Frequency of Even and Odd Numbers in Distance Matrices of Bipartite Graphs

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In a recent paper (Lukovits, I. *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 626–629) the frequency of even and odd numbers in distance matrices of trees was investigated. We now show that the regularities reported there apply to all (connected) bipartite graphs. Moreover, these regularities are easily envisaged by taking into account certain general structural features of bipartite graphs.

INTRODUCTION

In a recent paper,[1] the occurrence of even and odd entries in the distance matrices of trees was studied and several regularities for them were reported. The aim of this paper is to point out that the results obtained in ref 1 can be straightforwardly extended to all (connected) bipartite graphs. We also show that the same regularities are violated in the case of non-bipartite graphs.

The considerations in ref 1 utilize an auxiliary graph with colored edges that is associated to a tree in the following manner.

Let T be a tree (a connected acyclic graph) whose vertices are labeled by $v_1, v_2, ..., v_N$. The distance between the vertices v_i and v_j in T is denoted by $d(v_i,v_j|T)$. (Recall that the distance[2,3] between the vertices v_i and v_j in a graph is equal to the number of edges in the shortest path connecting v_i and v_j. In a connected graph the distance is a well-defined quantity for all pairs of vertices. In trees, there is just one path between any two vertices.)

Now, we associate to T an auxiliary graph CEC = CEC(T) whose vertices are the same as those of T (i.e., $v_1,v_2, ..., v_N$). CEC is a complete graph, i.e., any two of its vertices are connected. The edges of CEC(T) are "colored" by two "colors", *e* and *o*, in the following manner. The edge of CEC(T), connecting the vertices v_i and v_j, is colored by *e* and is said to be an *e*-edge if $d(v_i,v_j|T)$ is an even number. If $d(v_i,v_j|T)$ is an odd number, then the respective edge of CEC(T) is colored by *o* and is said to be an *o*-edge. Hence, CEC is a *complete edge-colored* graph.

The results of the paper[1] are stated in theorems 1, 2, and 3. For the purpose of this work, we formulate these theorems in a slightly different (but fully equivalent) way.

Theorem 1. Any three distinct vertices in CEC are connected either by three *e*-edges or by two *o*-edges and one *e*-edge.

As a consequence of theorem 1, the colors of the edges starting from a particular vertex of CEC determine the colors of all edges of CEC. It is also immediately clear that the structure of CEC is fully determined (up to isomorphism) by specifying the number of *e*- and *o*-edges which start from the vertex considered. If these numbers are *m* and *n*, respectively, we denote the corresponding complete edge-colored graph by CEC($e^m o^n$). Note that CEC($e^m o^n$) possesses $m + n + 1$ vertices. Note also that the concept of the CEC($e^m o^n$) graph is sound only provided theorem 1 is obeyed.

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Theorem 2. If $m \geq 0$ and $n \geq 1$, then CEC($e^m o^n$) and CEC($e^{n-1} o^{m+1}$) are isomorphic.

A vertex of CEC, incident to *m* *e*-edges and *n* *o*-edges is said[1] to be an $e^m o^n$ vertex.

Theorem 3. CEC($e^m o^n$) has $m + 1$ $e^m o^n$ vertices and n $e^{n-1} o^{m+1}$ vertices.

MAIN RESULTS

Our main results can now be expressed in the following form.

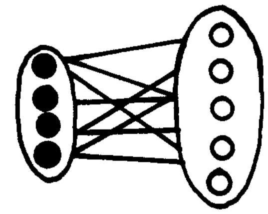
Theorem A. The statements of theorems 1, 2, and 3 remain valid if CEC corresponds to an arbitrary connected bipartite graph.

Theorem B. The statements of theorems 1, 2, and 3 are violated if CEC corresponds to any connected non-bipartite graph.

Recall that a graph is bipartite[2] if its vertices can be colored by two colors (say black and white) such that adjacent vertices are colored differently. A graph is bipartite if and only if it does not contain odd-membered cycles.[2] (Consequently, all trees are bipartite graphs.)

TWO AUXILIARY RESULTS

Consider a bipartite graph **B** and color its vertices by black and white so that the first neighbors of a black vertex are white and vice versa. Thus, no two black and no two white vertices are mutually adjacent. In view of this, the bipartite character of **B** is best visualized by means of the following diagram; the encircled vertices are mutually nonadjacent.



