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Distance Neighbourhood Pattern Matrices

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Abstract. Let $G = (V, E)$ be a given connected simple (p, q)-graph, and an arbitrary nonempty subset $M \subseteq V(G)$ of G and for each $v \in V(G)$, define $N_j^M[u] = \{v \in M : d(u, v) = j\}$. Clearly, then $N_j[u] = N_j^{V(G)}[u]$. B.D. Acharya [2] defined the *M-eccentricity* of u as the largest integer for which $N_j^M[u] \neq \emptyset$ and the $p \times (d_G + 1)$ nonnegative integer matrix $D_G^M = (|N_j^M[v_i]|)$, called the *M-distance neighborhood pattern* (or, *M-dnp*) *matrix* of G. The matrix D_G^{*M} is obtained from D_G^M by replacing each nonzero entry by 1. Clearly, $f_M(u) = \{j : N_j^M[u] \neq \emptyset\}$. Hence, in particular, if $f_M : u \mapsto f_M(u)$ is an injective function, then the set M is a *distance-pattern distinguishing set* (or, a 'DPD-set' in short) of G and G is a dpd-graph. If $f_M(u) - \{0\}$ is independent of the choice of u in G then M is an *open distance-pattern uniform* (or, ODPU) *set* of G. A study of these sets is expected to be useful in a number of areas of practical importance such as facility location [5] and design of indices of "quantitative structure-activity relationships" (QSAR) in chemistry [3, 10]. This paper is a study of M-dnp matrices of a dpd-graph.

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Key Words and Phrases: Distance-pattern distinguishing sets, distance neighborhood pattern matrix, M-distance neighborhood pattern matrix.

1. Introduction

For all terminology which are not defined in this paper, we refer the reader to F. Harary [5]. Unless mentioned otherwise, all the graphs considered in this paper are finite, simple and without self loops.
On 26th November 2006, B.D. Acharya [2] conveyed to the first author the following definitions and problems for a detailed study.

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Definition 1 ([2, 9])**.** *Let $G = (V, E)$ be a given connected simple (p, q)-graph, $M \subseteq V(G)$ and for each $u \in V(G)$, let $f_M(u) = \{d(u, v) : v \in M\}$ be the* distance-pattern *of u with respect to the* marker set M. *If f_M is injective then the set M is a* distance-pattern distinguishing set *(or, a "dpd-set" in short) of G and G is a* dpd-graph. *If $f_M(u) - \{0\}$ is independent of the choice of u in G then M is an open distance-pattern uniform (or, odpu) set of G and G is called an odpu-graph. The minimum cardinality of a dpd-set (odpu-set) in G, if it exists, is the* dpd-number*(odpu-number) of G and it is denoted by $\varrho(G)$.*

B.D. Acharya [2], raised the following problems during the conversation.

Problem 1. *For what structural properties of the graph G, the function f_M is injective?*

Problem 2. *Characterize dpd-graphs having the given dpd-number.*

Problem 3. *Which graphs G have the property that every k-subset of $V(G)$ is a dpd-set of G. Solve this problem in particular when $k = \varrho(G)$?*

Problem 4. *Which graphs G have exactly one $\varrho(G)$-set?*

Given a positive integer n, an *n-distance coloring* of a graph G is a coloring of the vertices of G in such a way that no two vertices at distance n are colored by the same color; G is *n-distance colorable* if it indeed admits such a coloring (*e.g., see* Sampathkumar, 1977 [13], 1988 [14]). Clearly, if G admits an n-distance coloring then $1 \leq n \leq diam(G)$.

Problem 5. *For which values of n it is possible to extract a proper n-distance coloring of a given graph G using a distance-pattern function as a listing of colors for the vertices?*

Problem 6. *Given any positive integer k, does there exist a graph G with $\varrho(G) = k$?*

Some of the above mentioned problems studied are reported in the Technical Report [9]. B.D. Acharya, while sharing his many incisive thoughts, during the discussion, in June 2008, introduced a new approach namely, distance neighborhood pattern matrices (dnp-matrices), to study dpd-graphs. In this paper we initiate a study of dnp-matrices of a graph.

