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Graphs with the Same Detour Matrix

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The detour matrix (***DD***) of a graph has for its (i,j) entry the length of the longest path between vertices i and j. The sum of all entries above the main diagonal gives the detour index dd. Distinct graphs that have the same detour index have been reported in the literature. We examined such graphs and others that we have found and report on some of their regularities. We noticed that many graphs have not only the same detour index but also the same detour matrix. We considered in particular graphs for which the elements of the detour matrix are maximal. Such graphs are called *saturated* graphs. The detour matrix of a saturated graph is the same as that of the complete graph having the same number or vertices.

INTRODUCTION

The detour matrix was introduced in graph theory some time ago by F. Harary[1] for describing the connectivity in directed graphs. The detour matrix, in contrast to the distance matrix that records the length of the shortest path between vertices, records the length of the longest distance between each pair of vertices. The detour matrix has recently received some attention in the chemical literature.[2–6] The revival of interest in the detour matrix reflects recent efforts to construct novel topological indices obtained by extracting invariants from new graph matrices.[7–14] Among the most popular graph invariants (for non-negative matrices which are of particular interest in chemical applications) are the average matrix element[15–23] and the

leading eigenvalue of the matrix.[10,12,24–26] The average matrix element is equivalent to the sum of matrix elements above the main diagonal; the two differ only in the normalization factor. In the case of the graph distance matrix the sum of the matrix elements above the diagonal gives the well-known Wiener number (*W*). This graph invariant was introduced in structure-property studies in 1947 by H. Wiener.[15] The detour matrix (for which we will use symbol (***DD***) is yet another matrix associated with graphs the elements of which are given by graph theoretical distances between the vertices, though now one is searching for the longest, rather then the shortest paths. Amić and Trinajstić[2] were first to consider the detour index defined as the sum of matrix elements above the main diagonal of the detour matrix, for which we will use symbol *dd*.

Use of the detour index in quantitative structure-activity relationship (QSAR) studies has been investigated by Lukovits.[5] In correlation with several other indices, he tested this index on the correlation of the boiling points of alkanes and cycloalkanes. A multiple regression analysis has shown that a combination of *W* and *dd* may give correlations for selected molecular properties which are size-dependent (as boiling points of alkanes). However, if one restricts attention to molecules of the same size (*e.g.*, isomers of octane and cyclic alkanes having eight carbon atoms) the index *dd* and its combinations with the other indices considered to not show such a good correlation. Hence, it yet remains to be seen if the detour index will become useful molecular descriptors of importance in QSAR.

The detour index certainly carries some interesting structural information for cyclic compounds. For acyclic structures the distance matrix and the detour matrix are the same and yield the same index, since there is only a single possible path connecting any pair of vertices. The construction of the distance matrix (from which the Wiener index follows) particularly for larger graphs is not trivial.[27–33] Construction of the detour matrix (from which the detour index *w* follows) is even more involved. According to Harary (Ref. 1, p. 203);

»There is no efficient method for finding the entries of the detour matrix. This problem is closely related to several other long-standing algorithmic questions of graph theory, such as finding spanning cycles and solving salesman problems«.[1]

Lukovits outlined a procedure for obtaining *dd* by using cut points,[15] while Nikolić and Trinajstić[34] outlined an algorithm for construction of the detour matrix based on screening spanning trees of a cyclic graph. Both these algorithms are consistent with the assertion that calculation of *dd* is a

[1] » ... The traveling salesman problem asks for an algorithm for finding a walk in a network whereby the salesman can visit each point and return to the starting point while traversing arcs with the minimal cost«.

NP-complete problem.[35] Our initial interest was on the problem of construction of graphs which have the same detour index. Finding such graphs and their properties may point to the limitations of this particular index.

