

Matching Energy of Unicyclic and Bicyclic Graphs with a Given Diameter

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Abstract

Gutman and Wagner proposed the concept of matching energy (ME) and pointed out that the chemical applications of ME go back to the 1970s. Let G be a simple graph of order n and $\mu_1, \mu_2, \dots, \mu_n$ be the roots of its matching polynomial. The matching energy of G is defined to be the sum of the absolute values of μ_i ($i = 1, 2, \dots, n$). In this paper, we characterize the graphs with minimal matching energy among all unicyclic and bicyclic graphs with a given diameter d .

Key words: graph; matching energy; energy; diameter

1 Introduction

In this paper, all graphs under our consideration are finite, connected, undirected and simple. For more notations and terminology that will be used in the sequel, we refer to [2]. Let G be a simple undirected graph with order n and $A(G)$ be the adjacency matrix of G . The characteristic polynomial of G , denoted by $\phi(G)$, is defined as

$$\phi(G) = \det(xI - A(G)) = \sum_{i=0}^n a_i(G)x^{n-i},$$

where I is the identity matrix of order n . The roots of the equation $\phi(G) = 0$, denoted by $\lambda_1, \lambda_2, \dots, \lambda_n$, are the eigenvalues of $A(G)$. The energy of

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G , denoted by $E(G)$, is defined as the sum of the absolute values of the eigenvalues of $A(G)$, that is,

$$E(G) = \sum_{i=1}^n |\lambda_i|.$$

The concept of the energy of simple undirected graphs was introduced by Gutman in [15] and now is well-studied. For more results about graph energy, we refer the readers to recent papers [8, 9, 12, 32, 34], two surveys [16, 17] and the book [31]. There are various generalizations of graph energy, such as Randić energy [3, 10], Laplacian energy [7], distance energy [36], incidence energy [4, 5], energy of matrices [14] and energy of a polynomial [33], etc.

Let G be a simple graph with n vertices and m edges. Denote by $m_k(G)$ the number of k -matchings (= the number of selections of k independent edges = the number of k -element independent edge sets) of G . Specifically, $m_1(G) = m$ and $m_k(G) = 0$ for $k > \lfloor \frac{n}{2} \rfloor$ or $k < 0$. It is both consistent and convenient to define $m_0(G) = 1$. The matching polynomial of the graph G is defined as

$$\alpha(G) = \alpha(G, \mu) = \sum_{k \geq 0} (-1)^k m_k(G) \mu^{n-2k}. \quad (1)$$

Recently, Gutman and Wagner [23] defined the matching energy of a graph G based on the zeros of its matching polynomial [13, 21].

Definition 1.1 *Let G be a simple graph with order n , and $\mu_1, \mu_2, \dots, \mu_n$ be the zeros of its matching polynomial. Then,*

$$ME(G) = \sum_{i=1}^n |\mu_i|. \quad (2)$$

Moreover, Gutman and Wagner [23] pointed out that the matching energy is a quantity of relevance for chemical applications. They arrived at the simple relation:

$$TRE(G) = E(G) - ME(G),$$

where $TRE(G)$ is the so-called “topological resonance energy” of G . About the chemical applications of matching energy, for more details see [18, 1, 20].

For the coefficients $a_i(G)$ of $\phi(G)$, let $b_i(G) = |a_i(G)|$, $i = 0, 1, \dots, n$. Note that $b_0(G) = 1$, $b_1(G) = 0$, and $b_2(G)$ is the number of edges of G . For convenience, let $b_i(G) = 0$ if $i < 0$. In [19, 24], we have

$$E(G) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{dx}{x^2} \ln \left[\left(\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} b_{2j}(G) x^{2j} \right)^2 + \left(\sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} b_{2j+1}(G) x^{2j+1} \right)^2 \right]. \quad (3)$$

Thus $E(G)$ is a monotonically increasing function of $b_i(G)$, $i = 0, 1, \dots, n$.

Being similar to Eq.(3), the matching energy also has a beautiful formula as follows[23]. Eq.(4) could be considered as the definition of matching energy, in which case Eq.(2) would become a theorem.

Theorem 1.1 *Let G be a simple graph of order n , and $m_k(G)$ be the number of its k -matchings, $k = 0, 1, 2, \dots, \lfloor \frac{n}{2} \rfloor$. The matching energy of G is given by*

$$ME = ME(G) = \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln \left[\sum_{k \geq 0} m_k(G) x^{2k} \right] dx. \quad (4)$$

By Eq.(4) and the monotony of the function logarithm, we can define a quasi-order “ \succeq ” as follows: If two graphs G_1 and G_2 have the same order and size, then

$$G_1 \succeq G_2 \iff m_k(G_1) \geq m_k(G_2) \quad \text{for all } k.$$

If $G_1 \succeq G_2$ and there exists some k such that $m_k(G_1) > m_k(G_2)$, then we write $G_1 \succ G_2$. Clearly, $G_1 \succ G_2 \implies ME(G_1) > ME(G_2)$.

Notice that when $ME(G_1) > ME(G_2)$, we may not deduce that $G_1 \succ G_2$. However, if G is any simple connected graph with n vertices other than S_n , where S_n is a star of order n , then not only $ME(G) > ME(S_n)$ [23] but also $G \succ S_n$. Based on the quasi-order, there are some more extremal results on matching energy of graphs [6, 26, 27, 30].

In this paper, we characterize the graphs with minimal matching energy among all unicyclic and bicyclic graphs with a given diameter d .

2 Preliminaries

The following result gives two fundamental identities for the number of k -matchings of a graph (see [13, 21]).

Lemma 2.1 *Let G be a simple graph, $e = uv$ be an edge of G , and $N(u) = \{v_1(=v), v_2, \dots, v_j\}$ be the set of all neighbors of u in G . Then we have*

$$m_k(G) = m_k(G - uv) + m_{k-1}(G - u - v), \quad (5)$$

$$m_k(G) = m_k(G - u) + \sum_{i=1}^j m_{k-1}(G - u - v_i). \quad (6)$$

From Lemma 2.1, we know that $m_k(P_1 \cup G) = m_k(G)$. And we can also obtain that

Lemma 2.2 *Let G be a simple graph and H be a subgraph(resp. proper subgraph) of G . Then $G \succeq H$ (resp. $\succ H$).*

A connected graph with n vertices and n edges is called a unicyclic graph. Obviously, a unicyclic graph has exactly one cycle. A connected graph with n vertices and $n + 1$ edges is called a bicyclic graph. Let $\mathcal{U}(n)$ be the class of connected unicyclic graphs with n vertices, $\mathcal{U}(n, d)$ be the class of unicyclic graphs with n vertices and diameter d , where $1 \leq d \leq n - 2$. Let $\mathcal{B}(n)$ be the class of bicyclic graphs with n vertices and $\mathcal{B}(n, d)$ be the class of bicyclic graphs in $\mathcal{B}(n)$ with diameter d , where $2 \leq d \leq n - 2$. Let P_n be the path with n vertices and K_n be the complete graph with n vertices.