For an arbitrarily fixed vertex u in G and for any nonnegative integer j, we let $N_j[u] = \{v \in V(G) : d(u, v) = j\}$. Clearly, $N_0[u] = \{u\}$, $\forall\ u \in V(G)$ and $N_j[u] = V(G) - V(\mathscr{C}_u)$ whenever j exceeds the eccentricity $\varepsilon(u)$ of u in the component $\mathscr{C}_u$ to which u belongs. Thus, if G is connected then, $N_j[u] = \emptyset$ if and only if $j > \varepsilon(u)$. If G is a connected graph then the vectors $\overline{u} = (|N_0[u]|, |N_1[u]|, |N_2[u]|, \ldots, |N_{\varepsilon(u)}[u]|)$ associated with $u \in V(G)$ can be arranged as a $p \times (d_G + 1)$ nonnegative integer matrix D_G given by

$$\begin{pmatrix} 1 & |N_1[v_1]| & |N_2[v_1]| & \ldots & |N_{\varepsilon(v_1)}[v_1]| & 0 & 0 & 0 \\ 1 & |N_1[v_2]| & |N_2[v_2]| & \ldots & \ldots & |N_{\varepsilon(v_2)}[v_2]| & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & |N_1[v_p]| & |N_2[v_p]| & \ldots & \ldots & \ldots & \ldots & |N_{\varepsilon(v_p)}[v_p]| \end{pmatrix}$$

where d_G denotes the diameter of G; we call D_G *distance neighborhood pattern* (or, *dnp*-) *matrix* of G.

For a dnp-matrix the following observations are immediate.

Observation 7. *Since $N_0[u] = \{u\}$ for all $u \in V(G)$, each entry in the first column of D_G is equal to* 1.

Observation 8. *Entries in the second column of D_G corresponds to the degree of the corresponding vertices in G.*

Observation 9. *In each row of D_G, the entry zero will be after the nonzero entries.*

Proposition 1. *For each $u \in V(G)$ of a connected graph G, $\{N_j[u] : N_j[u] \neq \emptyset,\ 0 \leq j \leq d_G\}$ gives a partition of $V(G)$.*

Proof. If possible, let $N_j[u] \bigcap N_k[u] = v$, for some $u, v \in V(G)$, which implies $d(u,v) = j$ and $d(u,v) = k$, and hence $j = k$. Therefore, $N_j[u] \bigcap N_k[u] = \emptyset$ for any (j,k) with $j \neq k$. Now, clearly, $\bigcup_{j=0}^{d_G} N_j[u] \subseteq V(G)$. Also, for any $v \in V(G)$, since G is connected, $d(u,v) = k$, for some $k \in \{0,1,2,\ldots,d_G\}$. That is, $v \in N_k[u]$ for some $k \in \{0,1,2,\ldots,d_G\}$, which implies $V(G) \subseteq \bigcup_{j=0}^{d_G} N_j[u]$. Hence, $\bigcup_{j=0}^{d_G} N_j[u] = V(G)$.

Corollary 1. *Each row of the dnp-matrix D_G of a graph G is the partition of the order of G. Hence, sum of the entries in each row of the dnp-matrix D_G of a graph G is equal to the order of G.*

2. M-distance Neighborhood Pattern Matrix of a Graph

Given an arbitrary nonempty subset $M \subseteq V(G)$ of G and for each $u \in V(G)$, define $N_j^M[u] = \{v \in M : d(u,v) = j\}$; clearly then $N_j^{V(G)}[u] = N_j[u]$. One can define the M-eccentricity of u as the largest integer for which $N_j^M[u] \neq \emptyset$ and the $p \times (d_G + 1)$ nonnegative integer matrix $D_G^M = (|N_j^M[u]|)$ is called the M-distance neighborhood pattern (or M-dnp) matrix of G. D_G^{*M} is obtained from D_G^M by replacing each nonzero entry by 1.
Acharya [2] defined dnp matrix of any graph and in particular, M-dnp matrix of a dpd-graph as follows:

Definition 2. *Let $G = (V,E)$ be a given connected simple (p,q)-graph, $\emptyset \neq M \subseteq V(G)$ and $u \in V(G)$. Then, the* M-distance-pattern *of u is the set $f_M(u) = \{d(u,v) : v \in M\}$. Clearly, $f_M(u) = \{j : N_j^M[u] \neq \emptyset\}$. Hence, in particular, if $f_M : u \mapsto f_M(u)$ is an injective function then the set M is a* distance-pattern distinguishing set *(or, a "dpd-set"in short) of G and if $f_M(u) - \{0\}$ is independent of the choice of u in G then M is an open distance-pattern uniform (or, odpu) set of G. A graph G with a dpd-set(odpu-set) is called a dpd-(odpu-)graph.*

Following are some interesting results on M-dnp matrix of a connected graph G.

