

ON BIPARTITE GRAPHS WHICH ATTAIN MINIMUM RANK AMONG BIPARTITE GRAPHS WITH A GIVEN DIAMETER*

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Abstract. The rank of a graph is defined to be the rank of its adjacency matrix. In this paper, the bipartite graphs that attain the minimum rank among bipartite graphs with a given diameter are completely characterized.

Key words. Bipartite graphs, Adjacency matrix, Nullity, Rank, Diameter.

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1. Introduction. All the graphs considered in this paper are finite, undirected and simple. Let $G = (V, E)$ be a graph of order n with vertex set $V = V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E = E(G)$. For any $v \in V$, the degree and neighborhood of v are denoted by $d_G(v)$ and $N_G(v)$ or simply $d(v)$ and $N(v)$ respectively, when just one graph is under discussion. The adjacency matrix $A = A(G) = (a_{ij})_{n \times n}$ of G is defined as follows: $a_{ij} = 1$ if v_i and v_j are adjacent, and $a_{ij} = 0$ otherwise. The *rank* of a graph G is the rank of its adjacency matrix $A(G)$ and is denoted by $r(G)$. The multiplicity of the eigenvalue zero in the spectrum of $A(G)$ is called the *nullity* of G and is denoted by $\eta(G)$. Observe that $\eta(G) = |V(G)| - r(G)$.

Recently the rank of graphs has received a lot of attention. On one hand, as the rank is such a fundamental algebraic concept, the relationship between the structure of a graph and its rank is a natural topic of study for algebraic graph theorists. One of the most well-known investigations in this direction is the study of the relationship between the rank and the chromatic number of a graph [1]. On the other hand, the nullity of a molecular graph has important applications to the Hückel theory of non-bonding molecular orbitals in chemistry [8]. A famous problem posed by Collatz et al. [7] is to characterize all graphs G with $\eta(G) > 0$, which is a very interesting one in chemistry as the occurrence of a zero eigenvalue in the spectrum of a bipartite

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graph (corresponding to an alternant hydrocarbon) indicates chemical instability of the molecule which such a graph represents.

The problem of classifying the graphs according to their rank or nullity seemed to appear initially in the work of Whitney [21]. Cheng and Liu [6] characterized the graphs of order n with nullity $n - 2$ or $n - 3$ or, equivalently, the graphs with rank 2 or 3. Fan and Qian [10] characterized all bipartite graphs with rank 4. Recently Chang, Huang, and Yeh characterized the graphs with rank 4 in [4] and also the graphs with rank 5 in [5]. Other works on the rank or nullity of graphs can be found in [2, 12, 14, 15, 16, 17, 18, 19, 20].

In Section 2, we give some basic notations and facts that will be used in the sequel. In Section 3, we focus ourselves on studying the bipartite graphs and completely characterize the bipartite graphs that attain the minimum rank among bipartite graphs with a given diameter. The case of non-bipartite graphs is still an open problem.

2. Preliminaries. For a graph G , an equivalence relation \sim on $V(G)$ is given by: $u \sim v$ if and only if $N(u) = N(v)$. Corresponding to this equivalence relation, we can define a graph, denoted by G/\sim , with the equivalence classes as its vertices such that $\{u/\sim, v/\sim\}$ is an edge in G/\sim if and only if $\{u, v\}$ is an edge in G (for details see [11]). If $u \sim v$ and $u \neq v$, then u and v are also said to be *duplicates*. If u is a vertex of G with a duplicate, then $G - u$ is called a *reduction* of G . A graph to which no reduction can be applied is *reduced*. From every graph G , we can obtain a unique (up to isomorphism) reduced graph $\mathcal{R}(G)$ (i.e., G/\sim) by successive reductions. If G is any graph and $\mathcal{R}(G)$ is the (unique) reduced graph obtained from G by reductions then G can be obtained from $\mathcal{R}(G)$ by multiplication of vertices (i.e., replacing each vertex by a stable set and an edge by the edges in the corresponding complete bipartite graph, for details see [13, p. 53]). Furthermore, we always have $r(G) = r(\mathcal{R}(G))$, $\text{diam}(G) = \text{diam}(\mathcal{R}(G))$ provided that $\text{diam}(G) \geq 3$, and also G is bipartite if and only if $\mathcal{R}(G)$ is bipartite. So we may restrict our attention to reduced bipartite graphs in the sequel.

A graph with vertex set $\{v_1, v_2, \dots, v_n\}$ and edge set $\{v_1v_2, v_2v_3, \dots, v_{n-1}v_n\}$ is called a *path* from v_1 to v_n and is denoted by P_n . The number of edges of the path is its *length*. The distance $d_G(x, y)$ (or simply $d(x, y)$) in G of two vertices x, y is the length of a shortest path from x to y in G ; if no such path exists, we define $d(x, y)$ to be infinite. The greatest distance between two vertices in G is the *diameter* of G , denoted by $\text{diam}(G)$.

As shown in [9], there are only finitely many reduced graphs with given rank. Let $\mathcal{BG}(d)$ denote the finite set of reduced bipartite graphs with diameter d and rank $r(P_{d+1})$. Note that $P_{d+1} \in \mathcal{BG}(d)$. Also, if G has diameter d then G must contain P_{d+1} as an induced subgraph and so we have $r(G) \geq r(P_{d+1})$. Hence, $\mathcal{BG}(d)$ consists

of all reduced bipartite graphs attaining minimum rank among all bipartite graphs of diameter d . We write $H \subseteq_I G$ to mean that H is an induced subgraph of G . The \subseteq_I -minimal element in $\mathcal{BG}(d)$ is unique and is precisely the path P_{d+1} . Instead of listing all elements of $\mathcal{BG}(d)$, we shall first give a complete characterization of \subseteq_I -maximal elements in $\mathcal{BG}(d)$ and then show that $\mathcal{BG}(d)$ consists of all graphs H satisfying $P_{d+1} \subseteq_I H \subseteq_I G$, for some \subseteq_I -maximal element G in $\mathcal{BG}(d)$. We will use the notation $\mathcal{MBG}(d)$ to denote the set of all \subseteq_I -maximal elements in $\mathcal{BG}(d)$.