GRAPHS WITH THE SAME TOPOLOGICAL INDEX

As is well known, topological indices show degeneracy, that is, two or more non-isomorphic graphs may have identical numerical values for an index. Sometimes this happens already for small graphs, sometimes for graphs of intermediate size. It is of interest for any graph invariant to find the size of the smallest graphs that show degeneracy. This indicates the limitations of the particular index (invariant descriptor) to differentiate structural variations among similar compounds. In Table I we list for a number of topological indices the size of the smallest graph for which the degeneracy occurs. The size of the graphs is given by n, the number of vertices. The last column in Table gives N, the total number of trees having n vertices. As we see the discrimination power of the Wiener index,[15] the Hosoya index,[36] and the connectivity index,[37] all of them being widely used in QSAR, is rather low. This, as is known, does not affect their performance in QSAR, because similar structures (that have overlapping topological indices) as a rule have also similar properties.[38,39]

The Balaban index[40,41] was one of the earlier indices which has shown greater discrimination power. It was followed by the molecular *ID* number,[16,42] and in particular the prime *ID* numbers[17] (the number in which the relative weights of different bonds were weighted with different prime numbers in order to maximize the numerical diversity of the bond contributions). An index *EA* (derived from an extended adjacency matrix) was proposed that shows high discrimination.[43] It was tested on all trees with $n = 16$ or less and no duplicate trees have been found. However, when tested against cyclic graphs with multiple bonds (which is a more stringent test to which many other indices were not tested), some duplicates have been de-

TABLE I

The discrimination power of various topological indices: n the largest tree for which no duplicates occur; N the total number of trees

Topological Index	Symbol	n	N
Connectivity index	χ	7	22
Balaban index	J	11	309
Identification number	ID	14	3,324
Prime number *ID*	P_{ID}	19	251,731
Extended adjacency index	$EAID$	22	3,807,434

tected. Recently, a new index (*EID*) was designed that surpassed both *EA* and prime-number *ID*. This index, derived from a modification of the extended adjacency matrix is a somewhat convoluted manner, was tested for all trees with $n = 22$ and has not as yet showed degeneracy.[44]

Simple indices, including the Wiener index, the Hosoya index, and the connectivity index, show low resolution, give good correlations and have a direct structural interpretation. More involved indices, like Balaban's *J*, molecular *ID* number, and in particular the latest index of Hu and Xu,[43] show very high resolution but have more convoluted structural interpretation. Is it possible to have a relatively *simple* index that can show an *impressive* discrimination power? Search for indices of high resolution and simple structural interpretation will continue. The novel branching index[25,26] based on the leading eigenvalue of paths may become one of the desired indices of this new class of indices that show higher resolution power and yet maintain relatively simple interpretation.

GRAPHS WITH THE SAME DETOUR INDEX

A number of graphs having the same detour index were reported by Amić and Trinajstić,[2] and by Lukovits.[5] Those reported by Amić and Trinajstić are illustrated in Figure 1 and Figure 2. The graphs of Figure 1 have the same detour index but different detour matrices, while those of Figure 2 have the same detour index because they also have identical detour matrices (assuming that the labeling of the vertices in the two graphs are preserved).

Let us examine the cases illustrated in Figure 1. The smallest graphs having the same detour index have five vertices. As we see from Figure 1 there are two such pairs: (G_1, G_2) and (G_3, G_4). The first pair corresponds to the molecular graphs of ethylcyclopropane and dimethylcyclopropane. The corresponding detour matrices are, respectively;

$$\boldsymbol{DD}_1 = \begin{pmatrix} 0 & 1 & 2 & 4 & 4 \\ & 0 & 1 & 3 & 3 \\ & & 0 & 2 & 2 \\ & & & 0 & 2 \\ & & & & 0 \end{pmatrix} \qquad \boldsymbol{DD}_2 = \begin{pmatrix} 0 & 1 & 3 & 3 & 4 \\ & 0 & 2 & 2 & 3 \\ & & 0 & 2 & 3 \\ & & & 0 & 1 \\ & & & & 0 \end{pmatrix}.$$

Because the detour matrix is symmetrical we have shown only the elements above the main diagonal. The detour index *dd*, given by the sum of these elements is in both cases $dd = 24$. The partition of w by adding the contributions of the atoms separated by one bond, then the contributions of