Observation 10. *Both D_G^M and D_G^{*M} do not admit null rows.*

Proposition 2. *For each $u_i \in V(G)$,*

$$N_0^M[u_i] = \begin{cases} u_i & \text{if } u_i \in M \\ \emptyset & \text{if } u_i \notin M \end{cases}$$

Therefore, the entries in the first column of D_G^M and D_G^{*M} will either be 0 *or* 1.

Remark 1. *It should note that Observation 9 is not true in the case of* D_G^M.

Corollary 2. *The sum of the entries in the first column of* D_G^M *and* D_G^{*M} *is equal to* $|M|$.

Lemma 1 is similar to Proposition 1.

Lemma 1. *For each* $u \in V(G)$*, of a connected graph G,* $\{N_j^M[u] : N_j^M[u] \neq \emptyset,\ 0 \leq j \leq d_G\}$ *is a partition of* M.

Proof. Let $N_j^M[u] \bigcap N_k^M[u] = v$, for some $u \in V(G)$, $v \in M$. Then $d(u,v) = j$ and $d(u,v) = k$, and hence $j = k$. Therefore, $N_j^M[u] \bigcap N_k^M[u] = \emptyset$ for $j \neq k$.
Now, $\bigcup_{j=0}^{d_G} N_j^M[u] \subseteq M$ is trivial. Also, for any vertex $v \in M$, since G is connected $d(u,v) = k$, for some $k \in \{0,1,2,\dots,d_G\}$. That is, $v \in N_k^M[u]$ for some $k \in \{0,1,2,\dots,d_G\}$. Hence, $v \in \bigcup_{j=0}^{d_G} N_j^M[u]$, which implies $M \subseteq \bigcup_{j=0}^{d_G} N_j^M[u]$. Hence, $\bigcup_{j=0}^{d_G} N_j^M[u] = M$.

Corollary 3. *Each row of* D_G^M *is a partition of* $|M|$.

Corollary 4. *Sum of the entries in each row of* D_G^M *gives* $|M|$ *and sum of the entries in each row of* D_G^{*M} *is less than or equal to* $|M|$.

3. M-dnp Matrix of a dpd-graph

In this section we investigate some interesting results of D_G^M (D_G^{*M}) of a dpd-graph. From the definition of D_G^{*M}, we have the following important observations.

Observation 11. *In any graph G, a nonempty* $M \subseteq V(G)$ *is a dpd-set if and only if no two rows of* D_G^{*M} *are identical.*

Observation 12. *If M is a dpd-set of a dpd-graph G, no row in* D_G^{*M} *is a scalar multiple of any other row.*

Remark 2. *For any* $\emptyset \neq M \subseteq V(G)$*, if the rows of* D_G^{*M} *are linearly independent, M is a dpd-set. However, the converse need not be true. For example, let G be a graph obtained by attaching two vertices* u_1 *and* u_2 *to two adjacent vertices* v_4 *and* v_5 *respectively of the cycle* $C_5 : v_1v_2v_3v_4v_5$. *Choose* $M = \{v_2, v_3, u_1\}$. *Then,*

$$D_G^{*M} = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

In D_G^{*M} *the third row is the sum of fifth and seventh rows.*

Lemma 2. *Let G be a graph with dpd-set M. If there exists a row say, R_m, in D_G^{*M} as the sum of any other rows, say, $R_1, R_2, \ldots, R_k$ then, each column sum of the sub matrix formed by $R_1, R_2, \ldots, R_k$ is either 0 or 1.*

Proof. Let $C_j : \ j = 1, 2, \ldots, (d_G + 1)$ be the j^{th} column sum of the sub-matrix formed by $R_1, R_2, \ldots, R_k$. Assume $C_j = c$ where c is a constant not equal to 0 or 1 for some j. Then the j^{th} entry in row R_m is, $c \neq 0, \ 1$, which is a contradiction to the fact that D_G^{*M} is a $(0,1)-$matrix.