It is clear that $\mathcal{BG}(1) = \{P_2\}$. According to a result of Cheng and Liu [6], for a graph G of order n (≥ 2), $r(G) = 2$ if and only if G is the union of a complete bipartite graph and possibly a null graph (i.e., a graph without edges). Thus, there exists no reduced bipartite graph with diameter 2 and rank $r(P_3)$ ($= 2$); hence, $\mathcal{BG}(2) = \emptyset$. So, hereafter, when considering the set $\mathcal{BG}(d)$, we always assume that $d \geq 3$.

Let S be a set and $A \subseteq S$. The characteristic function χ_A of A with respect to S is defined to be identically one on A , and is zero elsewhere. That is

$$\chi_A(x) = \begin{cases} 1, & \text{if } x \in A, \\ 0, & \text{if } x \in S \setminus A. \end{cases}$$

For convenience, χ_A may also be regarded as a column $(0, 1)$ -vector of length $|S|$. For a subset T of S , let $\chi_A \upharpoonright T$ denote the restriction of χ_A to T .

Let G be a graph and let α be a column $(0, 1)$ -vector indexed by the vertices of G . We use $G \oplus_\alpha v$ to denote the graph obtained from G by adding a vertex v and all edges joining v to those vertices u for which the component $\alpha(u) = 1$. When it is not essential to specify α explicitly, we write $G \oplus_\alpha v$ simply as $G \oplus v$. Note that α can be viewed as the characteristic function of the neighborhood $N(v)$ of v in $G \oplus_\alpha v$ with respect to vertex set $V(G)$. The exact effect on the rank of a graph when a single vertex is added has been examined in [3].

LEMMA 2.1 ([3]). *Let G be a graph and let A be the adjacency matrix of G . Then:*

- (1) $r(G \oplus_\alpha v) = r(G) + 2$ if and only if α is not a vector in $rs(A)$, where $rs(A)$ is the range space of A .
- (2) If $\alpha = A\beta$ is in $rs(A)$, then:
 - (a) $r(G \oplus_\alpha v) = r(G) + 1$ if and only if α is not orthogonal to β , and
 - (b) $r(G \oplus_\alpha v) = r(G)$ if and only if α is orthogonal to β .

3. Main results. In this section, we give a complete characterization of $\mathcal{BG}(d)$, that is we determine those (reduced) bipartite graphs that attain the minimum rank among all bipartite graphs with a given diameter. For this purpose, we need to investigate in depth the structure properties of the graphs in $\mathcal{BG}(d)$, especially the

\subseteq_I -maximal graphs in $\mathcal{BG}(d)$.

Let $G = (X, Y, U)$ be a connected bipartite graph, where (X, Y) is the bipartition and U is the edge set of G , respectively. The vertices of G may be numbered so that the adjacency matrix has its following form:

$$(3.1) \quad A = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix}.$$

The matrix B is the “incidence matrix” between the parts X, Y of the bipartition for G . It is easy to see that $r(G) = 2r(B)$; consequently, the rank of a bipartite graph is always even.

Recall that a graph is bipartite if and only if it contains no odd cycles. Let G be a connected bipartite graph with bipartition (X, Y) . It is easy to see that if a vertex v is added to G such that the resulting graph is still bipartite, then the vertices joined to v must all belong to X or Y . If v is joined to vertices in Y (respectively, X), we say that v is added to X (respectively, Y).

LEMMA 3.1. *Let $G \oplus_\alpha v$ be a bipartite graph obtained by adding a new vertex v to a connected bipartite graph G with bipartition (X, Y) . Then $r(G) = r(G \oplus_\alpha v)$ if and only if α is a linear combination of the $\chi_{N_G(u)}$ ’s, with u ’s all belonging to X (respectively, Y) if v is added to X (respectively, Y).*

Proof. Let A be the adjacency matrix of G with the form as given in Equation (3.1). It suffices to consider the case when v is added to X , as a similar argument applies to the case when v is added to Y . In this case, we have $x_u = 0$ for any $u \in X$, as u is not joined to vertices in X . So to conform with the bipartition (X, Y) , α may be partitioned as $\alpha = \begin{bmatrix} 0 & x_2^T \end{bmatrix}^T$.

Sufficiency: By Lemma 2.1, there exists a vector β such that $\alpha = A\beta$. Partitioning β conformally, let $\beta = \begin{bmatrix} y_1^T & y_2^T \end{bmatrix}^T$. Then

$$\begin{bmatrix} 0 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix},$$

which implies $x_2 = B^T y_1$; hence,

$$\alpha = \begin{bmatrix} 0 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ B^T \end{bmatrix} y_1.$$

As each column of $\begin{bmatrix} 0 \\ B^T \end{bmatrix}$ is a characteristic function of $N_G(u)$ for some u in X , our assertion follows.