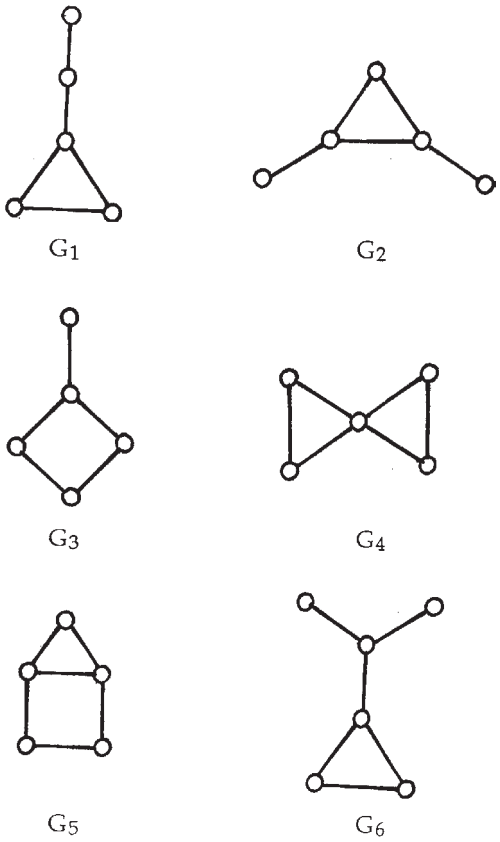


Figure 1. Three pairs of smaller graphs having the same detour index *dd*.

atoms separated by two bonds, then those separated by three bonds, and so on, gives:

ethylcyclopropane $dd = 8 + 12 + 4 = 24$

dimethylcyclopropane $dd = 8 + 8 + 8 = 24$

The other pair of pentanes whose graphs have the same w are 1-methylcyclobutane and spiropentane (G_3 and G_4, Figure 1). Their detour matrices are:

$$\boldsymbol{DD}_3 = \begin{pmatrix} 0 & 1 & 4 & 4 & 3 \\ & 0 & 3 & 3 & 2 \\ & & 0 & 2 & 3 \\ & & & 0 & 3 \\ & & & & 0 \end{pmatrix} \qquad \boldsymbol{DD}_4 = \begin{pmatrix} 0 & 2 & 2 & 2 & 2 \\ & 0 & 2 & 4 & 4 \\ & & 0 & 4 & 4 \\ & & & 0 & 2 \\ & & & & 0 \end{pmatrix}$$

with the partitions:

1-methylcyclobutane $dd = 13 + 12 + 3 = 28$

spiropentane $dd = 12 + 16 = 28$

Graphs G_5 and G_6 have the same detour index $dd = 37$ but are of different size. There are additional such examples. Such pairs are of lesser interest since the graphs can be easily differentiated by their size. Both G_5 and G_6 have the same number of edges, but there are cases of graphs having the same detour index which have neither the same number of edges nor the same number of vertices. One such example is the following set of graphs with $dd = 40$:

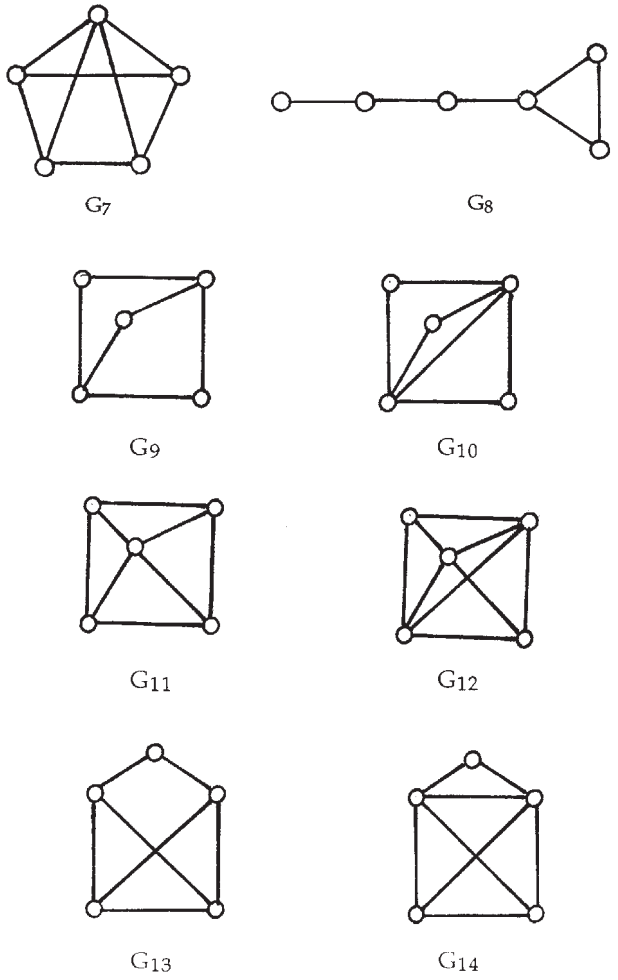


Figure 2. Three pairs of smaller graphs having the same detour matrix ***DD***.