When $d = 1$, $n = 3$, K_3 is the unique graph in $\mathcal{U}(3, 1)$. When $d = 1$, $n \geq 4$, $\mathcal{U}(n, 1)$ contains no graphs. When $d = 2$, $n = 4$, $\mathcal{U}(4, 2)$ has two graphs $G_{4,2}^1$ and $G_{4,2}^2$ (see Figure 1). Clearly, $ME(G_{4,2}^2) > ME(G_{4,2}^1)$, i.e., $G_{4,2}^1$ is the unique graph with minimal matching energy in $\mathcal{U}(4, 2)$. When $d = 2$, $n \geq 5$, the graph obtained by attaching $n - 3$ pendant vertices to a vertex of a triangle is the unique graph in $\mathcal{U}(n, 2)$. Thus, we just consider the case in which $3 \leq d \leq n - 2$. In section 3 of our paper, we will prove that for $3 \leq d \leq n - 2$, the graph $U_{n,d}$ is the unique graph in $\mathcal{U}(n, d)$ with minimal matching energy, where the graph $U_{n,d}$ is shown in Figure 2.

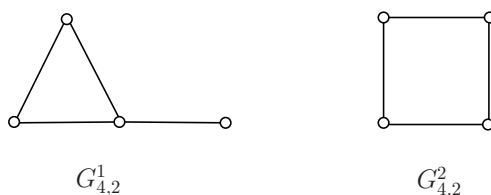


Figure 1: The two graphs in $\mathcal{U}(4, 2)$.

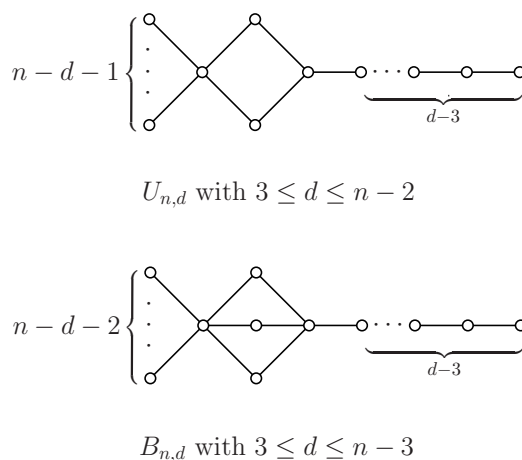


Figure 2: The graphs $U_{n,d}$ and $B_{n,d}$.

When $d = 2$, $n \geq 6$, $\mathcal{B}(n, 2)$ has two graphs $G_{n,2}^1$ and $G_{n,2}^2$ (see Figure 3). By Lemma 2.1 and simple calculation, we can get $G_{n,2}^1 \succ G_{n,2}^2$, hence $G_{n,2}^2$ is the unique graph in $\mathcal{B}(n, 2)$ with minimal matching energy. Therefore, we only consider the case in which $3 \leq d \leq n-2$. In section 4, we will show that $B_{n,d}$ is the unique graph with minimal matching energy for $3 \leq d \leq n-3$, where the graph $B_{n,d}$ is shown in Figure 2. Furthermore, we also pay our attention to the case $d = n-2$.

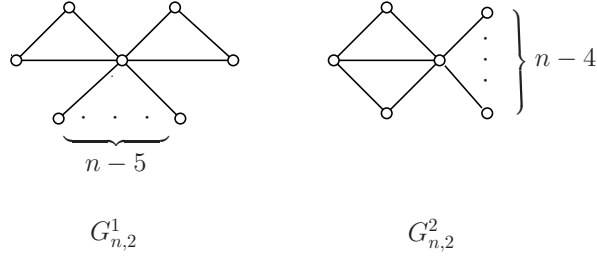


Figure 3: The two graphs in $\mathcal{B}(n, 2)$.

Let $\mathcal{T}(n, d)$ be the class of trees with $n \geq 2$ vertices and diameter d , where $1 \leq d \leq n-1$. If $T \in \mathcal{T}(n, 1)$, then $T = P_2$. For $1 \leq d \leq n-1$, let $T_{n,d}$ denote the graph obtained by attaching $n-d$ pendent vertices to an end vertex of P_d . Specially, $T_{n,1} = T_{n,2} = S_n$. Obviously, $T_{n,2}$ is the unique tree in $\mathcal{T}(n, 2)$ and $T_{n,n-1} = P_n$ is the unique tree in $\mathcal{T}(n, n-1)$.

Let G_1, G_2 be two graphs with n vertices. Now we introduce a *quasi-order* \succeq_1 defined in [31]: If $b_i(G_1) \geq b_i(G_2)$ for all $i \geq 0$, then we write $G_1 \succeq_1 G_2$. If $G_1 \succeq_1 G_2$ and there exists an i_0 such that $b_{i_0}(G_1) > b_{i_0}(G_2)$, then we write $G_1 \succ_1 G_2$. The following lemmas are relevant results on this quasi-order.

Lemma 2.3 ([22, 40]) For $2 \leq i \leq \lfloor \frac{n}{2} \rfloor$ and $n \geq 4$,

$$P_n \succ_1 P_i \cup P_{n-i} \succ_1 P_1 \cup P_{n-1}.$$

Lemma 2.4 ([19]) For $3 \leq d \leq n-2$, $P_n \succeq_1 T_{n,d} \succeq_1 S_n$.

Lemma 2.5 ([37]) Let $T \in \mathcal{T}(n, d)$ and $T \neq T_{n,d}$. Then $T \succ_1 T_{n,d}$.

Lemma 2.6 ([29]) If $d > d_0 \geq 3$, then $T_{n,d} \succ_1 T_{n,d_0}$.

Lemma 2.7 ([39]) For $2 \leq d_1 \leq n_1-2$, we have $T_{n_1,d_1} \cup T \succeq_1 T_{n_1+n_2-1,d_1+d_2}$, where $T = T_{n_2,d_2}$ if $2 \leq d_2 \leq n_2-2$, and P_2 if $n_2 = 2$ and $d_2 = 1$.

If G is an acyclic graph, then [22] $b_{2k}(G) = m_k(G)$ and $b_{2k+1}(G) = 0$ for all k . Thus, the quasi-order \succ_1 (resp. \succeq_1) in Lemmas 2.3–2.7 can be replaced by \succ (resp. \succeq), and the results also work.

By Lemma 2.1 and the definition of the quasi-order \succeq , it is easy to see that the following lemma holds.

Lemma 2.8 *Let $G, G' \in \mathcal{U}(n)$ and uv (resp. $u'v'$) be a pendant edge with the pendant vertex u (resp. u') of the graph G (resp. G'). If $G - u \succeq G' - u'$ and $G - u - v \succ G' - u' - v'$, or $G - u \succ G' - u'$ and $G - u - v \succeq G' - u' - v'$, then $G \succ G'$.*

The following lemmas will be needed in our paper, which are obtained based on the previous results.