B

For instance, the hydrogen-suppressed graphs of 4-isopropyl-3,6,7-trimethylnonane (G_1) and of bicyclo[2.2.2]octane (G_2) can be drawn as follows. (The vertices of G_1 are labeled in the same way as in the paper.[1])

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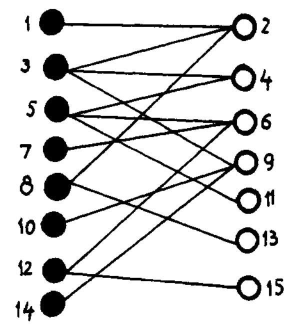
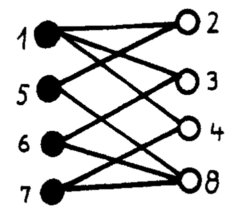
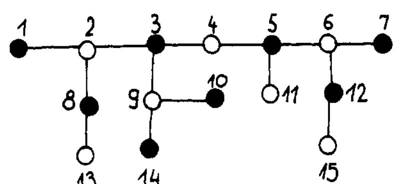


G_1

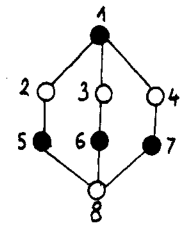


G_2

A more usual representation of the same graphs is, of course



G_1



G_2

It is evident that any path in a bipartite graph goes alternately through black and white vertices. Therefore the length of any path (not necessarily the shortest one) connecting two vertices of the same color is even, whereas the length of any path connecting vertices of different colors is odd. We thus arrive at[4]

Lemma 1. If **B** is a connected bipartite graph and v_i and v_j are two of its vertices, then $d(v_i,v_j|\mathbf{B})$ is even if v_i and v_j have the same colors and $d(v_i,v_j|\mathbf{B})$ is odd if v_i and v_j have different colors.

As already explained, every pair of vertices of **B** whose distance is even corresponds to an *e*-edge of CEC(**B**) and every pair of vertices of **B** whose distance is odd corresponds to an *o*-edge of CEC(**B**). The number of *e*- and *o*-edges in CEC(**B**) is denoted[1] by E_e and E_o, respectively. Then, bearing in mind lemma 1, we have

Lemma 2. (a) E_e is equal to the number of pairs of black vertices plus the number of pairs of white vertices of **B**; E_o is equal to the number of pairs of oppositely colored vertices of **B**. (b) If **B** has $m + 1$ vertices of one color and n vertices of the other color, then $E_e = \binom{m+1}{2} + \binom{n}{2}$ and $E_o = (m + 1)n$.

The results of lemma 2b should be compared with eqs 7 and 8 in the paper.[1] Recall that

$$E_e + E_o = \binom{m+n+1}{2} = \binom{N}{2}$$

because the complete graph on N vertices possesses $\binom{N}{2}$ edges.

PROOF OF THEOREMS A AND B

Let **B** be an arbitrary connected bipartite graph. Choose any three of its vertices. These vertices are either all of the same color or two of the same color and one of the other color. In the first case, according to lemma 1, any two of the chosen vertices are at even distance and thus correspond to an *e*-edge in CEC(**B**). In the second case, two pairs of the (oppositely colored) vertices are at odd distance and one pair (equally colored) at even distance, implying two *o*-edges and one *e*-edge in CEC(**B**). Hence, theorem 1 holds for **B**.

When coloring the vertices of **B**, the choice of the color (say, black) of the first vertex is arbitrary. However, once the color of a vertex is chosen, the colors of all other vertices are determined too.

Suppose that **B** has $m + 1$ vertices of one color and n vertices of the other color. Start the coloring procedure at a vertex from the first class. Then **B** will have $m + 1$ black and n white vertices. The initially colored (black) vertex is at even distance to m (black) vertices and at odd distance to n (white) vertices, implying the complete edge-colored graph CEC($e^m o^n$).

Start now the coloring procedure at a vertex from the second class. Then **B** will have n black and $m + 1$ white vertices, implying the complete edge-colored graph CEC($e^{n-1} o^{m+1}$).

Evidently, CEC($e^m o^n$) and CEC($e^{n-1} o^{m+1}$) correspond to the different colorings of the same graph **B** and are therefore mutually isomorphic. Hence, theorem 2 holds for **B**.

All the $m + 1$ black vertices of **B** have m (black) vertices at even distance and n (white) vertices at odd distance. Thus, the number of $e^m o^n$ vertices in CEC($e^m o^n$) is $m + 1$. In a similar way we see that the number of $e^{n-1} o^{m+1}$ vertices in CEC($e^m o^n$) is equal to n. Hence, also theorem 3 holds for any connected bipartite graph **B**.