Necessity: In this case we can find a vector y_1 such that $\alpha = \begin{bmatrix} 0 \\ B^T \end{bmatrix} y_1$. So

$$\begin{bmatrix} 0 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ 0 \end{bmatrix},$$

and hence, $\alpha \in rs(A)$. Since the rank of every bipartite graph is even and $G, G \oplus_\alpha v$ are bipartite, by Lemma 2.1(2) it follows that $r(G) = r(G \oplus_\alpha v)$. \square

LEMMA 3.2 ([17]). *If H is the graph obtained from a graph G by deleting a pendant vertex and its unique neighbor, then $\eta(G) = \eta(H)$ or, equivalently, $r(G) = r(H) + 2$.*

LEMMA 3.3. *Let G be a connected graph and H a connected induced subgraph of G satisfying $r(H) = r(G)$. Then for any subgraph F such that $H \subseteq_I F \subseteq_I G$, F is connected.*

Proof. Suppose that $F = W_1 \cup W_2 \cup \dots \cup W_t$ ($t \geq 2$), where W_1, \dots, W_t are the connected components of F . As $H \subseteq_I F$ and H is connected, H must be an induced subgraph of a connected component of F , say, $H \subseteq_I W_1$. Obviously, we have $r(F) = r(H)$ and $r(W_1) = r(H)$. But $r(F) = \sum_{i=1}^t r(W_i)$, it follows that $r(W_i) = 0$ and W_i is a null graph for $i = 2, \dots, t$. Hence, F can be written as $W_1 \cup \tilde{W}$, where \tilde{W} is a nonempty null graph. Take any vertex v in \tilde{W} . Since G is connected, we can find a vertex u in G adjacent to v . Note that $N_G(v) \cap V(W_1) = \emptyset$ as v is an isolated vertex in F and $F \subseteq_I G$, so $u \notin V(F)$. Now let F' denote the subgraph of G induced by $V(W_1) \cup \{u, v\}$. Then we have $H \subseteq_I F' \subseteq_I G$ and $r(F') = r(H)$. On the other hand, $d_{F'}(v) = 1$, u being the unique neighbor of v in F' . So by Lemma 3.2, $r(F') = r(W_1) + 2 = r(H) + 2$, which is a contradiction. Therefore, F must be connected. \square

Below we present a result more general than Lemma 3.1.

LEMMA 3.4. *Let G be a connected bipartite graph with bipartition (X_G, Y_G) . Let H be a connected induced subgraph of G with bipartition (X_H, Y_H) such that $X_H \subseteq X_G$ and $Y_H \subseteq Y_G$. Then $r(G) = r(H)$ if and only if for any $u \in V(G) \setminus V(H)$, $\chi_{N_G(u)}$ is a linear combination of the $\chi_{N_G(x)}$'s, where all x 's belong to X_H or Y_H depending on whether u belongs to $X_G \setminus X_H$ or $Y_G \setminus Y_H$.*

Proof. Sufficiency: It suffices to consider the case when $u \in X_G \setminus X_H$, as a similar argument applies to the case when $u \in Y_G \setminus Y_H$. For any $u \in X_G \setminus X_H$, let F_1 (respectively, F_2) denote the subgraph of G induced by $X_H \cup Y_G$ (respectively, $X_H \cup \{u\} \cup Y_G$). Clearly $H \subseteq_I F_1 \subseteq_I F_2 \subseteq_I G$, and as $r(G) = r(H)$ we have $r(F_1) = r(F_2)$. By Lemma 3.3, F_1 and F_2 are connected. So by Lemma 3.1, $\chi_{N_{F_1}(u)}$ is a linear combination of the $\chi_{N_{F_1}(x)}$'s, where $x \in X_H$. But $N_{F_1}(u) = N_G(u)$ and $N_{F_1}(x) = N_G(x)$ whenever $x \in X_H$, so the desired assertion follows.

Necessity: Let B denote the incidence matrix between the parts X_G, Y_G of the bipartition for G . Partition X_G as $X_H \cup (X_G \setminus X_H)$ and Y_G as $Y_H \cup (Y_G \setminus Y_H)$, and let the corresponding partitioned matrix for B be the following 2×2 block matrix:

$$\begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}.$$

Note that B_{11} is the incidence matrix between the parts X_H, Y_H of the bipartite graph H . For any $u \in X_G \setminus X_H$, the transpose of the row of B indexed by u is equal to the vector $\chi_{N(v)} \upharpoonright Y_G$. By the assumption, $\chi_{N_G(u)}$ is a linear combination of $\chi_{N_G(x)}$'s with $x \in X_H$. Hence, $\chi_{N_G(u)} \upharpoonright Y_G$ is also a linear combination of $\chi_{N_G(x)} \upharpoonright Y_G$'s with $x \in X_H$. In other words, every row of the matrix $\begin{bmatrix} B_{21} & B_{22} \end{bmatrix}$ belongs to the row space of $\begin{bmatrix} B_{11} & B_{12} \end{bmatrix}$. In a similar manner, we can show that every column of the matrix $\begin{bmatrix} B_{12} \\ B_{22} \end{bmatrix}$ belongs to the column space of $\begin{bmatrix} B_{11} \\ B_{21} \end{bmatrix}$; hence, every column of B_{12} belongs to the column space of B_{11} . Putting together, we have

$$r\left(\begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}\right) = r\left(\begin{bmatrix} B_{11} & B_{12} \end{bmatrix}\right) = r(B_{11}).$$

Note that $r(G) = 2r(B)$ and $r(H) = 2r(B_{11})$. Therefore $r(G) = r(H)$. \square

Let G be a graph with diameter d and suppose that v_1 is a vertex such that $\max_{v \in V} d(v_1, v) = d$. Now let $V_i = V_i(v_1) \equiv \{v \in V : d(v_1, v) = i-1\}$, $i = 2, \dots, d+1$. Clearly, $V(G) = \{v_1\} \cup V_2 \cup \dots \cup V_{d+1}$. We will refer to $\{v_1, V_2, \dots, V_{d+1}\}$ as the *distance partition* (of G) with respect to v_1 . The following fact, whose proof we omit, is an immediate consequence of the definition of distance partition.

