288, 1708, 1024
2,2,3,3-tetramethylbutane	7, 42, 192, 660, 1620, 2520, 1800

Some Regularities of Acyclic Codes

A glance at Table 1 - Table 4 immediately reveals several regularities of the proposed codes. First, and most significant, none of the codes so far reported appear more than once, but the sample of the structures considered is too small to make further generalizations. The first entry in each sequence indicates the number of terms in the sequence, and it is necessarily the same for all isomers since they have the same number of bonds. But we see also that the next entry, b_1 , the count of bonds in the collection of Ulam subgraphs is the same for all isomers; i.e., 6 for butanes, 12 for pentanes, 20 for hexanes, 30 for heptanes, 42 for octanes, 56 for nonanes and so on. The numbers can be recognized as given by $(n-1)(n-2)$ where n is the number of carbon atoms in the structure. Higher b_i numbers are not as transparent, but one can trace some regularity for b_2 when comparing different isomers and their skeletal branching. The number increases with the apparent degree of branching of the molecular graph. We will postpone discussion of b_2 until we consider cyclic graphs and will look closely at the b_i sequences for linear chains (i.e., normal alkanes). One can arrange the b_i values in a triangular form as follows:

n = 1				1								
n = 2			2		2							
n = 3			3		6		4					
n = 4		4		12		16		8				
n = 5		5		20		40		40	16			
n = 6	6		30		80		120		96	32		
n = 7	7		42		140		280		336		224	64

The regularity of the coefficients is readily deduced by examining the decomposition of a n -chain which always yields:

$2(n-1)\text{chain} + 2(n-2)\text{chain} + 2(n-3)\text{chain} + \dots + 2K_2$
with K_2 representing an edge. Therefore, except for the first term which equals n , the remaining coefficients are obtained by adding all previous sequences (term by term) and doubling the result.

One can obtain the same result by adding the preceding sequence to the sequence obtained from it by doubling terms, shifting one position to the right and appending 1 in the first position. For example, the last line in the triangle form is derived as a sum of:

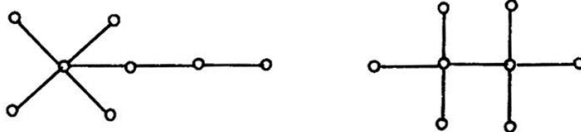
	6,	30,	80,	120,	96,	32	
+	1,	12,	60,	160,	240,	192,	64
<hr/>							
	7,	42,	140,	280,	336,	224,	64

In general, the b_i sequences appear sufficiently different that one is justified in further pursuit of their features. Since the coefficients increase rapidly, the probability of accidental coincidences among them is diminishing with the size of the graph. This may make it worthwhile to search for such coincidences in order to attempt to resolve the question of uniqueness. Alternatively, any occurrence of a coincidence might lead to some inherent structural features worth further investigation.

In view of the unlimited pool of graphs, even acyclic, it seems important to restrict attention to graphs of special interest and special properties first. Among these one should include isospectral graphs and graphs having the same path sequences as potential candidates for duplicate b_i sequences.

Isospectral Acyclic Graphs

The smallest connected isospectral graphs which are acyclic have eight points:²



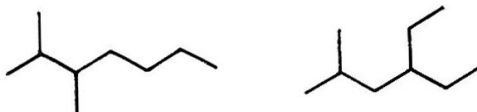
The corresponding bond sequences are respectively:

7, 42, 184, 596, 1532, 1776, 1008

and 7, 42, 192, 660, 1620, 2520, 1800 .

Clearly the present approach discriminates among (at least some) isospectral graphs. The above pair is of no direct chemical interest because the graph at left has valency greater than four, but it may be of interest in future extensions of graph theoretical considerations to inorganic chemistry.

