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PAIRS OF NON-ISOMORPHIC GRAPHS HAVING THE SAME PATH DEGREE SEQUENCE

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Abstract

The concept of the Path Degree Sequence for a graph is important because of its application in describing atomic environments and in various classification schemes for molecules. In general it provides a great deal of information and in particular provides more information than that yielded by the valence class (degree partition class) or even than that of the "shells of neighbors" system (Distance Degree Sequence) for a molecule. Thus, it is not surprising that it was hoped that the Path Degree Sequence would characterize molecules. We show here that, in general, this is not the case by exhibiting counterexamples to this conjecture for a variety of classes of graphs. In spite of this we support the opinion that the concept is still very useful. We close by noting that it is an open problem to find a pair of non-isomorphic regular graphs having the same Path Degree Sequence.

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1. Introduction

In a recent article M. Randić [1] discussed in some detail the uses of the enumeration of paths and neighbors in molecular graphs. Included in this study was an extensive survey of the work done and in progress by other researchers of this area. Also considered was the open problem of characterizing molecular graphs through the use of Path Degree Sequences. With respect to this we will show that a conjecture proposed in [1; p. 17] is not valid. Nevertheless, the importance of these invariants is not diminished as evidenced by the work cited in [1] as well as their role in other applications [2], [3], and [4]. In brief, Path Degree Sequences do not provide a "code" as defined in [4], not even for trees. However, while they fail in general to uniquely determine a graph up to isomorphism, they can be extremely useful in demonstrating the non-isomorphism of graphs. Furthermore, Path Degree Sequences do distinguish between graphs of certain specified types up to a large enough number of points so as to be of practical application. See for example our discussion in Section 3.

For our formulation of the problem and commentary we shall use the following graph theoretic language and notation.

Let G denote a finite connected graph with point set $\{v_1, v_2, \ldots, v_{|G|}\}$ and d_{ij} the number of points in G that are at distance j from v_i. Then, the sequence $(d_{i0}, d_{i1}, d_{i2}, \ldots, d_{ij}, \ldots)$ is called the distance degree sequence of v_i in G. The $|G|$-tuple of distance degree sequences of the points of G arranged in lexicographic order is the Distance Degree Sequence of G and is denoted DDS(G). Similarly, we define the path degree sequence of v_i in G as the sequence $(p_{i0}, p_{i1}, p_{i2}, \ldots, p_{ij}, \ldots)$ where p_{ij} is the number of paths in G having initial point v_i and length j. Here the $|G|$-tuple of path degree sequences of points of G arranged lexicographically is called the Path Degree Sequence of G and is denoted PDS(G).

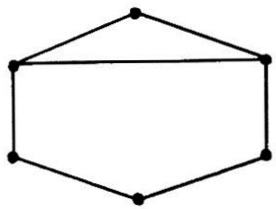
These concepts are illustrated via the graph G shown in FIGURE 1.1, where we have

$$DDS(G) = ((1,2,2,1,0,\dots)^2,(1,2,3,0,\dots)^2,(1,3,2,0,\dots)^2)$$

and

$$PDS(G) = ((1,2,2,4,6,2,0,\dots),(1,2,3,4,4,3,0,\dots)^2,$$
$$(1,2,4,4,4,4,0,\dots),(1,3,4,3,3,2,0,\dots)^2).$$

Note that the exponent notation is used to indicate repetitions of sequences.



G

FIGURE 1.1.

A considerable amount of information about a graph is contained in these sequences (see e.g., [1] and [2]). Here we shall only discuss that which is relevant to the present context. In particular we propose some problems which are natural to consider. Note that, when G is thought of as a molecular graph, PDS(G) is precisely the lexicographically ordered list of atomic codes [1] for the points, i.e., atoms of G.

2. The conjecture

It was noted in [1; p. 13] that "between pairs of atoms in acyclic structures there is a unique path so that the number of paths of a given length corresponds to the number of neighbors at a given distance". For our purposes we formulate this as follows.

(2.1) For a connected graph G, DDS(G) = PDS(G) if and only if G is a tree.

Proof. If G is a tree, then $d_{ij} = p_{ij}$ for all i and j, because there is exactly one path from v_i to each of the d_{ij} points which are at distance j from v_i. Thus, DDS(G) = PDS(G).

Clearly, for any graph $d_{ij} \leq p_{ij}$ for all i and j.

If G is not a tree, then G contains a cycle C of length g. Let v_i be any point of G which lies on C and let x be a second point on C such that x is adjacent to v_i. Since $d(v_i,x) = 1$, x is not among the points at distance g - 1 from v_i. However, there is a path of length g - 1 from v_i to x. Thus, $p_{ig-1} \geq d_{ig-1} + 1$ and DDS(G) ≠ PDS(G). □

In [1; p. 17] the following was conjectured.