Proposition 3. *Any dpd-graph G, with dpd-set M and the M-dnp matrix D_G^M as an identity matrix of order n is isomorphic to a path P_n on n vertices with dpd-set M as any of its pendent vertices.*

Proof. Let G be a graph with dpd-set M such that $D_G^M \cong I_n$, the identity matrix of order n. From Corollary 4, sum of the entries in each row of $D_G^M = |M|$. Hence $|M| = 1$, since, $D_G^M \cong I_n$. Since $|M| = 1$, $M = \{x\}$, where x is any vertex in G. We claim that x is a pendent vertex. If possible assume there exists at least two vertices $v_1, v_2 \in V(G)$ adjacent to x. Then the rows corresponding to v_1 and v_2 in D_G^M will be

$$\begin{pmatrix} 0 & 1 & 0 & \ldots & 0 & 0 \\ 0 & 1 & 0 & \ldots & 0 & 0 \end{pmatrix},$$

which is not possible since, $D_G^M \cong I_n$. Therefore, x is a pendent vertex.
Now we prove that $G \cong P_n$, a path on n vertices. Since, $D_G^M \cong I_n$, $O(G) = n$ and $d_G = n - 1$. Since $d_G = n - 1$, G contains a path of length $n - 1$. Since $O(G) = O(P_n) = n$, number of vertices of G and P_n are same. Now, if $G \ncong P_n$, G contains at least one edge other than the edges of P_n, which is not possible, since $d_G = n - 1$. Hence, $G \cong P_n$, the path on n vertices.
For the converse, consider the path $P_n = v_1 v_2 \ldots v_n$ with dpd-set M as any of its pendent vertices. Then,

$$D_G^M = I_n = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & 1 \end{pmatrix}$$

Proposition 4. *Let G be a dpd-graph. Then the dnp-matrix D_G^M of G is a diagonal matrix if and only if all the diagonal entries in D_G^M are unity. Also, D_G^M can neither be upper triangular nor lower triangular.*

Proof. Let G be graph with dpd-set M and M-dnp matrix D_G^M, a diagonal matrix say, D. By Proposition 2, entries in the first column of D_G^M are 0 or 1 and by Observation 10, D_G^M does not admit null rows, hence, $a_{11} = 1$. Also, by Corollary 4, the sum of the entries in each row of $D_G^M = |M|$. Therefore, from first row of D, $|M| = 1$ and hence $a_{ii} = 1 \ \forall \ i = 2, 3, \ldots, n$. Hence $D \cong I_n$. Converse part follows from Proposition 3.
For the second part of the theorem, assume that G is a graph with dpd-set M and D_G^M as an upper triangular matrix with atleast one nonzero entry above the main diagonal. From

Proposition 2, the entries in the first column of D_G^M are either 0 or 1. Also, from Corollary 2 sum of the entries in the first column of $D_G^M = |M|$. Hence $a_{11} = 1$ and $|M| = 1$. From Corollary 4, sum of the entries in each row of $D_G^M = |M|$. Hence, in each row, the nonzero entry appears in exactly one place and is unity. D_G^M being an upper triangular matrix, the entry 1 cannot be below the main diagonal and D_G^M contains atleast one nonzero entry above the main diagonal, which in turn implies, D_G^M contains identical rows, a contradiction.
By a similar argument, we can prove that D_G^M is not a lower triangular matrix.

4. Main Results

Theorem 13. *For any graph $G = (V, E)$, there exists no dpd-set M of cardinality 2.*

Proof. Suppose there exists a dpd-graph G with a dpd-set M of cardinality 2. Let us choose $M = \{x, y\}$, where x and y are arbitrary vertices in G. Then D_G^{*M} contains $2 \times (d_G + 1)$ sub-matrix so that rows of the sub-matrix represent the M-distance neighborhood pattern(M-dnp) of x and M-distance neighborhood pattern(M-dnp) of y in D_G^{*M}. Hence, the entry 1 can be only at the first and $(d(x, y) + 1)^{th}$ columns, and the rows will be of the following form

$$\begin{pmatrix} 1 & 0 & 0 & \dots & 1 & 0 & \dots & 0 \\ 1 & 0 & 0 & \dots & 1 & 0 & \dots & 0 \end{pmatrix}$$

Hence, D_G^{*M} contains identical rows and so M is not a dpd-set.

Theorem 14. *For any (p, q)-graph G, $V(G)$ is a dpd-set if and only if G is isomorphic to K_1, the trivial graph.*

Proof. Assume that G is isomorphic to K_1. Clearly, K_1 has the dpd-set $M = \{v\}$ where $V(K_1) = \{v\}$.
Converse follows from the fact when $M = V(G)$, the rows in the dnp-matrix D_G^{*M} corresponding to the diametrically opposite vertices are identical. Hence, G can have exactly one row and column (i.e., exactly one vertex) and hence is isomorphic to K_1.