In Table 5 we listed several pairs of isospectral graphs on nine points and corresponding to carbon skeletons. In some of these cases the corresponding bond sequences differ in the b_2 coefficient even though the corresponding graphs have a common partitioning of vertices. This is the case with:

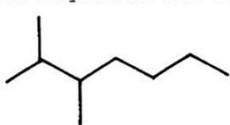


Hence, the b_i parameters appear to be quite sensitive on the details of the mode of branching and distribution of neighbors.

If b_i sequences are used for checking isomorphism (even though such application may produce inconclusive outcome; we have not yet accumulated sufficient evidence to guide one in such applications) one can proceed in stages by first deriving parameters b_0 for both

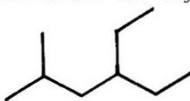
Table 5

Bond Sequences for Isospectral Trees Having Nine Vertices



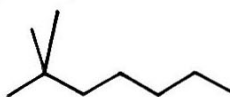
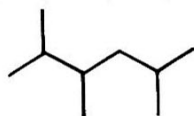
8, 56, 260, 846, 1904, 2788, 2356, 862

8, 56, 268, 906, 2120, 3268, 2892, 1236



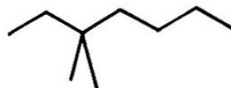
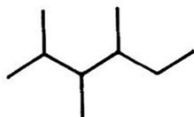
8, 56, 272, 952, 2364, 3930, 3884, 1708

8, 56, 256, 818, 1816, 2586, 2088, 720



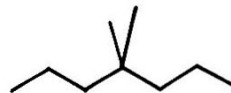
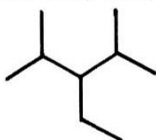
8, 56, 280, 1028, 2712, 4832, 5148, 2442

8, 56, 268, 922, 2216, 3470, 3132, 1218



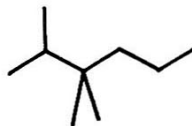
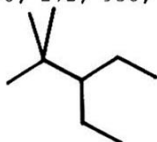
8, 56, 284, 1062, 2850, 5164, 5680, 2880

8, 56, 272, 956, 2352, 3488, 3536, 1440



8, 56, 288, 1108, 3096, 5880, 6696, 3456

8, 56, 284, 1074, 2812, 5394, 5896, 2840



graphs, then b_1 and so on. The advantage of such an approach is that one can interrupt the process (and save valuable effort in deriving higher b_i values) the first time one encounters different b_i values. It remains to be seen if such an isomorphism testing proves practical. It appears to satisfy the minimal conditions in that the procedure grows exponentially with the size of a graph; thus, the approach is not obviating the $n!$ difficulty characterizing the isomorphism problem.¹¹ This should be taken merely as a sign that the scheme may have merits and may have potential for unique characterization, but no such outcome is guaranteed. In practical terms it appears to us that an intensive search for a counterexample is the most efficient approach to upgrade present speculations to a conjecture -- effort that we intend to follow.

Isocodal structures

Enumeration of paths p_i of different length allows one to consider path sequences $p_0, p_1, p_2, \dots, p_k$. Path numbers p_0 and p_1 correspond to the count of vertices and edges and thus coincide with b_0 and b_1 , and the same numbers emerge in other constructions as the most obvious starting parameters. Paths p_2 represent two consecutive bonds and have been already suggested by Gordon and Scantlebury¹² as an index of molecular branching. On the other hand Platt anticipated their use in discussion of molecular (thermodynamical in particular) properties¹³ together with other higher p_i numbers. Wiener¹⁴ introduced p_3 as an important parameter for his additivities and discussion of isomeric variations. More recently p_2 and p_3 have been found to provide a frame for general discussion of trends in numerous molecular properties resulting in construction of the periodic table of Isomers.¹⁵ In another

direction of exploration of structure activity relationships it was demonstrated that sequences $p_0, p_1, p_2, \dots, p_k$ offer a basis for comparison of structures and subsequent quantification of the degree of structural resemblance¹⁶ as well as a means for pattern recognition (clustering of structures).¹⁷ Hence, interest in path numbers appears to be well justified despite the fact that it was found that some structures produce the same path counts. The smallest such isodocal pair are two nonane isomers: 2,3,4-trimethylhexane and 3-methyl-3-ethylhexane with the path numbers: 9, 8, 10, 6, 2