LEMMA 3.5. *Let G be a bipartite graph with diameter d . Let v_1 be a vertex such that $\max_{v \in V} d(v_1, v) = d$, and let $\{v_1, V_2, \dots, V_{d+1}\}$ be the distance partition with respect to v_1 . For any $v \in V_t$ ($2 \leq t < d+1$), v is adjacent to some vertex in V_{t-1} , possibly to some vertex in V_{t+1} , but not adjacent to vertices in V_i for $i \neq t-1, t+1$.*

LEMMA 3.6. *If G is a reduced connected bipartite graph and v is a non-cut vertex of G such that $r(G) = r(G-v)$ then $G-v$ is a reduced bipartite graph.*

Proof. Denote by (X, Y) the bipartition of G . Suppose that there exist duplicates u and w in $G-v$, say $u, w \in X$, without loss of generality. If $v \in X$ then, as $N_{G-v}(u) = N_G(u)$ and $N_{G-v}(w) = N_G(w)$, we have $N_G(u) = N_G(w)$, i.e., u and w are duplicates in G , which is a contradiction. If $v \in Y$, by Lemma 3.1, $\chi_{N_{G-v}(v)}$ is a linear combination of $\chi_{N_{G-v}(x)}$'s, where $x \in Y \setminus \{v\}$. Then v is adjacent to u if and only if it is adjacent to w . Therefore, $N_G(u) = N_G(w)$, which is again a contradiction. \square

LEMMA 3.7. *Let H be a graph satisfying $P_{d+1} \subseteq_I H \subseteq_I G$ for some $G \in \mathcal{BG}(d)$. Then:*

- (1) $r(H) = r(P_{d+1})$.
- (2) H is connected.
- (3) H is bipartite.
- (4) H is reduced.

Proof. Suppose that $V(G) \setminus V(H) = \{u_1, u_2, \dots, u_d\}$. Then we can construct graphs H_i , $0 \leq i \leq d$ such that $H = H_d \subseteq_I H_{d-1} \subseteq_I \dots \subseteq_I H_1 \subseteq_I H_0 = G$ with $H_i = H_{i-1} - u_i$ for $i = 1, \dots, d$. Consider any i , $1 \leq i \leq d$. Suppose we have already shown inductively that $H_0 (= G), \dots, H_{i-1}$ are all connected, bipartite, reduced and have the same rank as P_{d+1} . Since $P_{d+1} \subseteq_I H_i \subseteq_I H_{i-1}$, it is clear that $r(H_i) = r(P_{d+1})$. By Lemma 3.3 H_i is connected. As $H_i = H_{i-1} - u_i$ and H_i is connected, it is clear that u_i is a non-cut vertex of H_{i-1} . So by Lemma 3.6, H_i is a reduced bipartite graph. Therefore, H_i satisfies conditions (1)–(4). Proceeding in this way, after a finite number of steps, we conclude that H also satisfies conditions (1)–(4). \square

Let G be a bipartite graph with diameter d , and let $v_1 v_2 \dots v_{d+1}$ be a path in G such that $d(v_1, v_{d+1}) = d$. Let $\{v_1, V_2, V_3, \dots, V_{d+1}\}$ be the distance partition with respect to v_1 . The sequence $(v_i, v_{i+2}, \dots, v_{i+2k})$ is called *neighborhood compatible* (*N-compatible*, for short) in G if $N(v_{i+r}) \cap V_{i+r+1} = N(v_{i+r+2}) \cap V_{i+r+1}$ for $r = 0, 2, \dots, 2(k-1)$; the sequence $(v_i, v_{i+2}, \dots, v_{i+2k})$ is called *nearly neighborhood compatible* (*nearly N-compatible*, for short) if the subsequence $(v_{i+2}, \dots, v_{i+2k})$ is N-compatible and $N(v_i) \cap V_{i+1} \supseteq N(v_{i+2}) \cap V_{i+1}$.

We shall investigate the structure of the distance partition of the graphs in $\mathcal{BG}(d)$. The following result is key to the proofs of Theorems 3.9 and 3.10.

LEMMA 3.8. *Let $G \in \mathcal{BG}(d)$, let $v_1 v_2 \dots v_{d+1}$ be a path in G such that $d(v_1, v_{d+1}) = d$, and let $\{v_1, V_2, V_3, \dots, V_{d+1}\}$ be the distance partition with respect to v_1 . Then*

- (1) $|V_i| \leq 2$ for $i = 2, \dots, d+1$, $|V_2| = |V_3| = |V_{d+1}| = 1$, and when d is even, $|V_{2j}| = 1$ for all j .
- (2) If $|V_{2r}| = 2$ and d is odd, then $(v_{2r}, v_{2r+2}, \dots, v_{d+1})$ is nearly N-compatible. In this case, we have $N(v) = N(v_{2r}) \setminus N(v_{2r+2})$, where $v \in V_{2r} \setminus \{v_{2r}\}$.
- (3) If $|V_{2r+1}| = 2$, then $(v_1, v_3, \dots, v_{2r-1})$ is N-compatible. In this case, $N(v) = N(v_{2r-1}) \cap V_{2r}$, where $v \in V_{2r+1} \setminus \{v_{2r+1}\}$.
- (4) (i) For $4 \leq i \leq d-1$, if $(v_i, v_{i+2}, \dots, v_{d+1})$ is nearly N-compatible (so that i and d are of opposite parity) and $|V_i| = 1$, then $G \oplus v \in \mathcal{BG}(d)$, where v is a new vertex that satisfies $N(v) = N(v_i) \setminus N(v_{i+2})$.
 (ii) For any odd integer $i \geq 5$, if $(v_1, v_3, \dots, v_{i-2})$ is N-compatible and $|V_i| = 1$ then $G \oplus v \in \mathcal{BG}(d)$, where v is a new vertex that satisfies $N(v) = N(v_{i-2}) \cap V_{i-1}$.