Lemma 2.9 *For $3 \leq d \leq n - 2$, $B_{n,d} \succ U_{n,d} \succ T_{n,d}$.*

Proof. Since $U_{n,d}$ is a proper subgraph of $B_{n,d}$, then by Lemma 2.2, we can get $B_{n,d} \succ U_{n,d}$. Similarly, we also have $U_{n,d} \succ T_{n,d}$. ■

Lemma 2.10 *For $3 \leq d_0 < d \leq n - 2$, $U_{n,d} \succ U_{n,d_0}$.*

Proof. By Lemmas 2.1, 2.2 and 2.6,

$$\begin{aligned} m_k(U_{n,d}) &\geq m_k(U_{n-1,d-1}) + m_{k-1}(T_{n-2,d-2}) \\ &\geq m_k(U_{n-1,d-1}) + m_{k-1}(T_{d-1,d-3}) \\ &= m_k(U_{n,d-1}). \end{aligned}$$

Furthermore, $m_2(U_{n,d}) > m_2(U_{n,d-1})$. It follows that $U_{n,d} \succ U_{n,d-1}$. Therefore, $U_{n,d} \succ U_{n,d-1} \succ \cdots \succ U_{n,d_0}$. ■

Similarly, we have

Lemma 2.11 *For $3 \leq d_0 < d \leq n - 2$, $B_{n,d} \succ B_{n,d_0}$.*

3 Unicyclic graphs with a given diameter

Now we consider the minimal matching energy of graphs in $\mathcal{U}(n, d)$ with $3 \leq d \leq n - 2$. We first discuss the case $d = n - 2$.

Lemma 3.1 *Let $G \in \mathcal{U}(n, n - 2)$ with $n \geq 8$ and $G \neq U_{n,n-2}$. Then $G \succ U_{n,n-2}$.*

Proof. We will prove the lemma by induction on n .

If $n = 8$, then G is isomorphic to one of the following graphs (see Figure 4).

It is easy to get

$$\begin{aligned} \alpha(U_{8,6}^1) &= \mu^8 - 8\mu^6 + 19\mu^4 - 13\mu^2 + 1; & \alpha(U_{8,6}^2) &= \mu^8 - 8\mu^6 + 18\mu^4 - 11\mu^2 + 1; \\ \alpha(U_{8,6}^3) &= \mu^8 - 8\mu^6 + 18\mu^4 - 12\mu^2 + 1; & \alpha(U_{8,6}^4) &= \mu^8 - 8\mu^6 + 19\mu^4 - 14\mu^2 + 2; \end{aligned}$$

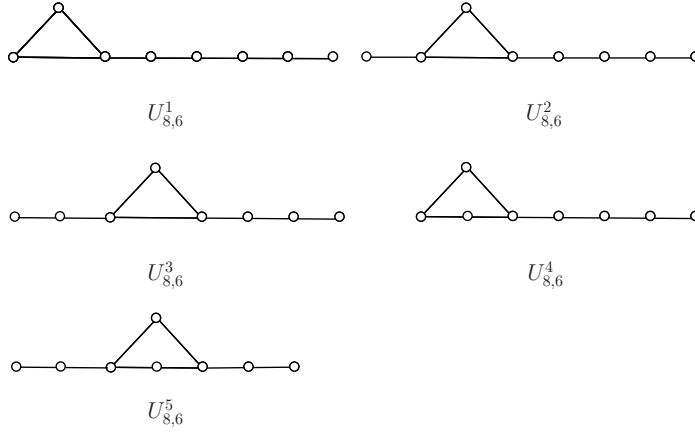


Figure 4: The graphs in $\mathcal{U}(8,6)$ except for $U_{8,6}$.

$$\alpha(U_{8,6}^5) = \mu^8 - 8\mu^6 + 18\mu^4 - 12\mu^2 + 2; \quad \alpha(U_{8,6}) = \mu^8 - 8\mu^6 + 18\mu^4 - 11\mu^2.$$

And then it is obvious that $U_{8,6}^i \succ U_{8,6}$ for $i = 1, 2, 3, 4, 5$, i.e., $U_{8,6}$ is the unique graph in $\mathcal{U}(8,6)$ with minimal matching energy.

If $n = 9$, then G is isomorphic to one of the following graphs (see Figure 5).

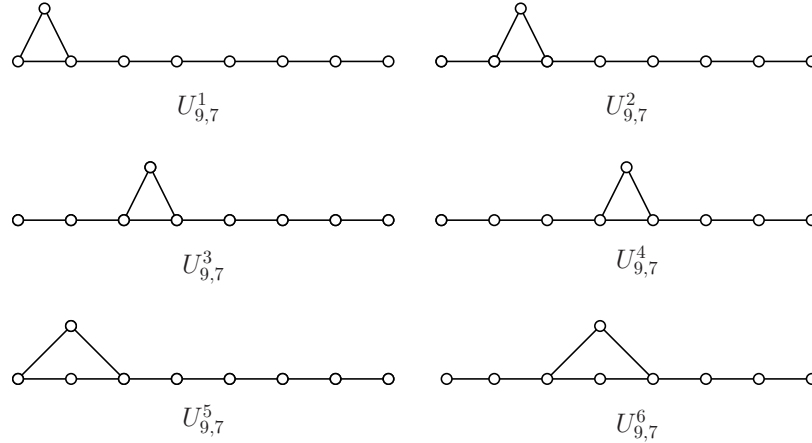


Figure 5: The graphs in $\mathcal{U}(9,7)$ except for $U_{9,7}$.

We can obtain that

$$\begin{aligned} \alpha(U_{9,7}^1) &= \mu^9 - 9\mu^7 + 26\mu^5 - 26\mu^3 + 6\mu; & \alpha(U_{9,7}^2) &= \mu^9 - 9\mu^7 + 25\mu^5 - 23\mu^3 + 5\mu; \\ \alpha(U_{9,7}^3) &= \mu^9 - 9\mu^7 + 25\mu^5 - 24\mu^3 + 6\mu; & \alpha(U_{9,7}^4) &= \mu^9 - 9\mu^7 + 25\mu^5 - 24\mu^3 + 5\mu; \\ \alpha(U_{9,7}^5) &= \mu^9 - 9\mu^7 + 26\mu^5 - 27\mu^3 + 8\mu; & \alpha(U_{9,7}^6) &= \mu^9 - 9\mu^7 + 25\mu^5 - 24\mu^3 + 6\mu; \end{aligned}$$

along with

$$\alpha(U_{9,7}) = \mu^9 - 9\mu^7 + 25\mu^5 - 23\mu^3 + 4\mu.$$

It now immediately follows that $U_{9,7}^i \succ U_{9,7}$ for $i = 1, 2, 3, 4, 5, 6$, i.e., $U_{9,7}$ is the unique graph in $\mathcal{U}(9, 7)$ with minimal matching energy.

Now suppose that the result holds for graphs in $\mathcal{U}(n-1, n-3)$ and $\mathcal{U}(n-2, n-4)$. Let $G \in \mathcal{U}(n, n-2)$ and $G \neq U_{n,n-2}$, where $n \geq 10$.

Let u (resp. u') be a pendant vertex, adjacent to v (resp. v'), which has the largest distance to a vertex on the unique cycle of G (resp. $U_{n,n-2}$). Then the degree of v is 2. So is v' . Hence $G - u \in \mathcal{U}(n-1, n-3)$, $G - u - v \in \mathcal{U}(n-2, n-4)$ and $U_{n,n-2} - u' = U_{n-1,n-3}$, $U_{n,n-2} - u' - v' = U_{n-2,n-4}$.