We find the following two bond-sequences for the above structures:

8, 56, 280, 1028, 2712, 4832, 5148, 2442, and

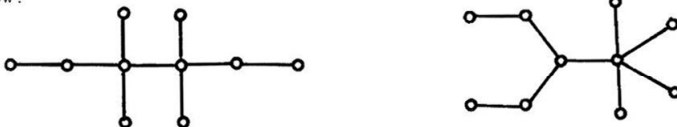
8, 56, 280, 1028, 2648, 4500, 4528, 2040

Observe the initial identical values for b_0, b_1, b_2 , and even b_3 .

Special applications

There are several special graphs of interest. These graphs exhibit greater structural similarity and, therefore they are more likely to offer a counterexample for a simple isomorphism test. However, the size of such graphs is relatively large, and the search for bond-sequences is recurrent and requires information on many graphs of small size. This makes such applications tedious unless an extensive catalogue becomes available or the task can be delegated to a computer. None of the prerequisites is currently available. Hence, more interesting applications have to wait for further development

of the proposed scheme. Nevertheless, we can illustrate one such special application: we will examine graphs having the same distance sequence $(d(v_1), d(v_2), d(v_3), \dots, d(v_n))$. Here v_i is i -th vertex of a graph and $d(v_i)$ is the sum of all paths between vertex i and the remaining vertices. The numbers $d(v_i)$ measure the "degree" of centrality of a vertex, vertices closer to the center of the graph having smaller sum $d(v_i)$. Some properties of $d(v_i)$ have been discussed in ref. 3b. Recently Seybold¹⁸ used $d(v_i)$ as an index of "connectedness" of atom i to the remainder of the carbon framework in study of substituent effect of aromatic carcinogens. Among all trees with 10 and less vertices there are only two graphs with the same distance sequence and they are shown below:



The result has been reported by Slater¹⁹ and independently verified by Miller.²⁰ The distance sequence is: (15, 15, 21, 21, 23, 23, 23, 23, 29, 29) and the entries are ordered in an increasing sequence. For the two graphs we obtain the following bond sequences respectively:

9, 72, 444, 2160, 8136, 22760, 43928, 42600, 13752

9, 72, 448, 2160, 8148, 23244, 44440, 50844, 27216

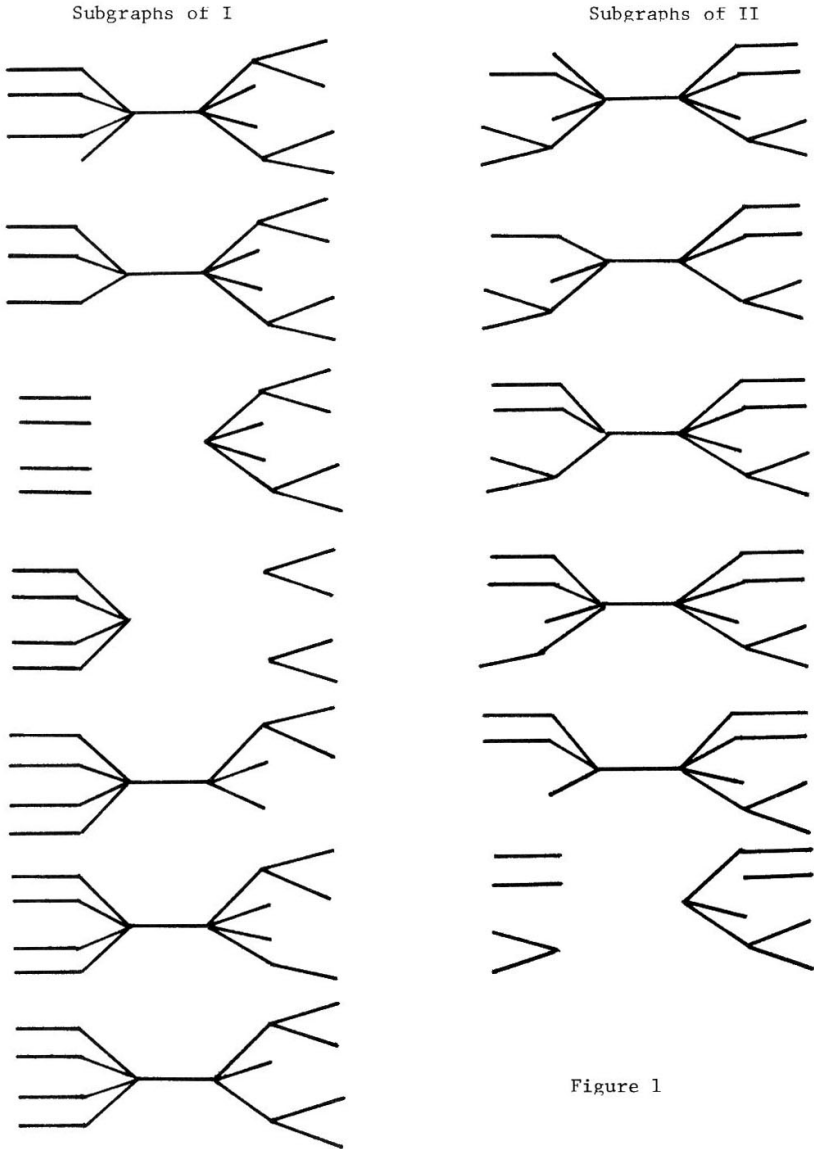
Clearly the discriminatory power of the proposed sequences is sufficient to resolve the two nonisomorphic graphs having the same distance sequence. A more critical test is provided by the graphs¹⁹



which have not only the same distance sequence but also common distance degree sequences for the collection of vertices. Thus, the graphs represent a counterexample to the conjecture that the collection of path numbers $(p_1, p_2, p_3, \dots, p_k)_i$ ($i = 1, 2, \dots, n$) characterizes graphs uniquely.²¹

In order to indicate a rather rare instance of an occurrence of a counterexample, we may mention that the conjecture has been proposed after verifying its validity on all acyclic graphs (with maximal valency of four) having 10 and less vertices; and, subsequently, Shelly and Trulson²² using program CASE (Computer Assisted Structure Elucidation) verified the conjecture on all C_{11} isomers (159 structures); all C_{12} isomers (355 structures); all C_{13} isomers (802 structures) and finally all C_{14} structures (1858 isomers). Thus, some 3000 graphs have been screened the smallest counterexample having 18 vertices and valency of five (which makes it irrelevant for carbon atom chemistry). Nevertheless, the existence of counterexamples is significant, and the graphs on 18 vertices represent a new test for validity of any subsequent isomorphism tests.

Because of the size of the graphs the answer is not readily available. Both graphs have some symmetry so instead of 18 Ulam's subgraphs for each we can consider fewer (seven and six respectively as illustrated in the Fig. 1). However, the examination of Ulam subgraphs will only yield b_1 , which will be the same since the structures are isomers. Determination of b_2 requires the construction of corresponding subgraphs for each of the thirteen graphs of Fig. 1. Although each such subgraphs will necessarily appear at least twice (because each is derived by erasure of two vertices i, j and the relative order is immaterial)²³ the Ulam subgraphs have little symmetry. Consequently the number of subgraphs to be considered proliferates.