Proof. Let $k = \lceil \frac{d}{2} \rceil$. Then d is $2k$ or $2k - 1$, depending on whether d is even or odd. Consider any r , $1 \leq r \leq k$, such that $|V_{2r}| \geq 2$. Let $v \in V_{2r} \setminus \{v_{2r}\}$. Since the connected bipartite graph G contains the connected bipartite graph P_{d+1} as an induced subgraph, by Lemma 3.4, we have

$$(3.2) \quad \chi_N(v) = a_2 \chi_N(v_2) + a_4 \chi_N(v_4) + \cdots + a_{2k} \chi_N(v_{2k})$$

for some real numbers a_2, a_4, \dots, a_{2k} . If there is some j , $1 \leq j \leq r - 1$, such that $a_{2j} \neq 0$, let j_0 be the smallest such j . In view of Lemma 3.5, among $v, v_2, v_4, \dots, v_{2k}$, only v_{2j_0} is adjacent to v_{2j_0-1} . By equating the values of the two sides of (3.2) at v_{2j_0-1} , we obtain $a_{2j_0} = 0$, which is a contradiction. So we must have $a_{2j} = 0$ for $1 \leq j \leq r - 1$ and (3.2) is reduced to $\chi_N(v) = \sum_{j=r}^k a_{2j} \chi_N(v_{2j})$. Since $\chi_N(v)$ takes the value 1 at some vertex in V_{2r-1} and for $j = r + 1, \dots, k$, $\chi_N(v_{2j})$ takes the value 0 at that vertex, we have $a_{2r} = 1$. So $\chi_N(v) = \chi_N(v_{2r}) + \sum_{j=r+1}^k a_{2j} \chi_N(v_{2j})$. By equating the values of the two sides of the preceding relation at v_{2r+1} , we obtain $\chi_N(v)(v_{2r+1}) = 1 + a_{2r+2}$. If $\chi_N(v)(v_{2r+1}) = 1$, then $a_{2r+2} = 0$ and by considering the values of $\chi_N(v)$ at $v_{2r+3}, v_{2r+5}, \dots, v_{2k-1}$ (in this order), we obtain successively that a_{2r+4}, \dots, a_{2k} are all equal to 0; hence, $\chi_N(v) = \chi_N(v_{2r})$ and so $N(v) = N(v_{2r})$, which contradicts the assumption that G is a reduced graph. So we must have $\chi_N(v)(v_{2r+1}) = 0$ and $a_{2r+2} = -1$. Then by considering the values of $\chi_N(v)$ at $v_{2r+3}, \dots, v_{2k-1}$ respectively (and in this order), we obtain respectively $a_{2r+4} = 1, \dots, a_{2k} = (-1)^{k-r}$. So we have

$$(3.3) \quad \chi_N(v) = \chi_N(v_{2r}) - \chi_N(v_{2r+2}) + \cdots + (-1)^{k-r} \chi_N(v_{2k}).$$

Using (3.3), we find that for any $u \in V_{2r+1}$, $u \in N(v)$ if and only if $\chi_N(v_{2r})(u) = 1$ and $\chi_N(v_{2r+2})(u) = 0$. Similarly, for any $u \in V_{2r-1}$, $u \in N(v)$ if and only if $u \in N(v_{2r})$. So we have $N(v) = N(v_{2r}) \setminus N(v_{2r+2})$. Furthermore, if there exists $u \in (N(v_{2r+2}) \cap V_{2r+1}) \setminus (N(v_{2r}) \cap V_{2r+1})$, then by (3.3) we obtain $\chi_N(v)(u) = -1$, which is a contradiction. Therefore, $N(v_{2r}) \cap V_{2r+1} \supseteq N(v_{2r+2}) \cap V_{2r+1}$. Also, for any $j = 1, \dots, k - 1 - r$ and any $u \in V_{2r+2j+1}$ we have $\chi_N(v)(u) = 0$ and hence $\chi_N(v_{2r+2j})(u)$ equals 1 or 0 depending on whether $\chi_N(v_{2r+2j+2})(u)$ equals 1 or 0. So we have $N(v_{2r+2j}) \cap V_{2r+2j+1} = N(v_{2r+2j+2}) \cap V_{2r+2j+1}$. This proves that $(v_{2r}, v_{2r+2}, \dots, v_{2k})$ is nearly N-compatible.

If V_{2r} contains an element, say w , different from v and v_{2r} , then by the same argument we obtain $N(w) = N(v_{2r}) \setminus N(v_{2r+2})$. Hence, $N(v) = N(w)$, which is a contradiction. This shows that if $|V_{2r}| \geq 2$ then necessarily $|V_{2r}| = 2$.

If d is even, then by (3.3) we have $\chi_N(v)(v_{2k+1}) = (-1)^{k-r}$, which implies $r = k$ and consequently $N(v) = N(v_{2k})$. So we arrive at a contradiction. This shows that when d is even, $|V_{2j}| = 1$ for $j = 1, \dots, k$.

Next, we note that we always have $|V_{2k}| = 1$; in other words, we have $|V_d| = 1$

when d is even and $|V_{d+1}| = 1$ when d is odd. Otherwise, by (3.3) (with $r = k$) we have $\chi_{N(v)} = \chi_{N(v_{2k})}$ or $N(v) = N(v_{2k})$, which is a contradiction.