Since $G \neq U_{n,n-2}$, we have either $G - u \neq U_{n-1,n-3}$ or $G - u - v \neq U_{n-2,n-4}$. By the induction hypothesis, we have $G - u \succ U_{n-1,n-3}$ and $G - u - v \succeq U_{n-2,n-4}$, or $G - u \succeq U_{n-1,n-3}$ and $G - u - v \succ U_{n-2,n-4}$. By Lemma 2.8, $G \succ U_{n,n-2}$. \blacksquare

Theorem 3.2 *Let $G \in \mathcal{U}(n, d)$ with $n \geq 8$, $3 \leq d \leq n-2$ and $G \neq U_{n,d}$. Then $ME(G) > ME(U_{n,d})$.*

Proof. We prove the result by induction on $n-d$.

When $n-d = 2$, by Lemma 3.1, we have $G \succ U_{n,d}$. Let $t \geq 3$ and suppose that the result holds for $n-d < t$. Now suppose that $n-d = t$. Let u' be the vertex of degree 3 in $U_{n,d}$ and v' be a vertex on the quadrangle that is adjacent to u' . By Lemma 2.1,

$$\begin{aligned} m_k(U_{n,d}) &= m_k(U_{n,d} - u'v') + m_{k-1}(U_{n,d} - u' - v') \\ &= m_k(T_{n,d}) + m_{k-1}(P_{d-3} \cup S_{n-d+1}). \end{aligned}$$

For C_n , $m_k(C_n) = m_k(P_n) + m_{k-1}(P_{n-2})$. By Lemma 2.4, $P_n \succ T_{n,d}$. And by Lemmas 2.3 and 2.4, $P_{n-2} \succeq P_{d-3} \cup P_{n-d+1} \succ P_{d-3} \cup S_{n-d+1}$. Thus $C_n \succ U_{n,d}$. Therefore, we may suppose that the unique cycle of G is C_r with $r < n$. Let $P(G) = v_0v_1 \dots v_d$ be a diametrical path of G . Then one of v_0 and v_d must be a pendant vertex.

Case 1 All pendant vertices are on $P(G)$.

Since $t = n-d \geq 3$, then $|V(P(G))| = d+1 \leq n-2$. Thus there are at least two adjacency vertices, say u and v , on C_r which lie outside $P(G)$ such that $G - uv \in \mathcal{T}(n, d_1)$, and $G - u - v \in \mathcal{T}(n-2, d_2)$, where $d_1, d_2 \geq d$. By Lemmas 2.5 and 2.6, $G - uv \succeq T_{n,d_1} \succeq T_{n,d}$, $G - u - v \succeq T_{n-2,d_2} \succeq T_{n-2,d}$. We also have $T_{n-2,d} \succ P_{d-3} \cup T_{n-d+1,3} \succ P_{d-3} \cup S_{n-d+1}$ by Lemmas 2.2 and 2.4. Hence, $G - u - v \succ P_{d-3} \cup S_{n-d+1}$.

Note that $m_k(G) = m_k(G - uv) + m_{k-1}(G - u - v)$, so $m_k(G) \geq m_k(U_{n,d})$ for all k . Moreover, since $T_{n-2,d} \succ P_{d-3} \cup S_{n-d+1}$, there exists some k_0 such that $m_{k_0-1}(G - u - v) > m_{k_0-1}(P_{d-3} \cup S_{n-d+1})$, i.e., $m_{k_0}(G) > m_{k_0}(U_{n,d})$. Thus $G \succ U_{n,d}$.

Case 2 There is at least one pendant vertex outside $P(G)$.

Let u' be a pendant vertex of $U_{n,d}$ adjacent to the vertex v' of degree $n-d+1$. Then $U_{n,d}-u' = U_{n-1,d}$, and $U_{n,d}-u'-v' = (n-d-2)P_1 \cup T_{d,d-2}$.

Subcase 2.1 There is a pendant vertex u outside $P(G)$ such that its neighbor v lies on C_r .

Since u outside $P(G)$, then $G-u \in \mathcal{U}(n-1, d)$. Consequently, by the induction hypothesis, $G-u \succeq U_{n-1,d}$.

If v lies outside $P(G)$, then $G-u-v \supseteq P_{d+1}$. Thus $G-u-v \succeq P_{d+1} \succ T_{d,d-2}$.

Suppose that v lies on $P(G)$, then $P(G)$ and C_r have common vertices, say v_i, \dots, v_{i+j} with $j \geq 0$.

If $j = 0$, i.e., $v = v_i$ is the unique common vertex of $P(G)$ and C_r , then $G-u-v \supseteq P_i \cup P_{d-i} \cup P_2$. Since

$$m_k(P_i \cup P_{d-i} \cup P_2) \geq m_k(P_d) \geq m_k(T_{d,d-2})$$

and $m_2(P_i \cup P_{d-i} \cup P_2) > m_2(T_{d,d-2})$, then $P_i \cup P_{d-i} \cup P_2 \succ T_{d,d-2}$. Therefore, $G-u-v \succeq P_i \cup P_{d-i} \cup P_2 \succ T_{d,d-2}$.

If $j > 0$. For $v \neq v_i, v_{i+j}$, $G-u-v \supseteq P_{d+1}$. So $G-u-v \succeq P_{d+1} \succ T_{d,d-2}$. Otherwise, for $v = v_i$ or v_{i+j} , say $v = v_i$. Then $G-u-v \supseteq P_i \cup T_1$, where $T_1 \in \mathcal{T}(d-i+1, d-i-1)$ is obtained by attaching a pendant vertex to vertex v_{i+j} of the path $P = v_{i+1} \cdots v_d$. For $k \geq 0$,

$$m_k(P_i \cup T_1) \geq m_k(P_i \cup T_{d-i+1, d-i-1}) \geq m_k(T_{d,d-2}).$$

If $(i, j) \neq (1, 2)$, then $m_2(P_i \cup T_1) > m_2(T_{d,d-2})$, hence $G-u-v \succeq P_i \cup T_1 \succ T_{d,d-2}$. Otherwise, $P_i \cup T_1$ is a proper subgraph of $G-u-v$, then $G-u-v \succ P_i \cup T_1 \succeq T_{d,d-2}$. Thus we always have $G-u-v \succ T_{d,d-2}$. Therefore, $G-u-v \succ U_{n,d}-u'-v'$.

We have proved that $G-u \succeq U_{n-1,d}$. Then by Lemma 2.8, we obtain $G \succ U_{n,d}$.

Subcase 2.2 The neighbor of any pendant vertex outside $P(G)$ also lies outside C_r .

If there is a pendant vertex u such that its neighbor v lies outside $P(G)$, then $G-u-v \supseteq C_r \cup P_{d+1} \supseteq C_r \cup P_j \cup P_{d-j}$ or $G-u-v \supseteq G'$, where $G' \in \mathcal{U}(s, d)$ with $d+2 \leq s \leq n-2$.

If every pendant vertex outside $P(G)$ is adjacent to a vertex on $P(G)$, then we choose a pendant vertex u , adjacent to $v = v_j$ such that $G-u-v \supseteq C_r \cup P_j \cup P_{d-j}$ or $G-u-v \supseteq P_j \cup G''$, where $G'' \in \mathcal{U}(s', d')$ with $d' \geq d-j-1$, $s' \geq d'+2$ and $s'+j \leq n-2$.