One sees that the $n!$ character of the problem will eventually make applications to large graphs prohibitive. However, in checking on isomorphism of graphs I and II we can carry the search for b_i numbers in stages. We have constructed all subgraphs required for the count of b_2 (there being 42 such subgraphs for I occurring with weights 1, 2, 3 or 4 and there being 61 subgraphs for II with weights 1, 2 or 3). By counting bonds in corresponding graphs we find the b_2 coefficients different. The two sequences start as follows:

graph I: 17, 272, 3312,

graph II: 17, 272, 3656,

Although a count of bonds b_i is an error prone assignment there are some checks which can reduce the number of oversights. These include the observation that the result is an even number, and that the number of contributions equals the number of vertices of the graph considered.

The above demonstration that even graphs having equal distance degree sequences, besides already considered graphs having the same distance sequences, having same path numbers, and having same characteristic polynomial have different bond-sequences appears sufficiently encouraging to tempt us to propose, for acyclic graphs only, the following Conjecture:

Conjecture: Acyclic graphs which are nonisomorphic have different Bond-Sequences $(b_0, b_1, b_2, \dots, b_k)$, where b_i is the count of bonds (edges) derived at i -th successive erasure of vertices of the graph.

The search for counterexamples is, of course, open. Providing none is found the next important step is to examine the validity or limitations of the Conjecture to a more general class of polycyclic graphs.

Concluding Remarks

Bond-sequences appear to hold promise as a characterization of graphs, and as conjectured here for acyclic graphs may provide a unique name for such structures which are devoid of vertex labels. This is an important goal with great potential in chemical documentation for instance where so far no scheme has been proposed in which some necessity for labels did not occur. Before further accumulation of experience with the proposed characterization we should indicate a modification that may be also of interest.

As described here we count at each stage of the dissection process the number of bonds in all the fragments present, but when disjoint bonds (subgraphs K_2) appear they are eliminated from further considerations. This is in part consistent with the desire for reconstruction of graphs from such sequences (which may or may not be possible, certainly the problem being more complicated than the reconstruction of graph from Ulam's subgraphs!) since K_2 is not reconstructable. However, one may consider sequences of subgraphs $G^{(i)}$, $G^{(i,j)}$, $G^{(i,j,k)}$, etc in which one vertex at a time is erased (i); two vertices are erased (i,j); three vertices are erased (i,j,k) etc. This will produce different sequences from those here reported, with the property that all subgraphs (at each stage of the dissection process) would carry the same weight (as reflected by the number of components they generate). We have mentioned this alternative not as a replacement of the proposed scheme but merely to indicate that not all possibilities have yet been explored and exhausted.

It seems that the present work, as is quite typical of many graph

theoretical studies, while solving one problem at the same time points to several others yet to be considered. It is useful therefore to conclude the present exposition with a list of pending problems to be resolved. Besides considering the alternative count of bonds in each stage of the dissection this includes the question of reconstruction of graphs from the bond-sequences. Because, as is known, Ulam's conjecture is true in the case of acyclic graphs at least this can be viewed as the necessary condition for our reconstruction being satisfied.

Perhaps a more practical problem is that of relating numbers b_i among similar structures, relating b_i with similar values in sub-graphs and a search for a possible connection of b_i values of a graph and some of its components. If this can be resolved one could anticipate construction of the bond-sequences of larger structures without necessarily requiring an extensive cataloguing of all preceding structures. Another important aspect of unique codes is their use for ordering of structures and construction of graphs of desired properties. All these topics will benefit from a development of a computer program for construction of b_i even if it remains to be essentially an intractable task, i.e., even if it can be demonstrated that there cannot be a polynomial in time algorithm to accomplish the task. Much of the Chemistry is contained in structures having a dozen and two dozen atoms and if such systems can be considered within practical computer times the NP-character of the problem, though of fundamental interest, becomes hardly relevant for chemical applications.

Acknowledgment: This work was supported in part by the Office of Director, Ames Laboratory (Operated for the U. S. Department of Energy by Iowa State University under contract no, W-7405-ENG-82).

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