It is also not possible that $r = 1$. Otherwise, by (3.3) we have $\chi_{N(v)} = \chi_{N(v_2)} - \chi_{N(v_4)} + \cdots + (-1)^{k-1} \chi_{N(v_{2k})}$. If the shortest path from v to v_{d+1} contains v_1 then $d(v, v_{d+1}) = d + 1$ and so $\text{diam}(G) \geq d + 1$, which is a contradiction. So the shortest path from v to v_{d+1} must go through a vertex in V_3 . By (3.3) v is not adjacent to v_3 . So there exists $u_3 \in V_3 \setminus \{v_3\}$ such that v is adjacent to u_3 . Since $N(v) = N(v_2) \setminus N(v_4)$ (as $(v_2, v_4, \dots, v_{2k})$ is nearly N-compatible), u_3 is not adjacent to v_4 . But the shortest path from v to v_{d+1} must go through V_4 , so V_4 contains a vertex different from v_4 , say u_4 , which is adjacent to u_3 . By what we have done above (with $r = 2$ and $v = u_4$), $(v_4, v_6, \dots, v_{2k})$ is nearly N-compatible; hence, $N(u_4) \cap V_3 = N(v_4) \cap V_3$. But we have $u_3 \in V_3$, u_3 is adjacent to u_4 and u_3 is not adjacent to v_4 , which is a contradiction. This proves that we always have $|V_2| = 1$.

Now let r be a positive integer such that $|V_{2r+1}| \geq 2$. Consider any $v \in V_{2r+1} \setminus \{v_{2r+1}\}$. By Lemma 3.4 we have

$$(3.4) \quad \chi_{N(v)} = a_1 \chi_{N(v_1)} + a_3 \chi_{N(v_3)} + \cdots,$$

where the last term of the sum on the right side is $a_{2k-1} \chi_{N(v_{2k-1})}$ when d is odd and is $a_{2k+1} \chi_{N(v_{2k+1})}$ when d is even.

When d is odd, by considering the values of $\chi_{N(v)}$ at $v_{2k}, v_{2k-2}, \dots, v_{2r+4}$, we find that $a_{2j+1} = 0$ for $j \geq r + 1$. In this case (3.4) becomes

$$\chi_{N(v)} = a_1 \chi_{N(v_1)} + a_3 \chi_{N(v_3)} + \cdots + a_{2r+1} \chi_{N(v_{2r+1})}.$$

Since $\chi_{N(v)}(v_{2r+2}) = a_{2r+1}$, a_{2r+1} equals 1 or 0, depending on whether v is adjacent or not adjacent to v_{2r+2} . Consider the former case first. Note that $\chi_{N(v)}(v_{2r}) = 1 + a_{2r-1}$. If $\chi_{N(v)}(v_{2r}) = 1$ then $a_{2r-1} = 0$ and by considering the values of $\chi_{N(v)}$ at $v_{2r-2}, v_{2r-4}, \dots, v_2$, we infer that $a_{2r-3} = \cdots = a_1 = 0$; hence, $\chi_{N(v)} = \chi_{N(v_{2r+1})}$, which is a contradiction. So we must have $\chi_{N(v)}(v_{2r}) = 0$ and $a_{2r-1} = -1$. Now v must be adjacent to some vertex in V_{2r} , different from v_{2r} , say u . Then we have $1 = \chi_{N(v)}(u) = \chi_{N(v_{2r+1})}(u) - \chi_{N(v_{2r-1})}(u)$, which implies $\chi_{N(v_{2r+1})}(u) = 1$ and $\chi_{N(v_{2r-1})}(u) = 0$. As $|V_{2r}| \geq 2$, by what we have done, $N(u) = N(v_{2r}) \setminus N(v_{2r+2})$. So we arrive at a contradiction. This shows that the case $a_{2r+1} = 1$ cannot happen and we must have $a_{2r+1} = 0$. Then by the previous argument we can show that

$$(3.5) \quad \chi_{N(v)} = \chi_{N(v_{2r-1})} - \chi_{N(v_{2r-3})} + \cdots + (-1)^{r-1} \chi_{N(v_1)}.$$

When d is even, as we have shown, $|V_{2j}| = 1$ for $j = 1, \dots, k$. In view of these relations, we readily verify the equality relation

$$(3.6) \quad \chi_{N(v_1)} - \chi_{N(v_3)} + \cdots + (-1)^k \chi_{N(v_{2k+1})} = 0.$$

So we can rewrite $\chi_{N(v)}$ as a linear combination of $\chi_{N(v_1)}, \chi_{N(v_3)}, \dots, \chi_{N(v_{2k-1})}$. Using the kind of arguments we have used to obtain (3.3) from (3.2), we can show that in this case (3.5) still holds.

By (3.5) we readily deduce that $(v_1, v_3, \dots, v_{2r-1})$ is N -compatible and $N(v) = N(v_{2r-1}) \cap V_{2r}$. Hence, it also follows that if $|V_{2r+1}| \geq 2$ then necessarily we have $|V_{2r+1}| = 2$. If $|V_3| = 2$ then by (3.5) (with $r = 1$), we have $\chi_{N(v)} = \chi_{N(v_1)}$, which is a contradiction. We have already shown that $|V_{d+1}| = 1$ when d is odd. Now we contend that when d is even we still have $|V_{d+1}| = 1$. Assume to the contrary that there exists $v \in V_{d+1} \setminus \{v_{d+1}\}$. Then by (3.5) (with $r = k$) and (3.6) we obtain $\chi_{N(v)} = \chi_{N(v_{2k+1})}$, which is a contradiction.

In the above we have established (1), (2), and (3).

(4)(i) It is readily checked that we have

$$\chi_{N(v)} = \chi_{N(v_i)} - \chi_{N(v_{i+2})} + \dots + (-1)^{\frac{d+1-i}{2}} \chi_{N(v_{d+1})},$$

as the two sides of relation agree at v_1 and on V_i for $i = 2, 3, \dots, d+1$. So by Lemma 3.4, $G \oplus v \in \mathcal{BG}(d)$.