Hence there are three possibilities: $G-u-v \supseteq C_r \cup P_j \cup P_{d-j}$, $G-u-v \supseteq G'$ or $G-u-v \supseteq P_j \cup G''$.

First, suppose that $G-u-v \supseteq C_r \cup P_j \cup P_{d-j}$, then

$$m_k(C_r \cup P_j \cup P_{d-j}) \geq m_k(P_3 \cup P_j \cup P_{d-j}) \geq m_k(T_{d,d-2}).$$

In particular, $m_1(C_r \cup P_j \cup P_{d-j}) > m_1(T_{d,d-2})$. Thus, $G - u - v \succeq C_r \cup P_j \cup P_{d-j} \succ T_{d,d-2}$.

Next, suppose that $G - u - v \supseteq G'$, then $G - u - v \succeq U_{s,d} \succeq U_{d+2,d} \succ T_{d+2,d}$.

Finally, suppose that $G - u - v \supseteq P_j \cup G''$. For $G'' \in \mathcal{U}(s', d')$ with $s' - d' \leq n - 2 - j - (d - j - 1) = n - d - 1$. By the induction hypothesis, $G'' \succeq U_{s',d'} \succeq U_{d-j+1,d-j-1}$. Thus

$$G - u - v \succeq P_j \cup G'' \succeq P_j \cup U_{s',d'} \succeq P_j \cup U_{d-j+1,d-j-1}.$$

For $k \geq 0$,

$$m_k(P_j \cup U_{d-j+1,d-j-1}) \geq m_k(P_j \cup T_{d-j+1,d-j-1}) \geq m_k(T_{d,d-2}).$$

Furthermore, $m_1(P_j \cup U_{d-j+1,d-j-1}) > m_1(T_{d+2,d})$. It follows that $G - u - v \succeq P_j \cup U_{d-j+1,d-j-1} \succ T_{d+2,d}$.

According to the arguments above, we have proved that $G - u - v \succ U_{n,d} - u' - v'$. On the other hand, $G - u \succeq U_{n-1,d}$. Thus by Lemma 2.8, $G \succ U_{n,d}$.

Combining Cases 1 and 2, we conclude that $G \succ U_{n,d}$ also holds for $G \in \mathcal{U}(n, d)$ with $3 \leq d \leq n - 3$ and $G \neq U_{n,d}$, which yields the result. \blacksquare

4 Bicyclic graphs with a given diameter

In what follows we state some new definitions and notations. For a graph $G \in \mathcal{B}(n)$, it has either two or three distinct cycles. If G has exactly two cycles, suppose that the lengths of them are a and b respectively. If G has three cycles, then any two cycles must have at least one edge in common, and we may choose two cycles of lengths of a and b with t common edges such that $a - t \geq t$ and $b - t \geq t$. Then, in any case, we choose two cycles C_a and C_b in G . For convenience, let $C_a = v_0 v_1 \cdots v_{a-1} v_0$ and $C_b = u_0 u_1 \cdots u_{b-1} u_0$. If C_a and C_b have no common edges, then C_a and C_b are connected by a unique path P , say from v_0 to u_0 . Let $l(G)$ be the length of P . If C_a and C_b have exactly $t (\geq 1)$ common edges, and thus have exactly $t + 1$ common vertices, say, $v_0 = u_0, v_1 = u_1, \dots, v_t = u_t$, then $C_c = u_0 u_{b-1} \cdots u_{t+1} u_t v_{t+1} v_{t+2} \cdots v_{a-1} v_0$ is the third cycle of G , where $c = b + a - 2t$. If we write $w_0 = u_0, w_1 = u_{b-1}, \dots, w_{c-1} = v_{a-1}$, then $C_c = w_0 w_1 \cdots w_{c-1} w_0$. Denote by $d(G)$ the diameter of G .

Now we turn our attention to the minimal matching energy of graphs in $\mathcal{B}(n, d)$ with $3 \leq d \leq n - 2$. We first deal with the case $d = n - 3$.

Lemma 4.1 *Let $G \in \mathcal{B}(n, n - 3)$ with $n \geq 7$, and $G \neq B_{n,n-3}$. Then $G \succ B_{n,n-3}$.*

Proof. By induction on n to prove this fact.

For $n = 7$ and $n = 8$, there are only finitely many graphs we need to consider. Then by Lemma 2.1 and direct check, we can get $G \succ B_{n,n-3}$.

Suppose that the result holds for all graphs in $\mathcal{B}(n-1, n-4)$ and $\mathcal{B}(n-2, n-5)$, where $n \geq 9$. Let $G \in \mathcal{B}(n, n-3)$ and $G \neq B_{n,n-3}$.

Case 1 There is a pendent vertex u in G such that the degree of its neighbor v is 2.

In this case, $G - u \in \mathcal{B}(n-1, n-4)$ and $G - u - v \in \mathcal{B}(n-2, n-5)$. Since $G \neq B_{n,n-3}$, then $G - u \neq B_{n-1,n-4}$ or $G - u - v \neq B_{n-2,n-5}$. By the induction hypothesis, $G - u \succ B_{n-1,n-4}$ and $G - u - v \succeq B_{n-2,n-5}$, or $G - u \succeq B_{n-1,n-4}$ and $G - u - v \succ B_{n-2,n-5}$. Hence, $G \succ B_{n,n-3}$.

Case 2 The neighbor of any pendent vertex has degree at least 3 or there is no pendent vertex.

Then G is isomorphic to some H_j , $j = 1, 2$ (see Figure 6), or G contains one triangle or one quadrangle which has at most one common vertex with the other cycle that is a triangle or a quadrangle.

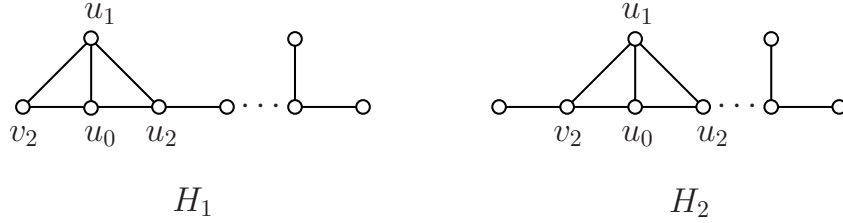


Figure 6: The graphs H_i for $i = 1, 2$.

If G is isomorphic to H_1 , then by Lemmas 2.1, 2.5, 2.6 and Theorem 3.2,

$$\begin{aligned}
m_k(G) &= m_k(G - u_1 v_2) + m_{k-1}(G - u_1 - v_2) \\
&\geq m_k(U_{n,n-3}) + m_{k-1}(T_{n-2,d-1}) \\
&\geq m_k(U_{n,n-3}) + m_{k-1}(P_{n-6} \cup S_4) \\
&= m_k(B_{n,n-3}).
\end{aligned}$$

Moreover, $m_2(G) > m_2(B_{n,n-3})$, thus $G \succ B_{n,n-3}$.