(2.2) Conjecture (Randić). Two graphs G_1 and G_2 are isomorphic if and only if $PDS(G_1) = PDS(G_2)$.

This conjecture is not valid as was shown in [5], where there is exhibited an infinite class of pairs of non-isomorphic trees having the property that the two members of each pair have the same Path Degree Sequence. In FIGURE 2.1 we show the smallest order pair of this class.

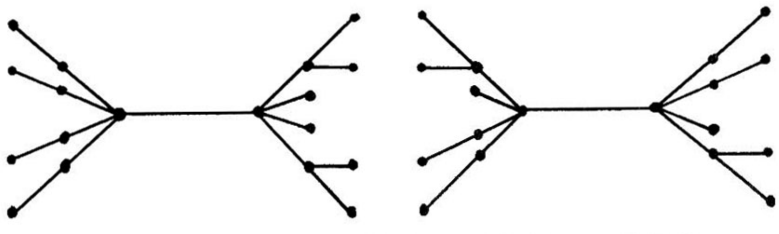


FIGURE 2.1. A pair of non-isomorphic trees with the same Path Degree Sequence.

Using this example it is easy to construct pairs of non-isomorphic non-tree graphs having a variety of properties and which invalidate the conjecture. As an illustration, consider the two graphs in FIGURE 2.2. These are non-isomorphic, each has a cycle of length g, and they have the same Path Degree Sequence. (The girth of a graph is defined to be the length of its smallest cycle.)

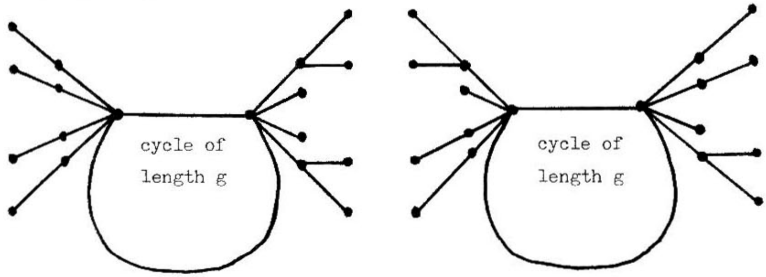


FIGURE 2.2. A pair of non-isomorphic graphs of girth g with the same Path Degree Sequence.

A second example is that of the two graphs in FIGURE 2.3. These graphs are non-isomorphic, have the same cycle rank β and the same Path Degree Sequence, where β equals the number of lines less the number of points plus the number of components of a graph. Note that β is also interpreted as the number of independent cycles of a graph (see [6; pp. 37-39]).

3. Some problems

As noted in Section 2, a tree is not, in general, characterized by its Path (= Distance) Degree Sequence. The least order for which there exists a pair of non-isomorphic trees with the same Path Degree Sequence has been shown to be ≥ 15 for acyclic alkanes, i.e., trees with no point of degree > 4 (see [1; p. 17]) and ≤ 18 for trees without point degree restrictions (see FIGURE 2.1).

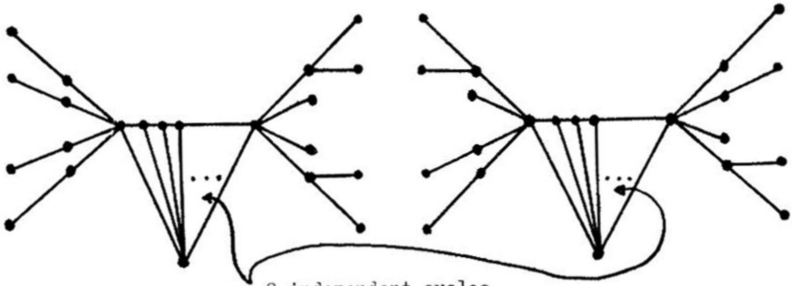


FIGURE 2.3. A pair of non-isomorphic graphs with β independent cycles and the same Path Degree Sequence.