Similarly, (4)(ii) also follows from the relation

$$\chi_{N(v)} = \chi_{N(v_{i-2})} - \chi_{N(v_{i-4})} + \dots + (-1)^{\frac{i-3}{2}} \chi_{N(v_1)}.$$

Therefore, we have established the conclusions (1)–(4). \square

Now we are ready to give a complete characterization of the set $\mathcal{MBG}(d)$. The next two results deal with the case when d is odd and when d is even respectively.

THEOREM 3.9.

$$\mathcal{MBG}(2k-1) = \begin{cases} \{P_4\}, & k = 2, \\ \{G_6^{(4)}\}, & k = 3, \\ \{G_{2k}^{(2i)} \mid i = \lceil \frac{k+1}{2} \rceil, \dots, k-1\}, & k \geq 4. \end{cases}$$

Proof. Let $G \in \mathcal{MBG}(2k-1)$. Let $v_1 v_2 \dots v_{2k}$ be a path in G such that $d(v_1, v_{2k}) = 2k-1$ and let $\{v_1, V_2, V_3, \dots, V_{2k}\}$ denote the distance partition of G with respect to v_1 . By Lemma 3.8, we have $|V_i| \leq 2$ for $i = 2, \dots, 2k$ and $|V_j| = 1$ for $j = 2, 3, 2k$. If $k = 2$ then clearly $G = P_4$; that is, $\mathcal{MBG}(3) = \{P_4\}$. Hereafter, we assume that $k \geq 3$.

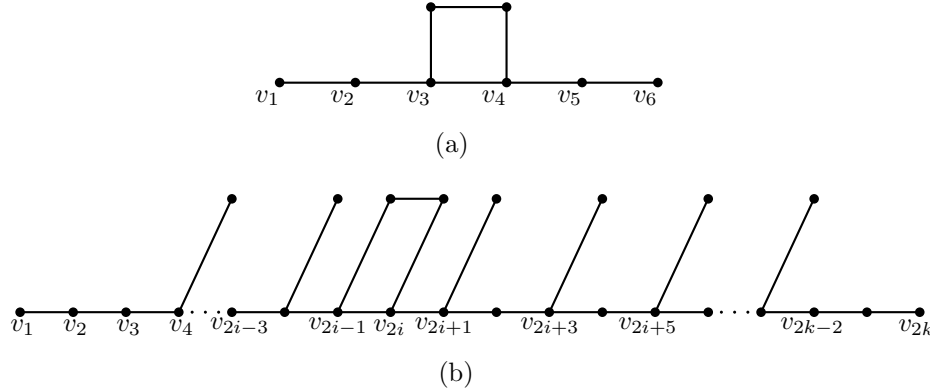


Figure 1. (a) $G_6^{(4)}$ and (b) $G_{2k}^{(2i)}$.

Next we show that there exists at least one j such that $|V_{2j}| = 2$. Assume that the contrary holds. Then $(v_1, v_3, \dots, v_{2k-3})$ is clearly N -compatible. If $|V_{2k-1}| = 1$, then by Lemma 3.8(4)(ii), we can add a new vertex v to G such that $G \oplus v \in \mathcal{BG}(2k-1)$, which contradicts the maximality assumption on G . So $|V_{2k-1}| = 2$ and by Lemma 3.8(3) we have $N(u_{2k-1}) = N(v_{2k-3}) \cap V_{2k-2} = v_{2k-2}$, where $u_{2k-1} \in V_{2k-1} \setminus \{v_{2k-1}\}$. But then $N(v_{2k-2}) \cap V_{2k-1} = V_{2k-1} \supseteq N(v_{2k}) \cap V_{2k-1}$, so (v_{2k-2}, v_{2k}) is nearly N -compatible. In view of the maximality of G , by Lemma 3.8(4)(i) it follows that $|V_{2k-2}| = 2$, which is a contradiction. This proves that $|V_{2j}| = 2$ for at least one j . Let i be the smallest such j . By Lemma 3.8(2) $(v_{2i}, v_{2i+2}, \dots, v_{2k})$ is nearly N -compatible. As $G \in \mathcal{MBG}(2k-1)$, by Lemma 3.8(4)(i), for $j = i, \dots, k-1$, we have $|V_{2j}| = 2$ and $N(u_{2j}) = N(v_{2j}) \setminus N(v_{2j+2})$, where $u_{2j} \in V_{2j} \setminus \{v_{2j}\}$; hence, u_{2j} is adjacent to v_{2j-1} .

By the assumption on i , we have $|V_{2j}| = 1$ for $j = 1, \dots, i-1$. This implies that $(v_1, v_3, \dots, v_{2i-1})$ is N -compatible. In view of the maximality of G , by Lemma 3.8(4)(ii) for $j = 2, \dots, i$, we have $|V_{2j+1}| = 2$ and $N(u_{2j+1}) = N(v_{2j-1}) \cap V_{2j}$, where $u_{2j+1} \in V_{2j+1} \setminus \{v_{2j+1}\}$; hence, u_{2j+1} is adjacent to v_{2j} .

Since $N(u_{2i}) = N(v_{2i}) \setminus N(v_{2i+2})$ and v_{2i+2} is adjacent to v_{2i+1} , u_{2i} and v_{2i+1} must be non-adjacent. Furthermore, we have $u_{2i} \in N(v_{2i-1})$. Hence, $N(v_{2i-1}) \cap V_{2i} \neq N(v_{2i+1}) \cap V_{2i}$. So $(v_1, v_3, \dots, v_{2i+1})$, and hence also, $(v_1, v_3, \dots, v_{2j+1})$ for any $j > i$, is not N -compatible. By Lemma 3.8(3) it follows that $|V_{2i+3}| = |V_{2i+5}| = \dots = |V_{2k-1}| = 1$.