In Figure 2 we show graphs which have not only the same detour index but also the identical detour matrix (assuming that the labeling of vertices between the two graphs is suitably selected). Amić and Trinajstić apparently overlooked or choose not to pay attention to this fact. The occurrence of identical matrices for non-isomorphic graphs represents a novel and interesting situation not previously encountered for other graph matrices. We will examine more closely this interesting novelty in a later section of this report. As one can see upon inspection of Figure 2 the graphs having the same detour matrix are closely related. They have the same connectivity, except for the presence of a single additional edge in one of the two graphs. We may refer to graphs G_{10} and G_{14} (and graphs that can be obtained from these graphs by introducing additional edges) as *replete* graphs, because introduction of additional edges do not generate different detour matrix.

We now proceed to consider the following questions;

(1) What structural factors introduce the degeneracy of the detour matrix?

(2) How can one construct graphs showing identical detour index?

REGULARITIES OF THE DETOUR INDEX

We have examined additional graphs in order to find the structural factors causing the graphs to have the same detour index. The smallest pair of polycyclic graphs having the same detour index (but distinct detour matrix) and not having pending bonds are illustrated in Figure 3. The correspond-

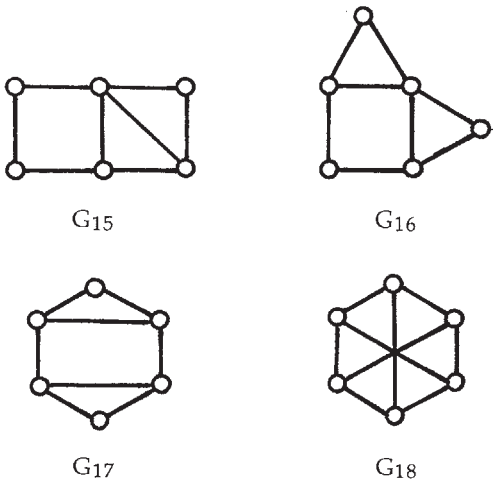


Figure 3. The smallest polycyclic graphs having no pending bonds and having the same detour matrix.

ing detour indices are 67 and 69 respectively. The first pair of graphs has the same number of vertices and the same number of edges, while the second pair has the same number of vertices but different number of edges.

Several regularities for the detour index *dd* can be observed from the reported smaller graphs having the same detour index, some of which are shown in Figures 1–3. Often by adding an edge to a graph the index *dd* increases by one, particularly when the added edge is a diagonal of a four member cycle. In Figure 4 we selected few graphs from the paper of Lukovits which have identical detour index and show a similar bonding pattern.

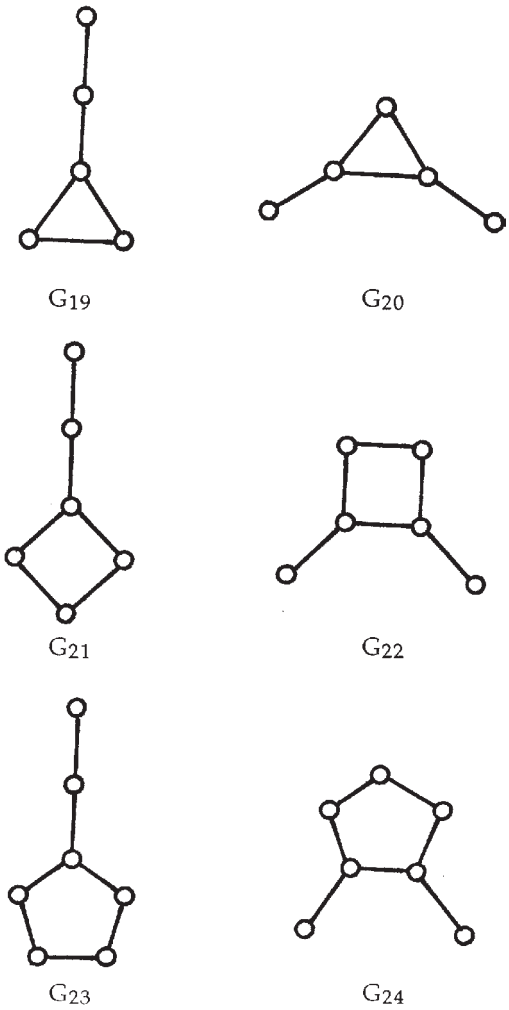


Figure 4. Structurally related graphs having the same detour index.