Theorem 15. *The complete graph K_n possess a dpd-set if and only if $n \leq 2$.*

Proof. Suppose $G \cong K_n$ has a dpd-set M with cardinality k. Then the first k rows of D_G^M represent the M-dnp of those vertices which belongs to M and the remaining $n - k$ rows represent the M-dnp of those vertices which are not in M.

That is,

$$D_G^M = \begin{pmatrix} 1 & k-1 \\ 1 & k-1 \\ \cdots & \cdots \\ \cdots & \cdots \\ 1 & k-1 \\ 0 & k \\ 0 & k \\ \cdots & \cdots \\ \cdots & \cdots \\ 0 & k \end{pmatrix}$$

Hence,

$$D_G^{*M} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \\ \cdots & \cdots \\ \cdots & \cdots \\ 1 & 1 \\ 0 & 1 \\ \cdots & \cdots \\ \cdots & \cdots \\ 0 & 1 \end{pmatrix}$$

Clearly, when $n \geq 3$, D_G^{*M} contains identical rows and hence M is not a dpd-set. Converse follows from Theorem 14 and proposition 3.

Theorem 16. *Complete bipartite graph $K_{m,n}$ possess a dpd-set M if and only if either $m = n = 1$ or $m = 1, n = 2$.*

Proof. Let $G \cong K_{m,n}$ be a complete bipartite graph with partition of the vertex set as P_1 and P_2 with $|P_1| = m$ and $|P_2| = n$. Assume $K_{m,n}$ possess a dpd-set M such that $|M| = k$. Let $M = \{v_1, v_2, \ldots, v_k\}$ where $\{v_1, v_2, \ldots, v_r\} \in P_1$ and $\{v_{r+1}, v_{r+2}, \ldots, v_k\} \in P_2$. Then the first k rows of D_G^{*M} represent the M-dnp of the vertices in M. In this k rows, the first r rows represent the M-dnp of the vertices which are in P_1 and the remaining $k - r$ rows represent the M-dnp of the vertices which are in P_2. The remaining $(m + n) - k$ rows represent the M-dnp of the vertices which are not in M. Now, in this $(m + n) - k$ rows, the first $m - r$ rows represent the M-dnp of the vertices in P_1 and the remaining $n-(k-r)$ rows represent the M-dnp of vertices which are in P_2.

Case 1: $r \geq 2$ and $k - r \geq 2$

Then,

$$D_G^{*M} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ \cdots & \cdots & \cdots \\ 1 & 1 & 1 \\ 0 & 1 & 1 \\ \cdots & \cdots & \cdots \\ 0 & 1 & 1 \end{pmatrix}$$

Since $r \geq 2$ and $k - r \geq 2$, D_G^{*M} contains identical rows and hence, M is not a dpd-set.

Case 2: $r = 1$ and $k - r \geq 2$

$$D_G^{*M} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ \cdots & \cdots & \cdots \\ 1 & 1 & 1 \\ 0 & 1 & 1 \\ \cdots & \cdots & \cdots \\ 0 & 1 & 1 \end{pmatrix}$$

Since, $k - r \geq 2$, D_G^{*M} contains identical rows and hence, M is not a dpd-set.

Case 3: $r = 0$ and $k - r \geq 2$

$$D_G^{*M} = \begin{pmatrix} 1 & 0 & 1 \\ \cdots & \cdots & \cdots \\ 1 & 0 & 1 \\ 0 & 1 & 0 \\ \cdots & \cdots & \cdots \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \cdots & \cdots & \cdots \\ 0 & 0 & 1 \end{pmatrix}$$

Since, $k - r \geq 2$, D_G^{*M} will have identical rows and hence, M is not a dpd-set.

Case 4: $r = 1$ and $k - r = 1$
In this case, $k = |M| = 2$. Therefore, by Theorem 13, M is not a dpd-set.

Case 5: $r = 0$ and $k - r = 1$

$$D_G^{*M} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \cdots & \cdots & \cdots \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \cdots & \cdots & \cdots \\ 0 & 0 & 1 \end{pmatrix}$$

Hence, from D_G^{*M} it is clear that D_G^{*M} contains nonidentical rows only if either $m = 1, n = 1$ or $m = 1, n = 2$.

Converse follows from proposition 3.