Since $N(u_{2i+1}) = N(v_{2i-1}) \cap V_{2i}$, u_{2i+1} is not adjacent to v_{2i+2} . On the other hand, we have shown that u_{2i+1} is adjacent to v_{2i} , and as $N(u_{2i}) = N(v_{2i}) \setminus N(v_{2i+2})$, it follows that u_{2i} is adjacent to u_{2i+1} . We have proved that G is precisely the graph $G_{2k}^{(2i)}$ (or the graph $G_6^{(4)}$ in case $k = 3$).

In the above, we have shown that every maximal element of $\mathcal{BG}(2k-1)$ is equal to some $G_{2k}^{(2i)}$ (or $G_6^{(4)}$ in case $k=3$). To complete the argument, we note that by applying Lemma 3.4 one can show that each $G_{2k}^{(2i)}$ indeed belongs to $\mathcal{BG}(2k-1)$. So the maximal elements in $\mathcal{BG}(2k-1)$ are exactly $G_{2k}^{(2i)}$, $i=2, \dots, k-1$. On the other hand, it can be verified that $G_{2k}^{(2i)}$ is isomorphic to $G_{2k}^{(2k-2i+2)}$ for $i=2, \dots, k-1$ —one way to see this is to consider the distance partition with respect to v_{2k} instead of v_1 . Therefore, (up to isomorphism) the \subseteq_I -maximal elements in $\mathcal{BG}(2k-1)$ are precisely $G_{2k}^{(2i)}$ for $\lceil \frac{k+1}{2} \rceil, \dots, k-1$. \square

THEOREM 3.10. *The \subseteq_I -maximal element in $\mathcal{BG}(2k)$ ($k \geq 2$) is unique: it is the path P_5 if $k=2$ and is the graph G_{2k+1} , which is given by Figure 2, if $k \geq 3$.*

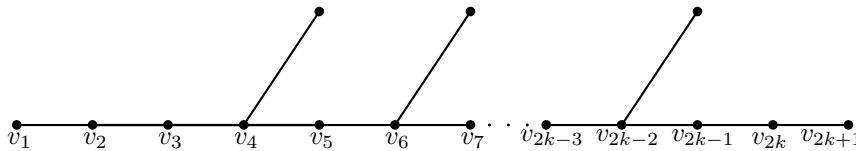


Figure 2. Graph G_{2k+1} .

Proof. Let $G \in \mathcal{MBG}(2k)$, let $v_1 v_2 \cdots v_{2k+1}$ be a path in G with $d(v_1, v_{2k+1}) = 2k$, and let $\{v_1, V_2, V_3, \dots, V_{2k+1}\}$ denote the distance partition of G with respect to v_1 . If $k=2$, then by Lemma 3.8(1) we have $|V_2| = |V_3| = |V_4| = |V_5| = 1$ and so G must be the path P_5 . Hereafter, we assume that $k \geq 3$. By Lemma 3.8(1), we have $V_3 = \{v_3\}$, $V_{2k+1} = \{v_{2k+1}\}$ and also $V_{2j} = \{v_{2j}\}$ for $j=1, 2, \dots, k$. In view of the latter relations, clearly $(v_1, v_3, \dots, v_{2k-1})$ is N-compatible. As $G \in \mathcal{MBG}(2k)$, by Lemma 3.8(4)(ii), we have $|V_{2r+1}| = 2$ for $r=2, \dots, k-1$; say, $V_{2r+1} = \{v_{2r+1}, u_{2r+1}\}$ for all such r . So G is obtained from the path $v_1 v_2 \cdots v_{2k+1}$ by adding the new vertices $u_5, u_7, \dots, u_{2k-1}$. By Lemma 3.8(3) and the fact that $V_{2j} = \{v_{2j}\}$ for $j=1, 2, \dots, k$, we also have $N(u_{2r+1}) = N(v_{2r-1}) \cap V_{2r} = \{v_{2r}\}$ for $r=2, \dots, k-1$. Now it should be clear that G is the graph G_{2k+1} . Our above argument proves that $\mathcal{BG}(2k)$ has a unique \subseteq_I -maximal element, namely, G_{2k+1} . \square

LEMMA 3.11. *Let H be a graph satisfying $P_{d+1} \subseteq_I H \subseteq_I G$, where G is an element in $\mathcal{MBG}(d)$ ($d \geq 3$). Then $\text{diam}(H) = d$.*

Proof. As before, let d be $2k$ or $2k-1$ according to whether d is even or odd. One can check that for any graph H that satisfies $P_{d+1} \subseteq_I H \subseteq_I G$, where G is one of P_4 and $G_{2k}^{(2i)}$ with $i = \lceil \frac{k+1}{2} \rceil, \dots, k-1$ when d is odd and is P_5 or G_{2k+1} when d is even, we have $d_H(v_1, v_{d+1}) = d$ and $d_H(v, w) < d$ for any other pair of vertices v, w of H . Thus, $\text{diam}(H) = d$. \square

Now we can conclude with the following main result of this paper.

THEOREM 3.12. *For $d \geq 3$, we have*

$$\mathcal{BG}(d) = \bigcup_{G \in \mathcal{MBG}(d)} \{H : P_{d+1} \subseteq_I H \subseteq_I G\}.$$

Proof. The inclusion $\bigcup_{G \in \mathcal{MBG}(d)} \{H : P_{d+1} \subseteq_I H \subseteq_I G\} \subseteq \mathcal{BG}(d)$ follows from Lemma 3.7 and Lemma 3.11, whereas the reverse inclusion is obvious as $\mathcal{BG}(d)$ is finite. \square

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