One may anticipate that graphs obtained by further enlarging the ring will also have the same detour index. We verified that this is the case on few additional examples. Is there a general route to find graphs having the same detour index, beside a brute-force search for such graphs?

CONSTRUCTION OF GRAPHS WITH THE SAME DETOUR INDEX

We start this section by exhibiting the detour matrices for the two graphs in the center of Figure 4, both of which have detour index 45. For each detour matrix we also form the row sums.

$$\boldsymbol{DD}_{19} = \begin{array}{c} \\ \begin{pmatrix} 0 & 1 & 2 & 5 & 4 & 5 \\ 1 & 0 & 1 & 4 & 3 & 4 \\ 2 & 1 & 0 & 3 & 2 & 3 \\ 5 & 4 & 3 & 0 & 3 & 2 \\ 4 & 3 & 2 & 3 & 0 & 3 \\ 5 & 4 & 3 & 2 & 3 & 0 \end{pmatrix} \end{array} \begin{array}{c} \text{Row sum} \\ 17 \\ 13 \\ 11 \\ 17 \\ 15 \\ 17 \end{array} \qquad \boldsymbol{DD}_{20} = \begin{array}{c} \\ \begin{pmatrix} 0 & 1 & 4 & 3 & 4 & 5 \\ 1 & 0 & 3 & 2 & 3 & 4 \\ 4 & 3 & 0 & 3 & 2 & 3 \\ 3 & 2 & 3 & 0 & 3 & 4 \\ 4 & 3 & 2 & 3 & 0 & 1 \\ 5 & 4 & 3 & 4 & 1 & 0 \end{pmatrix} \end{array} \begin{array}{c} \text{Row sum} \\ 17 \\ 13 \\ 15 \\ 15 \\ 13 \\ 17 \end{array}$$

Notice now that if we attach a new vertex to an existing vertex i of a graph of detour index dd, the addition

(a) Will not change any element of the detour matrix not involving the new vertex;

(b) Will add a new last row (and last column) containing as off-diagonal elements the corresponding elements of row (or column) i but with each entry augmented by unity, and zero as the new diagonal element;

(c) The new detour index *d,d', will be* dd + row sum (i) + n, where n is the number of vertices before enlargement.

It is thus apparent that if a graph has two symmetry non-equivalent vertices with the same detour-matrix sum, addition of a new vertex to either will produce two graphs of identical detour matrix. In addition, if two graphs of the same size and identical detour index each have a vertex with the same row sum, attachment of a new vertex to each of these vertices will produce new graphs of identical detour index. This process will fail only in the exceptional case that the pair of vertex additions produce identical graphs.

Extending the above analysis, we note the attachment of any graph to each of the pair of vertices meeting the conditions of the proceeding para-

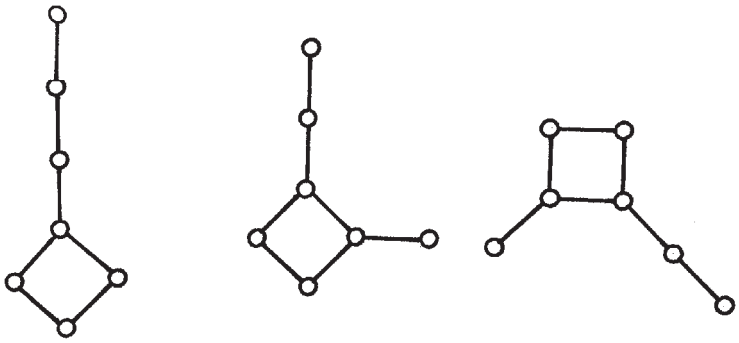


Figure 5. Illustration of graphs having the same detour index constructed by attachment of an edge to the vertices having the same row sum.