Corollary 5. *The star graph $K_{1,n}$ admits a dpd-set M if and only if $n \leq 2$.*

Theorem 17. *For a dpd-graph G with a dpd-set M of $|M| = 3$, the vertices in M should be at distinct distances from each other.*

Proof. Let G be a dpd-graph with dpd-set $M = \{v_1, v_2, v_3\}$.
Let us denote $d(v_1, v_2) = k_1$, $d(v_2, v_3) = k_2$ and $d(v_1, v_3) = k_3$.

Case 1: $d(v_1, v_2) = d(v_2, v_3) = d(v_1, v_3) = k$
In this case D_G^{*M} has a $3 \times (d_G + 1)$ sub-matrix where the rows represent the M-dnp of the vertices v_1, v_2 and v_3 respectively, with entries 1 only at the first and $(k+1)^{th}$ columns.

$$\begin{pmatrix} 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 \end{pmatrix}$$

Therefore, D_G^{*M} contains identical rows and hence, M is not a dpd-set.

Case 2: $k_1 = k_2 \neq k_3$
In this case, D_G^{*M} has a $2 \times (d_G + 1)$ sub-matrix where the rows represent the M-dnp of the vertices v_1 and v_3 respectively with entries 1 only at the first, $(k_1+1)^{th}$ and $(k_3+1)^{th}$ columns.

$$\begin{pmatrix} 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 \end{pmatrix}$$

Hence, D_G^{*M} has identical rows and M is not a dpd-set.

Case 3: $k_1 \neq k_2 \neq k_3$
In this case, the first, second and the third rows represent the M-dnp of the vertices v_1, v_2 and v_3 respectively in D_G^{*M}, with entries 1 only at the first, $(k_1+1)^{th}$, $(k_2+1)^{th}$ and the $(k_3+1)^{th}$ columns.

$$\begin{pmatrix} 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & 1 & 0 & \dots & 0 & 1 & 0 & \dots & 0 \end{pmatrix}$$

Hence, it is possible to form a dpd-set M with $|M| = 3$ in this case.

However, any subset $M = \{v_1, v_2, v_3\} \subseteq V(G)$, satisfying the condition stated in Theorem 17, is not a sufficient condition for M to be a dpd-set. Consider $C_6 = (v_1 v_2 \dots v_6)$, with $M = \{v_1, v_2, v_4\}$ which are at distinct distances, but clearly do not form a dpd-set.

Theorem 18. *A cycle $G \cong C_n$ of order n admits a dpd-set if and only if $n \geq 7$.*

Proof. Let $C_n = (v_1 v_2 \ldots v_n v_1)$ be a cycle on n vertices.

Case 1: n, an even integer and $n \geq 8$
Let $M = \{v_1, v_2, v_4\}$. Then,

$$D_G^{*M} = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 1 & 1 & 0 & 1 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 1 & 1 & 0 & 1 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

where the rows of D_G^{*M} represent the M-dnp of the vertices $v_1, v_2, \ldots, v_n$ taken in order. Now, we can partition D_G^{*M} in to two sub-matrices say, A and B where A is a $\frac{n}{2} \times (\frac{n}{2} + 1)$ sub-matrix of the form

$$\begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & \ldots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & \ldots & 0 & 0 & 0 & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 & 0 & 0 & \ldots & 1 & 0 & 1 & 1 & 0 \end{pmatrix},$$

If we denote the columns of A as $(c_1, c_2, \ldots, c_{d_G+1})$, then B is such that, the columns of B are $(c_{d_G+1}, \ldots, c_2, c_1)$. Looking at the rows of A and B, it is clear that the rows of D_G^{*M} are not identical, and hence, $\{v_1, v_2, v_4\}$ form a dpd-set.

Case 2: n, an odd integer and $n \geq 7$

Let $M = \{v_1, v_2, v_4\}$. Then,

$$D_G^{*M} = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & \dots & 0 & 0 & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 1 & 1 & 0 & 1 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 1 & 1 & 0 & 1 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

where rows of D_G^{*M} represent the M-dnp of the vertices $v_1, v_2, \dots, v_n$ taken in order. In this case, D_G^{*M} can have three sub-matrices A, B, C as its partition as described below. Choose the sub-matrix $A \ulcorner \frac{n}{2} \urcorner \times (d_G + 1)$ as

$$\begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & \dots & 0 & 0 & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 1 & 0 & 1 & 1 \end{pmatrix}$$

We choose B as $3 \times (d_G + 1)$ sub-matrix of D_G^{*M}, which is of the form

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 1 & 1 & 1 \end{pmatrix}$$

Also, choose C as $((n-3) - \ulcorner \frac{n}{2} \urcorner) \times (d_G + 1)$ sub-matrix of D_G^{*M}, which is of the form,

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \dots & 1 & 1 & 0 & 1 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 1 & 1 & 0 & 1 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

None of the rows of the sub-matrices of A, B and C are identical and hence the rows of D_G^{*M} are not identical. Therefore, for any cycle $C_n, n \geq 7$ there exist a dpd-set.
Now to complete the proof of the theorem it is enough to prove that C_n is not a dpd-graph for $n \leq 6$.