With respect to non-tree graphs, it is asserted in [1; p.17] that no pair of graphs on ≤ 11 points have the same Path Degree Sequence. The pair of graphs in FIGURE 2.2 shows that $16 + g$ is an upper bound for the least order realizable by a pair of non-isomorphic graphs of girth g with the same Path Degree Sequence. FIGURE 2.3 shows that $18 + \beta$ is an upper bound for the least order possible for a pair of non-isomorphic graphs having β independent cycles and the same Path Degree Sequence. However, these bounds can be improved. For example, if the β independent cycle subgraphs of FIGURE 2.3 are replaced by a smaller order and appropriately symmetric graph having β independent cycles, then the bound $18 + \beta$ can be lowered. Specifically, if one uses the complete n-point graph K_n as shown in FIGURE 3.1 the bound on the number of points is improved to $16 + n$ for the cases where $\beta = \binom{n}{2} - n + 1 = \binom{n-1}{2}$. For example, when $\beta = \binom{9}{2} = 36$, the graphs of FIGURE 3.1 have only 26 points and this is considerably smaller than the corresponding 54 point 36 independent cyles graphs of FIGURE 2.3.

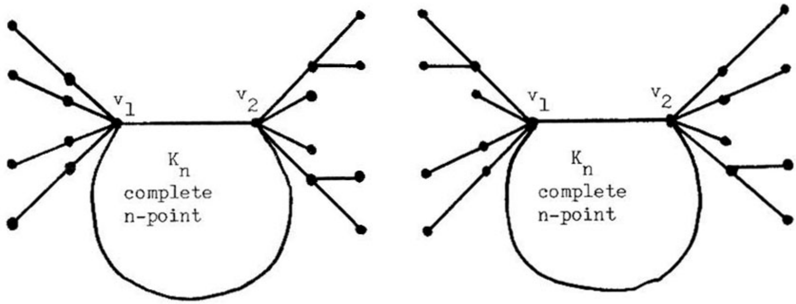


FIGURE 3.1. A pair of non-isomorphic graphs on 16 + n points with $\binom{n-1}{2}$ independent cycles and the same Path Degree Sequence.

The example just cited can be developed to yield the following result which gives a bound on the order for all values of β.

(3.1) Let $p(\beta)$ denote the smallest order for which there exists at least two non-isomorphic connected graphs having β independent cycles and the same Path Degree Sequence. Then,

$$p(\beta) \leq 16 + \left\lceil \frac{3 + \sqrt{1 + 8\beta}}{2} \right\rceil \qquad \text{for} \quad \beta = 0,1,2,\ldots$$

where $\lceil s \rceil$ denotes the least integer greater than or equal to s.

Proof. The asserted upper bound is obtained by exhibiting graphs with the specified number of independent cycles and order.

If $\beta = 0$, the trees of FIGURE 2.1 yield the upper bound 18; if $\beta = 1$, the graphs of FIGURE 2.2 with a cycle of length $g = 3$, yield the upper bound 19. Equivalently, these are the graphs of FIGURE 3.1 with $n = 2$ and $n = 3$ respectively.

If $\beta \geq 2$, we note that the graphs of FIGURE 3.1 have order 16 + n ($n = 4,5,\ldots$) and β independent cycles with

$$\beta = \binom{n}{2} - n + 1 = \binom{n-1}{2} = 3,6,10,\ldots \quad .$$

For values of β that lie between the values $\binom{n-2}{2}$ and $\binom{n-1}{2}$, i.e., the values that correspond to K_{n-1} and K_n, we modify the graphs of FIGURE 3.1 by deleting lines from their K_n subgraphs. If this is done as will be indicated, the Path Degree Sequence will be the same for these two graphs and the upper bound produced will be 16 + n for the values of β which are strictly between $\beta = \binom{n-2}{2}$ and $\beta = \binom{n-1}{2}$. The procedure for deleting lines from the graphs of FIGURE 3.1 is as follows.

(1) To reduce β by one, delete the line (v_1,v_2) from the K_n subgraphs, and

(2) to reduce β by two, delete any two lines of the K_n subgraph which are symmetrically located with respect to the line (v_1,v_2).

In general, to reduce β by an even number, apply (2) the appropriate number of times; to reduce β by an odd number, apply (1) and then apply (2) the appropriate number of times.

The gap between $\beta = \binom{n-2}{2}$ and $\beta = \binom{n-1}{2}$ is such that there are always enough lines in the K_n subgraph to lower β to the value $\binom{n-2}{2} + 1$. Specifically, the maximum number of lines that has to be deleted from the K_n subgraph is $\binom{n-1}{2} - \binom{n-2}{2} - 1 = n - 3$ and K_n has $\binom{n}{2}$ lines. Therefore, if we solve $\beta = \binom{n-1}{2}$ for n we will have the order of K_n which will give us β independent cycles. This equation is equivalent to $0 = n^2 - 3n + (2 - 2\beta)$ and taking into account that n must be an integer greater than or equal to the positive root of this quadratic, we have

$$n = \left\lceil \frac{3 + \sqrt{1 + 8\beta}}{2} \right\rceil$$

Finally, note that although this formula is derived with $\beta \geq 2$ in mind it yields the values n = 2 and 3 for $\beta = 0$ and 1 respectively.