If G is isomorphic to H_2 , then by Lemmas 2.1, 2.3 and Theorem 3.2,

$$\begin{aligned}
m_k(G) &= m_k(G - u_1 u_0) + m_{k-1}(G - u_1 - u_0) \\
&\geq m_k(U_{n,n-3}) + m_{k-1}(P_2 \cup T_{n-4,n-6}) \\
&\geq m_k(U_{n,n-3}) + m_{k-1}(P_2 \cup P_{n-5}) + m_{k-2}(P_2 \cup P_{n-7}) \\
&\geq m_k(U_{n,n-3}) + m_{k-1}(P_3 \cup P_{n-6}) + m_{k-2}(P_{n-6}) \\
&= m_k(B_{n,n-3}).
\end{aligned}$$

Similarly, $m_2(G) > m_2(B_{n,n-3})$, thus $G \succ B_{n,n-3}$.

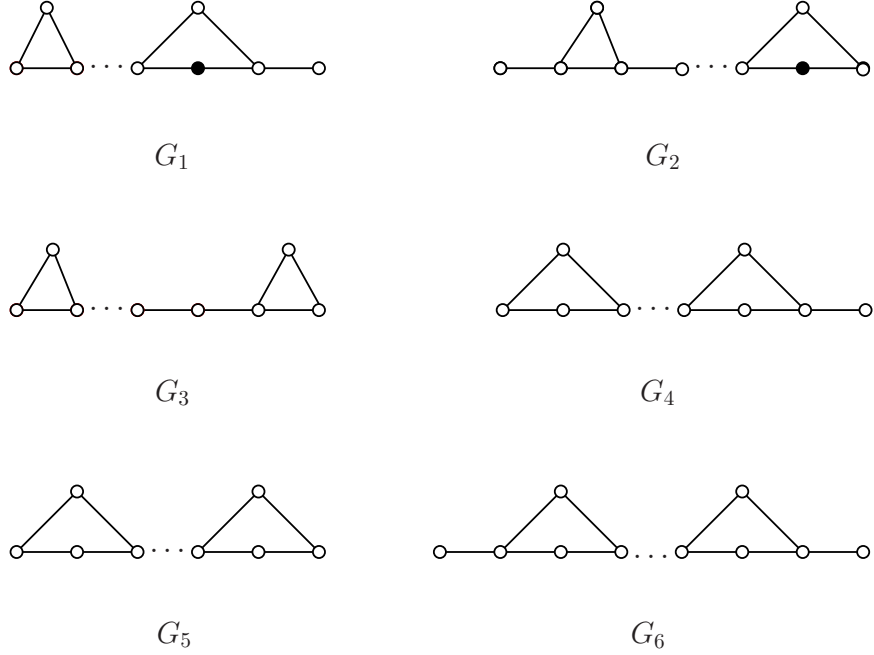


Figure 7: The graphs G_i for $i = 1, 2, 3, 4, 5, 6$.

Otherwise, G contains one triangle or one quadrangle which has at most one common vertex with the other cycle that is a triangle or a quadrangle. Choose C_a and C_b as above. Let $b \geq a$.

If $a = 3$, then G is isomorphic to G_1 , G_2 or G_3 in Figure 7, where the black vertices may not occur. Similarly, we can obtain that $G \succ B_{n,n-3}$.

If $a = 4$, then G is isomorphic to G_4 , G_5 or G_6 in Figure 7. We can show that $G \succ B_{n,n-3}$ in the same way.

Hence the conclusion follows. ■

Lemma 4.2 *Let $G \in \mathcal{B}(n, d)$ with $n \geq 8$ and $3 \leq d \leq n - 4$. If G contains no pendent vertices, then $G \succ B_{n,d+1}$.*

Proof. We choose C_a, C_b in G and if there exists the third cycle, then we choose C_c and t as above. Let $b \geq a$. Since $d \leq n - 4$, we have $b \geq 5$.

Case 1 C_a and C_b have no common edges.

Then $d = \lfloor \frac{a}{2} \rfloor + \lfloor \frac{b}{2} \rfloor + l(G)$, $d(G - u_1 u_2) = \lfloor \frac{a}{2} \rfloor + l(G) + b - 2 \geq d + 1$, $d(G - u_1 - u_2) = \lfloor \frac{a}{2} \rfloor + l(G) + b - 3 \geq d$. According to Lemmas 2.1, 2.2,

2.10 and Theorem 3.2,

$$\begin{aligned}
m_k(G) &= m_k(G - u_1u_2) + m_{k-1}(G - u_1 - u_2) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(U_{n-2,d}) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(P_{d-2} \cup S_{n-d}) \\
&= m_k(B_{n,d+1}).
\end{aligned}$$

Further, we have $m_2(G) > m_2(B_{n,d+1})$, thus $G \succ B_{n,d+1}$.

Case 2 C_a and C_b have at least one common edge.

Notice that $a - t \geq t, b - t \geq t$, where $t \geq 1$. It follows that $c \geq b + 1$, $d = \lfloor \frac{c}{2} \rfloor = \lfloor \frac{a+b}{2} \rfloor - t$, $d(G - w_0 - w_1) = c - 3 \geq d$ and $d \geq 3$.

If $b > 5$ or $b = 5$ and a is even, then $d(G - w_0w_1) = \lfloor \frac{a}{2} \rfloor + b - t - 1 \geq d + 1$, by Lemmas 2.1, 2.2, 2.9 and Theorem 3.2,

$$\begin{aligned}
m_k(G) &= m_k(G - w_0w_1) + m_{k-1}(G - w_0 - w_1) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(U_{n-2,d}) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(T_{n-2,d}) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(P_{d-2} \cup S_{n-d}) \\
&= m_k(B_{n,d+1})
\end{aligned}$$

together with $m_2(G) > m_2(B_{n,d+1})$, hence $G \succ B_{n,d+1}$.

If $b = 5$ and a is odd, then G is isomorphic to the two graphs in Figure 8, it is easy to verify that $G \succ B_{n,d+1}$ and the proof is complete. \blacksquare

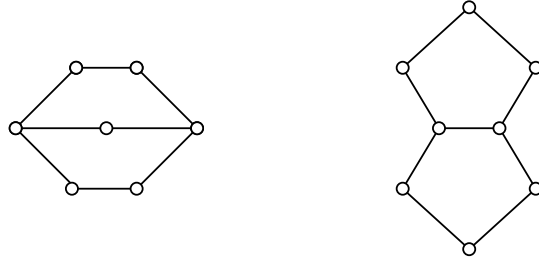


Figure 8: The graphs isomorphic to G when $b = 5$ and a is odd.

Lemma 4.3 *Let $G \in \mathcal{B}(n, d)$ with $n \geq 8$ and $3 \leq d \leq n - 4$. If G contains exactly one pendent vertex u on all diametrical paths of G such that $G - u$ contains no pendent vertices, then $G \succ B_{n,d+1}$.*

Proof. We choose C_a, C_b in G and if there exists the third cycle, then we choose C_c and t as above. Let $b \geq a$. Since $d \leq n - 4$, we have $b \geq 5$. Let v be the neighbor of u .

Case 1 C_a and C_b have no common edges.

Then $d = \lfloor \frac{a}{2} \rfloor + \lfloor \frac{b}{2} \rfloor + l(G) + 1$.