Case 3: $n = 3$.
Since C_3 is a complete graph by Theorem 15, C_3 is not a dpd-graph.

Case 4: $n = 4$ or n = 5.

Subcase 1: $|M| = 1$.
Let $M = \{v\}$; $v \in V(G)$. Then the rows represent the M-dnp of the adjacent vertices of v gives a $2 \times (d_G + 1)$ sub-matrix of D_G^{*M} of the form

$$\begin{pmatrix} 1 & 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & 0 & \dots & 0 \end{pmatrix}$$

in which the rows are identical. Hence, M is not a dpd-set.

Subcase 2: $|M| = 2$.
By Theorem 13, there exist no dpd-set M of cardinality 2.

Subcase 3: $|M| = 3$
For C_4 and C_5 we cannot find a dpd-set M with $|M| = 3$, in which the vertices of M are at distinct distances from each other. Hence, by Theorem 17 there exist no dpd-set M with $|M| = 3$ for C_4 and C_5.

Subcase 4: $|M| = 4$.
By Theorem 14, C_4 doesn't have a dpd-set M with $|M| = 4$ and for C_5, M with any four vertices of C_5 gives D_G^{*M} as:

$$D_G^{*M} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

in which the rows are identical. Hence, M is not a dpd-set.

Subcase 5: $|M| = 5$.
By Theorem 14, C_5 cannot have a dpd-set M with $|M| = 5$.
Thus C_4 and C_5 are not dpd-graphs.

Case 5: $n = 6$.
As in Case 4, M with $|M| = 1$ and $|M| = 2$ are not possible.

Let $|M| = 3$. Then, any dpd-set M satisfies Theorem 17, has D_G^{*M} as:

$$D_G^{*M} = \begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

in which third and sixth rows are identical. Hence, M with $|M| = 3$, is not a dpd-set for C_6.
Let C_6 has a dpd-set M with $|M| = 4$.

Subcase 1: Let $M = \{v_1, v_2, v_3, v_4\}$

$$D_G^{*M} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix}$$

in which there are identical rows and hence, M is not a dpd-set.

Subcase 2: $M = \{v_1, v_3, v_4, v_5\}$

$$D_G^{*M} = \begin{pmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \end{pmatrix}$$

in which there are identical rows and hence, M is not a dpd-set.

Subcase 3: $M = \{v_1, v_3, v_4, v_6\}$

$$D_G^{*M} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

in which there are identical rows and hence, M is not a dpd-set. By symmetry, similar argument follows for the other choices of four vertices in M and hence, C_6 doesn't have a dpd-set with $|M| = 4$.

Now, let C_6 has a dpd-set M of $|M| = 5$. Then,

$$D_G^{*M} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \end{pmatrix}$$

in which there are identical rows and hence, M is not a dpd-set. Thus, for C_6, a dpd-set M with $|M| = 5$ is not possible.

By Theorem 14, C_6 cannot possess a dpd-set M with $|M| = 6$. Thus C_6 is not a dpd-graph.

Theorem 19. *The set of all vertices in a diametrical path of a graph G cannot form a dpd-set.*

Proof. Let $P_n = v_1, v_2, \ldots, v_n$ be an arbitrary diametrical path of G, where $M = \{v_1, v_2, \ldots, v_n\}$ be a dpd-set of G. Then, the rows representing the M-dnp of the antipodal vertices v_1 and v_n in D_G^{*M} forms a $2 \times (d_G + 1)$ sub matrix as

$$\begin{pmatrix} 1 & 1 & \ldots & 1 & 1 \\ 1 & 1 & \ldots & 1 & 1 \end{pmatrix}$$

Hence, M is not a dpd-set.