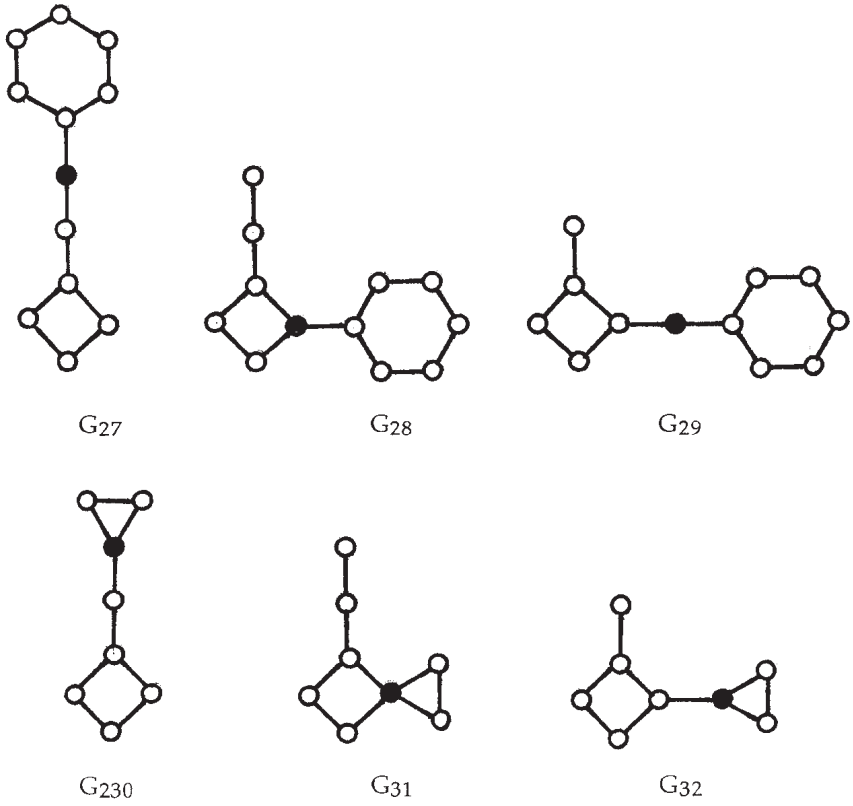


Figure 6. Illustration of graphs having the same detour index constructed by attachment of a larger fragment (a ring) to the vertices having the same row sum.

graph will result in new graphs of identical detour matrix. This observation continues to apply even if the new graph is attached to each identified vertex by identical sets of multiple edges.

Using the graph in the center of Figure 4 as starting points, we note that vertices 1 and 4 of G_{21} both have the row sum 17 and while not being symmetrically equivalent. Also the vertex 1 of G_{22} graph has row sum 17. In Figure 5 we illustrate graphs having the detour index 68 that are formed by adding an edge to vertices 1 and 4 of G_{21} and vertex 1 of G_{22}. Note that only two of these three graphs are distinct. In Figure 6 we present sets $\{G_{27}, G_{28}, G_{29}\}$ and $\{G_{30}, G_{31}, G_{32}\}$, each set having an identical detour index. The graphs are constructed by appending more complex fragment to the structures at the identified vertices having the same row sums.

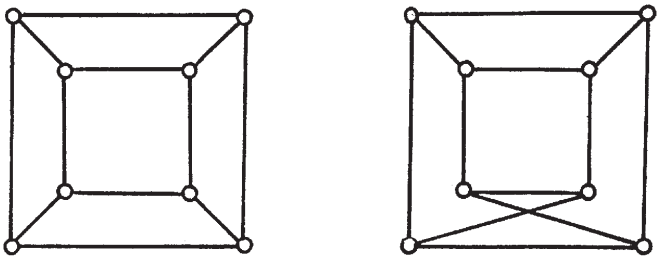
SATURATED AND MAXIMALLY REPLETE GRAPHS

The detour matrix of the complete graph K_5(which is at the same time also the detour matrix of G_{11} and G_{12} in Figure 2) is:

$$\begin{pmatrix} 0 & 4 & 4 & 4 & 4 \\ & 0 & 4 & 4 & 4 \\ & & 0 & 4 & 4 \\ & & & 0 & 4 \\ & & & & 0 \end{pmatrix}$$

As we see all the matrix elements for the graph of K_5 have the maximal possible value for a graph having five vertices and the graph therefore has the largest possible detour index for a graph of this size, namely 40. We refer to a graph of maximum possible detour index for its size as *saturated*. Because K_5 (and also G_{12} have more edges than necessary to yield this detour index, both are also *replete* (as that term was defined earlier). Since K_5 has the largest possible number of edges among graphs of this size and detour index, we can characterize it as *maximally replete* as well as *saturated*.