If $b \geq 7$, then $d(G - u_1u_2) \geq \lfloor \frac{a}{2} \rfloor + l(G) + b - 2 \geq d + 1$.

If v lies on C_a and $b = 5$ or 6 , then $d(G - u_1u_2) = \lfloor \frac{a}{2} \rfloor + l(G) + b - 1 = d + 1$.

If v lies on C_b , $a = 5$ and $b = 6$, then $d(G - v_1v_2) = \lfloor \frac{b}{2} \rfloor + l(G) + a - 1 = d + 1$.

In these cases, the proof is the same as Case 1 of Lemma 4.2.

Otherwise, v lies on C_b , $a = 3$ or 4 and $b = 5$ or 6 .

If $l(G) = 0$, then G is isomorphic to finitely many graphs. Apply Lemma 2.1 and direct calculation, we can get $G \succ B_{n,d+1}$.

So suppose that $l(G) \geq 1$. If $a = 3$ and $b = 5$, then $G - v_0v_1 \in \mathcal{U}(n, d+1)$. $G - v_0 - v_1 = P_1 \cup G_0$, where $G_0 \in \mathcal{U}(n-3, d-2)$. Since $d(G_0) = d-2$, $n(G_0) = n-3$, then $n-3 = d-2+3$, that is, $n-d = 4$, meanwhile, $l(G) - 1 = d-2-3 = d-5$, i.e., $l(G) = d-4$. Thus $G_0 - u_0u_1 \supseteq P_{d-2} \cup S_3$, $G_0 - u_0 - u_1 = P_{d-5} \cup P_4$. Therefore, by Lemmas 2.1, 2.2, 2.3 and Theorem 3.2,

$$\begin{aligned}
m_k(G) &= m_k(G - v_0v_1) + m_{k-1}(G - v_0 - v_1) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(G_0 - u_0u_1) + m_{k-2}(G_0 - u_0 - u_1) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(P_{d-2} \cup S_3) + m_{k-2}(P_{d-2}) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(P_{d-2} \cup S_{n-d}) \\
&= m_k(B_{n,d+1}).
\end{aligned}$$

In particular, $m_2(G) > m_2(B_{n,d+1})$, thus $G \succ B_{n,d+1}$.

If $a = 3$ and $b = 6$, by similar arguments, we can obtain that $G \succ B_{n,d+1}$.

If $a = 4$ and $b = 5$, then $n = d + 1 + 3 = d + 4$, i.e., $n - d - 1 = 3$, $G - v_0v_1 \in \mathcal{U}(n, d+1)$ and $G - v_0 - v_1 = P_2 \cup G_0$, where $G_0 \in \mathcal{U}(n-4, d-3)$. Similarly,

$$\begin{aligned}
m_k(G) &= m_k(G - v_0v_1) + m_{k-1}(G - v_0 - v_1) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(P_2 \cup G_0 - u_0u_1) + m_{k-2}(P_2 \cup G_0 - u_0 - u_1) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(P_2 \cup P_{d-2}) + m_{k-2}(P_2 \cup P_{d-6} \cup P_4) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(P_3 \cup P_{d-3}) + m_{k-2}(P_{d-2}) \\
&= m_k(B_{n,d+1}).
\end{aligned}$$

Moreover, $m_2(G) > m_2(B_{n,d+1})$, hence $G \succ B_{n,d+1}$.

If $a = 4$ and $b = 6$, we can verify that $G \succ B_{n,d+1}$ in the same way.

Case 2 C_a and C_b have at least one common edge.

Then $d = \lfloor \frac{c}{2} \rfloor + 1 = \lfloor \frac{a+b}{2} \rfloor - t + 1$. Since $b \geq 5$, $w_0, w_1 \neq v$ and $d(G - w_0w_1) = \lfloor \frac{a}{2} \rfloor + b - t - 1$. When $b \geq 6$, $d(G - w_0w_1) \geq d + 1$,

$d(G - w_0w_1) \geq d - 1$. And then

$$\begin{aligned}
m_k(G) &= m_k(G - w_0w_1) + m_{k-1}(G - w_0 - w_1) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(T_{n-2,d-1}) \\
&\geq m_k(U_{n,d+1}) + m_{k-1}(P_{d-2} \cup S_{n-d}) \\
&= m_k(B_{n,d+1})
\end{aligned}$$

along with $m_2(G) > m_2(B_{n,d+1})$, hence $G \succ B_{n,d+1}$. Now, we are left with the cases:

- (i) $b = 5, t = 2, a = 4, uv \in C_b$;
- (ii) $b = 5, t = 2, a = 4, uv \in C_a$;
- (iii) $b = 5, t = 2, a = 5$.

It can be checked directly that $G \succ B_{n,d+1}$ in these cases.

Combining Cases 1 and 2, we arrive at the result. \blacksquare

Theorem 4.4 *Let $G \in \mathcal{B}(n, d)$ with $n \geq 8$ and $3 \leq d \leq n - 3$. If there are two vertex-disjoint cycles in G , then $G \succ B_{n,d}$.*

Proof. The proof proceeds by induction on $n - d$. By Lemma 4.1, the result holds for $n - d = 3$. Let $h \geq 4$ and assume that the result holds for $n - d < h$. Suppose that $G \in \mathcal{B}(n, d)$ with $n - d = h$.

Case 1 There is no pendent vertex in G .

Then by Lemmas 2.11 and 4.2, $G \succ B_{n,d+1} \succ B_{n,d}$.

Case 2 There is a pendent vertex outside some diametrical path $P(G) = x_0x_1 \cdots x_d$.

Let u , adjacent to v , be a pendent vertex outside $P(G)$ in G . Then $G - u \in \mathcal{B}(n - 1, d)$. Since $(n - 1) - d < h$, by the induction hypothesis, $G - u \succ B_{n-1,d}$.

By Lemma 2.1,

$$m_k(B_{n,d}) = m_k(B_{n-1,d}) + m_{k-1}(T_{d+1,d-2}) \quad (*)$$

Meanwhile, let $H = G - u - v$, then

$$\begin{aligned}
m_k(G) &= m_k(G - u) + m_{k-1}(G - u - v) \\
&= m_k(G - u) + m_{k-1}(H) \\
&\geq m_k(B_{n-1,d}) + m_{k-1}(H).
\end{aligned}$$

Hence, to complete the proof we shall show that $m_k(H) \geq m_k(T_{d+1,d-2})$. Select C_a and C_b as above.

Subcase 2.1 v lies on some cycle, say C_a . Then $H \supseteq C_b$.

First, suppose that $P(G)$ and C_b have no common vertices. Then $H \supseteq P_i \cup P_{d-i} \cup C_b$ when v lies on $P(G)$, say $v = v_i$. Otherwise, $H \supseteq P_{d+1} \cup C_b \supseteq P_i \cup P_{d-i} \cup C_b$. Thus

$$\begin{aligned}
m_k(H) &\geq m_k(P_i \cup P_{d-i} \cup C_b) \geq m_k(P_{d-1} \cup S_b) \geq m_k(P_{d-1} \cup P_3) \\
&\geq m_k(P_{d+1}) \geq m_k(T_{d+1,d-2}).
\end{aligned}$$

Next, suppose that $P(G)$ and C_b have common vertices x_l, \dots, x_{l+q} , where $q \geq 0$.