Thus, it can be used for the two cases considered at the beginning of the proof, where it can be seen that the graphs are of the same type as the general case. □

PROBLEM. Prove or disprove the following statements (1) and (2). The smallest order for which there exists at least two non-isomorphic connected graphs having the same Path Degree Sequence is

(1) $16 + g$, if the two graphs are also required to have girth g, and

(2) $16 + \left\lceil \frac{3 + \sqrt{1 + 8\beta}}{2} \right\rceil$, if the two graphs are also required to have β independent cycles.

We conclude by turning our attention to r-regular graphs, i.e., graphs in which each point has exactly r points adjacent to it. We first make two observations with respect to Distance Degree Sequences.

First, the smallest order for which there exists a pair of non-isomorphic graphs having the same Distance Degree Sequence is exemplified by the pair of five point graphs shown in FIGURE 3.2.

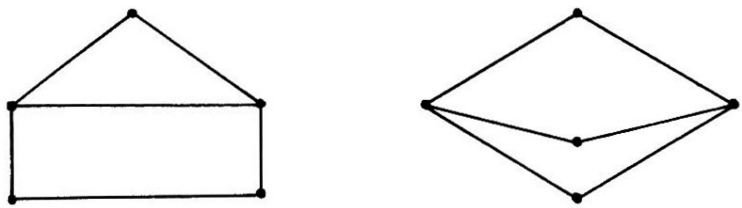


FIGURE 3.2. The smallest order pair of non-isomorphic graphs with the same Distance Degree Sequence.

Second, if one asks for the smallest order for which the Distance Degree Sequence fails to distinguish between r-regular graphs we respond with the following statement.

(3.2) Let $R(r)$ denote the smallest order for which there exists at least two non-isomorphic connected r-regular graphs on $R(r)$ points such that each has the same Distance Degree Sequence. Then,

$$R(r) = \begin{cases} \text{does not exist} & \text{if } r = 0,1, \text{ or } 2 \\ r + 3 & \text{if } r = 3,4,5,\ldots \end{cases}$$

Proof. If $r = 0,1$, or 2, the only connected r-regular graphs are respectively K_1, K_2, and the n-cycles. Thus, for these values of r, there are no pairs of non-isomorphic r-regular graphs having the same Distance Degree Sequence.

For $r \geq 3$, we note that K_{r+1} is the unique smallest order r-regular graph. Thus, $R(r) \geq r + 2$.

If G is an r-regular graph on $r + 2$ points, then $\overline{G}$, the complement of G, is an $(r + 2 - 1 - r)$-regular graph, i.e., a 1-regular graph, on $r + 2$ points. Since the only 1-regular graphs are those that are the union of K_2's, we find that $r + 2$ must be even and $\overline{G}$ is unique. The latter implies $R(r) \geq r + 3$.

If G is an r-regular graph on $r + 3$ points, then $\overline{G}$ is a 2-regular graph on $r + 3$ points. For $r + 3 \geq 6$, there are at least two non-isomorphic 2-regular graphs on $r + 3$ points, namely, the $(r + 3)$-cycle C_{r+3} and the graph consisting of the r-cycle C_r and the 3-cycle K_3. Since the diameters of these graphs are $\left[\frac{r+3}{2}\right]$ and ∞ respectively, their complements (the graphs we seek) have diameter 2 and are r-regular graphs on $r + 3$ points. Since every point of every such r-regular graph has its distance degree sequence equal to $(1,r,2,0,\ldots)$, the complements of C_{r+3} and $C_r \cup K_3$ have the same Distance Degree Sequence. Therefore, $R(r) = r + 3$ for $r = 3,4,5,\ldots$. $\square$

It is clear that Path Degree Sequences distinguish among r-regular graphs to a much greater extent than do Distance Degree Sequences. As we have noted in the first part of this section, there does not exist a pair of non-isomorphic graphs with the same Path Degree Sequence on less than 12 points. It also follows from the proof of (3.2) that the least order for which such an r-regular pair of graphs can exist is at least $r + 3$ for $r \geq 3$ and that none exist if $r = 0,1,$ or 2. Our investigation has thus far failed to produce even one pair of non-isomorphic r-regular graphs having the same Path Degree Sequence.

PROBLEM. For $r \geq 3$, does there exist a pair of non-isomorphic connected r-regular graphs having the same Path Degree Sequence? If the answer is yes, what is the smallest order $p(r)$ realizable by such a pair?

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