It may be of interest to ask how many edges can be removed from a maximally replete graph while retaining the property of saturation. It is convenient to cast this question in terms of the minimum density at which a graph can remain saturated, where the density may be defined as the ratio of the number of edges (E) to the number of vertices (V), namely E/V.[1] Some workers[44,45] have defined the density as the ratio E/E^*, where E^* is the number of edges in the complete graphs having the same number of vertices. It may be useful to note that there is not a unique correlation between density and saturation, as illustrated by the following pair of graphs on eight vertices:

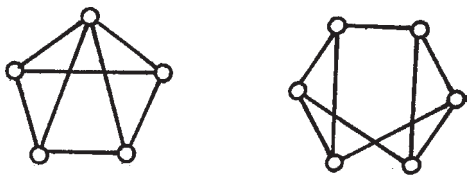


G_{33} G_{34}

Both these graphs have density $E/V = 3/2$, but the graph on the right is saturated while the graph of a cube (on the left) is not. This observation is indicative of the fact that density is a global property of a graph, while saturation depends on the details of the connectivity and, hence, has local characteristics.

ON CONSTRUCTION OF SATURATED GRAPHS

A route to the graphs having the maximal detour matrix is as follows; Start with the complete graph K_n and consider graphs derived from the complete graph by erasure of one or more edges, one at a time. How many bonds we can erase from a complete graph K_n and still have the same (maximal) detour matrix? When $n = 4$ not a single edge can be erased without changing the detour matrix. One can easily find that one can erase two edges from K_5 without changing the detour matrix. The derived has the density $E/V = 5$. Further reduction in graph density would change the detour matrix (and the detour index). In Figure 7 we also have illustrated graph G_{36} that is derived from K_6 by successive bond erasure. The density of G_{36} is $E/V = 3/2$. In the case of K_7 we can similarly construct several graphs with the same detour matrix until we arrive at a graph obtained by erasing almost half of



G_{35} G_{36}

$E/V = 8/5$ $E/V = 3/2$

Figure 7. Graphs derived by erasing edges of K_5 and K_6 but having the same ***DD*** matrix as K_5 and K_6 respectively.

the edges that still allows one to connect any pair of vertices by the longest path possible (here $d_{ij} = 6$). The corresponding density is 11/7. This appears to be an upper bound on the critical density for graphs having $n = 7$ vertices. Removal of any additional edge would produce a bridging vertex, or bridging vertices (of degree two) the presence of which shortens the longest paths for some pairs of vertices.

Such considerations can be extended to large K_n graphs. In Figure 8 we illustrate steps in reducing K_8 to the planar cubic graph related to trigonal prism. It is not difficult to verify that each pair of vertices in the polyhedral cubic graph are connected by the Hamiltonian path. In Table II we list for each vertex one such Hamiltonian path. The cubic graphs with $n = 6$ and

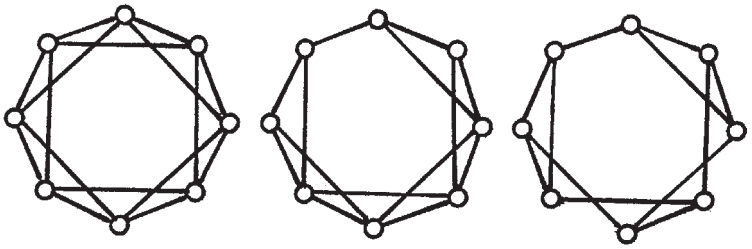


Figure 8. Reduction of K_8 to cubic graph having the same ***DD*** matrix.