By this we completed the proof of theorem A.

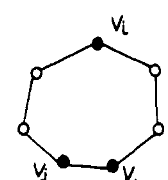
In order to verify theorem B recall that every non-bipartite graph possesses an odd-membered cycle.[2] Without loss of generality we may consider just the odd-membered cycle $\mathbf{C}_N$.

Let v_i by an arbitrary vertex of $\mathbf{C}_N$, N = odd. Select the vertices v_i, v_j, v_k so that $d(v_i,v_j|\mathbf{C}_N) = d(v_i,v_k|\mathbf{C}_N)$ is maximum. It is easy to see that then $d(v_i,v_j|\mathbf{C}_N) = d(v_i,v_k|\mathbf{C}_N) = (N-1)/2$ and, furthermore, $d(v_j,v_k|\mathbf{C}_N) = 1$. Consequently, if N = 3, 7, 11, 15, ..., then the vertices v_i, v_j, v_k correspond to an *ooo*-triad in CEC($\mathbf{C}_N$).

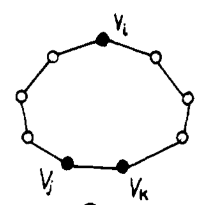
For instance, an *ooo*-triad is formed by the vertices v_i, v_j, v_k of $\mathbf{C}_7$ (see below); the respective distances are 3, 3, and 1.

If, on the other hand, N = 5, 9, 13, 17, ..., then the vertices v_i, v_j, v_k of $\mathbf{C}_N$ correspond to an *eeo*-triad. This case is illustrated on the cycle $\mathbf{C}_9$ (see below); the respective distances are 4, 4, and 1.

Hence, for the graph $\mathbf{C}_N$, N = odd, theorem 1 is violated.



C_7



C_9

It has already been pointed out that the concept of the complete edge-colored graph CEC($e^m o^n$) is meaningful only if theorem 1 is obeyed. Because theorem 1 is violated for non-bipartite graphs, theorems 2 and 3 are also not applicable to non-bipartite graphs. By this theorem B is confirmed.

CONCLUDING REMARKS

Our approach sheds some more light on the results communicated by I. Lukotivs.[1] In particular, the parameters m and n have now a simple interpretation: they pertain to the number of differently colored vertices ($m + 1$ and n, respectively) of the tree considered. We also easily understand why the operator e^{N-1} is exceptional (see in ref 1 the corollary of theorem 2). Namely, this operator would correspond to a bipartite graph in which all the vertices were of the same color, contradicting the requirement that the graphs considered are connected.

Similarly, the condition $m \geq 0$ and $n \geq 1$ in theorem 2 simply means that the graph has to contain at least one vertex of each color.

The above discussion straightforwardly leads to the following conclusion:

Theorem C. (a) The number of black and white vertices of a bipartite graph **B** completely determines CEC(**B**) (up to isomorphism). (b) All connected bipartite graphs with the same numbers of black ($m + 1$) and white (n) vertices have the same auxiliary graph CEC (up to isomorphism); this graph is just CEC($e^m o^n$). (c) The only property of **B** that can be reconstructed from CEC(**B**) is the number of black and white vertices.

In ref 1 also the number of *eee*- and *eoo*-triads in CEC($e^m o^n$) was calculated. Bearing in mind theorem C, we immediately see that the number T_e of *eee*-triads is just the number of selections of triplets of equally colored vertices of **B**. There are $\binom{m+1}{3}$ such black triplets and $\binom{n}{3}$ such white triplets, resulting in

$$T_e = \binom{m+1}{3} + \binom{n}{3}$$

a formula which should be compared with eq 11 in ref 1. The number T_o of *eoo*-triads is equal to the number of triplets of differently colored vertices of **B**. By an easy combinatorial reasoning we obtain

$$T_o = (m + 1)\binom{n}{2} + n\binom{m+1}{2}$$

Of course,

$$T_e + T_o = \binom{m+n+1}{3} = \binom{N}{3}$$

We have demonstrated (by means of counterexamples) that the theorems 1, 2, and 3 fail in the case of non-bipartite graphs. Yet, if G is a non-bipartite graph, CEC(G) is still well-defined. This complete edge-colored graph may contain both *eee*-, *eoo*-, *eeo*-, and *ooo*-triads. The number and distribution of these triads seem to depend in a somewhat complicated way on the structure of G. The elucidation of these dependencies remains a challenging task for the future.

REFERENCES AND NOTES

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