Theorem 20. *For all non-trivial dpd-graphs G, the number of nonzero entries in the first column of D_G^M is less than the number of rows. In particular, all the nonzero entries in the first column of D_G^M are unity.*

Proof. By Proposition 2, all the nonzero entries in the first column are unity. If possible, let the number of entries in the first column of D_G^M is equal to the number of rows. Since, all the nonzero entries in the first column are unity, $|N_0^M(u_i)| = 1 \;\; \forall u_i \in \; V(G)$, which implies, $N_0^M(u_i) = \{u_i\} \;\; \forall u_i \in V(G)$. Hence, $u_i \in M \;\; \forall u_i \in V(G)$. Therefore, by Theorem 14, $G \cong K_1$.

Corollary 6. *Let G be a nontrivial graph with dpd-set M and M-dnp matrix D_G^M as an $n \times n$ square matrix. Then, the number of nonzero entries in the first column $\leqq n - 1$.*

Theorem 21. *Let G be a graph with a dpd-set M. Then, the M-dnp matrix D_G^M is a square matrix of order n if and only if $G \cong P_n$, path on n vertices.*

Proof. Assume that the M-dnp matrix D_G^M of dpd-graph G is a square matrix of order n. Then $O(G) = n$ and $d_G = n - 1$. Since $d_G = n - 1$, G contains a path P of length $n - 1$. Since $O(G) = O(P) = n$, the number of vertices of G and P are same. Therefore, if $G \ncong P$, G contains at least one edge connecting the nonadjacent vertices of P, which is not possible since, in this case $d_G < n - 1$, a contradiction. Hence, $G \cong P_n$.

Conversely, let G be a path on n vertices with dpd-set M and M-dnp matrix D_G^M. Then, D_G^M is a square matrix of order n, since the number of vertices of G is n and $d_G = n - 1$.

Corollary 7. *Let G be a graph with dpd-set M and the M-dnp matrix D_G^M as an invertible matrix. Then $G \approxeq P_n$, a path on n vertices.*

Theorem 22. *Let G be a graph with dpd-set M and the M-dnp matrix D_G^M is such that the rows of D_G^M are the elements of a basis of the Euclidean space $\mathbb{R}^n$. Then $G \approxeq P_n$, a path on n vertices.*

Proof. Since the rows of D_G^M are the elements of a basis of $\mathbb{R}^n$, D_G^M is a square matrix of order n. Therefore, $G \approxeq P_n$, a path on n vertices.

Remark 3. *In Proposition 3, we proved that if the rows of D_G^{*M} are the elements of the standard basis of the Euclidean space $\mathbb{R}^n$, then G is a path P_n on n vertices with the dpd-set M as one of its pendent vertices.*

Remark 4. *The converse of Theorem 22 and Corollary 7 need not be true. Consider the path $P_7 = v_1v_2v_3\ldots v_7$. Let $M = \{v_1, v_2, v_3, v_4, v_5, v_7\}$. Then, M is a dpd-set. Now D_G^M is a square matrix, but the rows of D_G^M are not linearly independent. Therefore, the rows cannot form the basis elements of $\mathbb{R}^7$. Also note that D_G^M is not invertible.*

Remark 5. *All invertible matrices need not be a M-dnp matrix D_G^M of a graph G. For example*

$$A = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

is invertible but not a M-dnp, since the row sums are not equal.

From above discussion, it is interesting to investigate those $M-$dnp matrices D_G^M that are invertible. Also, distinguishing those invertible matrices which are M-dnp matrix of a graph is an open problem.

Problem 23. *Characterize those invertible matrices, which are the M-dnp of some graph G.*

5. Conclusion and Scope

As well known, apart from theoretical interest in the study of the distance matrix, such as the realization of a given matrix as the distance matrix of a graph [12], it has found applications in many practically interesting areas such as Quantitative Structure-Activity Relation (QSAR) in discrete mathematical chemistry [3] and studies on the effect of indirect qualitative relationships between individuals in a social network [7, 11]. Also, the *M-Weiner index $W_M(G)$* may be defined as the sum of the entries in the upper triangular half of the M-distance matrix D_G^M; by a *partial Weiner index $W'(G)$*, we mean the M-Weiner index of G for some nonempty proper subset M of $V(G)$ and the well known *Weiner index $W(G)$* [11] is then seen as the M-Weiner index with $M = V(G)$.

An interesting question for chemists would be the following.

Problem 24. *Consider any structure-activity relationship $\mathscr{R}$ of a molecular graph that has been identified to be well correlated with the Weiner index. Is it possible to achieve such a correlation using M-Weiner index for as low cardinality (dpd-)sets M as possible? [Choice of marker sets M in the molecular graph might be very crucial and hence might involve deeper insights into the molecular characteristics.]*

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