TABLE II

Hamiltonian paths for reduced graph having eight vertices

Vertices	Hamiltonian paths	Vertices	Hamiltonian paths
1–2	1–3–5–7–8–6–4–2	2–3	2–1–8–7–6–4–5–3
1–3	1–2–4–6–8–7–5–3	2–4	2–3–1–8–6–7–5–4
1–4	1–2–3–5–7–8–6–4	2–5	2–3–1–8–7–6–4–5
1–5	1–8–7–6–4–2–3–5	2–6	2–3–1–8–7–5–4–6
1–6	1–3–2–4–5–7–8–6	2–7	2–3–1–8–6–4–5–7
1–7	1–2–3–5–4–6–8–7	2–8	2–1–3–5–4–6–7–8
1–8	1–2–3–5–4–6–7–8		
3–4	3–2–1–8–6–7–5–4	4–5	4–2–3–1–8–6–7–5
3–5	3–2–1–8–7–6–4–5	4–6	4–5–3–2–1–8–7–6
3–6	3–2–1–8–7–5–4–6	4–7	4–5–3–2–1–8–6–7
3–7	3–2–1–8–6–4–5–7	4–8	4–2–1–3–5–7–6–8
3–8	3–2–1–4–5–7–6–8		

$n = 8$ vertices can be generalized to similar graphs having even number of vertices as illustrated in Figure 9 for K_{10}, K_{12} and K_{14}. The graphs of Figure 9, all of which have density $E/V = 3n/2n = 3/2$, represent the lowest possible density for graphs on n vertices with the detour matrix same as K_n. Hence, as n, the size of the graphs, increases, the number of graphs that have sufficient density to produce the same detour matrix as K_n increases rapidly.

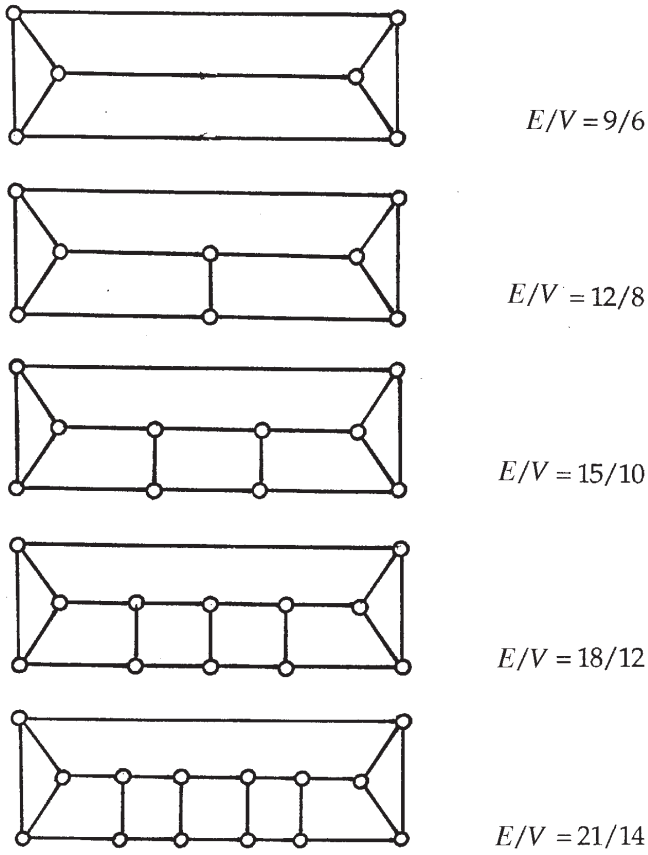


Figure 9. Generalization of the graph of trigonal prism to larger graphs having ***DD*** matrix as the corresponding complete graphs.

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SAŽETAK

Grafovi s istom matricom zaobilaženja

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Matrica zaobilaženja (***DD***) grafa ima ulaz (*i*,*j*) duljinu najduže staze izmedju čvorova *i* i *j*. Zbroj svih vrijednosti iznad glavne dijagonale daje indeks zaobilaženja *dd*. U literaturi su zabilježeni različiti grafovi koji imaju isti indeks zaobilaženja. Ispitavši takove grafove kao i druge grafove koje smo pronašli, izvješćujemo o nekim njihovim pravilnostima. Mnogi grafovi nemaju samo isti indeks zaobilježanja, već također i istu matricu zaobilaženja. Posebno smo razmatrali grafove za koje su elementi matrice zaobilažnja maksimalni. Takovi se grafovi zovu *zasićeni* grafovi. Matrica zaobilaženja zasićenog grafa ista je kao i matrica zaobilažnja potpunog grafa koji ima isti broj čvorova.