If v lies outside $P(G)$, then $H \supseteq G_1$, where $G_1 \in \mathcal{U}(s_1, d)$ with $s_1 \geq d+2$. Hence,

$$m_k(H) \geq m_k(G_1) \geq m_k(U_{s_1, d}) \geq m_k(T_{s_1, d}) \geq m_k(P_{d+1}) \geq m_k(T_{d+1, d-2}).$$

So suppose that v lies on $P(G)$. Then $P(G)$ and C_a have common vertices, say x_i, \dots, x_{i+p} , where $p \geq 0$.

When $p = 0$, then $i \geq 1$, thus $H \supseteq P_2 \cup P_i \cup G_2$, where $G_2 \in \mathcal{U}(s_2, d_2)$, $d_2 \geq d - i - 1 \geq 1$ and $s_2 \geq d_2 + 2$. If $d_2 = 1, i = d - 2$, then $G_2 = C_3$. Therefore,

$$m_k(H) \geq m_k(P_2 \cup P_{d-2} \cup C_3) \geq m_k(P_{d-1} \cup P_3) \geq m_k(P_{d+1}) \geq m_k(T_{d+1, d-2}).$$

If $d_2 = 2$, then $s_2 \geq 4, i \geq d - 3$. Consequently,

$$\begin{aligned} m_k(H) &\geq m_k(P_2 \cup P_i \cup G_2) \geq m_k(P_2 \cup P_i \cup S_{s_2}) \geq m_k(P_2 \cup P_i \cup T_{4,2}) \\ &\geq m_k(T_{i+4, i+2}) \geq m_k(T_{d+1, d-1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

If $d_2 \geq 3$, then $s_2 \geq 5$. Thus

$$\begin{aligned} m_k(H) &\geq m_k(P_2 \cup P_i \cup G_2) \geq m_k(P_2 \cup P_i \cup U_{s_2, d_2}) \geq m_k(P_2 \cup P_i \cup T_{s_2, d_2}) \\ &\geq m_k(T_{s_2+i, d_2+i}) \geq m_k(T_{d_2+i+2, d_2+i}) \geq m_k(T_{d+1, d-1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

When $p = 1$. If $v = v_i$, then $i \geq 1$ and $H \supseteq P_i \cup G_3$, where $G_3 \in \mathcal{U}(s_3, d_3)$, $d_3 \geq d - i \geq 3, s_3 \geq d_3 + 2$. Accordingly,

$$\begin{aligned} m_k(H) &\geq m_k(P_i \cup G_3) \geq m_k(P_i \cup U_{s_3, d_3}) \geq m_k(P_i \cup T_{s_3, d_3}) \geq m_k(T_{s_3+i-1, d_3+i-1}) \\ &\geq m_k(T_{d_2+i+2, d_2+i}) \geq m_k(T_{d+1, d-1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

If $v = v_{i+1}$, then $H \supseteq P_{i+2} \cup G_4$, where $G_4 \in \mathcal{U}(s_4, d_4)$, $d_4 \geq d - (i+1) - 1 = d - i - 2 \geq 1, s_4 \geq d_4 + 2$.

If $d_4 = 1$, then $i = d - 3, G_4 = C_3$, we have

$$m_k(H) \geq m_k(P_{d-1} \cup C_3) \geq m_k(P_{d-1} \cup P_3) \geq m_k(P_{d+1}) \geq m_k(T_{d+1, d-2}).$$

If $d_4 = 2$, then $s_4 \geq 4, i \geq d - 4$. Consequently,

$$\begin{aligned} m_k(H) &\geq m_k(P_{i+2} \cup G_4) \geq m_k(P_{i+2} \cup S_{s_4}) \geq m_k(P_{i+2} \cup T_{4,2}) \\ &\geq m_k(T_{i+5, i+3}) \geq m_k(T_{d+1, d-1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

If $d_4 \geq 3$. Then

$$\begin{aligned} m_k(H) &\geq m_k(P_{i+2} \cup G_4) \geq m_k(P_{i+2} \cup U_{s_4, d_4}) \geq m_k(P_{i+2} \cup T_{s_4, d_4}) \\ &\geq m_k(T_{s_4+i+1, d_4+i+1}) \geq m_k(T_{d+1, d-1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

Now suppose that $p \geq 2$. If $v \neq x_i, x_{i+p}$, then $H \supseteq G_5$, where $G_5 \in \mathcal{U}(s_5, d_5), d_5 \geq d, s_5 \geq d_5 + 2$. Hence

$$m_k(H) \geq m_k(G_5) \geq m_k(U_{s_5, d_5}) \geq m_k(T_{s_5, d_5}) \geq m_k(T_{d+1, d-2}).$$

If $v = x_i$, then $H \supseteq P_i \cup G_6$, where $G_6 \in \mathcal{U}(s_6, d_6), d_6 \geq d - i - 1 \geq 3, s_6 \geq d_6 + 3$. Therefore,

$$\begin{aligned} m_k(H) &\geq m_k(P_i \cup G_6) \geq m_k(P_i \cup U_{s_6, d_6}) \geq m_k(P_i \cup T_{s_6, d_6}) \\ &\geq m_k(T_{s_6+i-1, d_6+i-1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

If $v = x_{i+p}$, then $H \supseteq T_1 \cup G_7$ or $P_{i+p+1} \cup G_7$, where $G_7 \in \mathcal{U}(s_7, d_7), d_7 \geq d - i - p - 1 \geq 1, s_7 \geq d_7 + 2, T_1 \in \mathcal{T}(i+p+1, d_{T_1}), d_{T_1} \geq i+p-1$. If $d_7 = 1$, then $i+p = d-2, G_7 = C_3$, thus

$$m_k(H) \geq m_k(T_{d-1, d-3} \cup C_3) \geq m_k(T_{d-1, d-3} \cup P_3) \geq m_k(T_{d+1, d-2})$$

or

$$\begin{aligned} m_k(H) &\geq m_k(P_{i+p+1} \cup G_7) \geq m_k(P_{i+p+1} \cup C_3) \geq m_k(P_{i+p+1} \cup P_3) \\ &\geq m_k(P_{i+p+3}) = m_k(P_{d+1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

If $d_7 = 2$, then $i+p \geq d-3, s_7 \geq 4$, accordingly,

$$\begin{aligned} m_k(H) &\geq m_k(T_{i+p+1, i+p-1} \cup S_{s_7}) \geq m_k(T_{i+p+1, i+p-1} \cup T_{4, 2}) \\ &\geq m_k(T_{i+p+4, i+p+1}) \geq m_k(T_{d+1, d-2}) \end{aligned}$$

or

$$m_k(H) \geq m_k(P_{i+p+1} \cup S_{s_7}) \geq m_k(P_{i+p+1} \cup T_{4, 2}) \geq m_k(T_{i+p+4, i+p+2}) \geq m_k(T_{d+1, d-2}).$$

If $d_7 \geq 3$, then

$$\begin{aligned} m_k(H) &\geq m_k(T_{i+p+1, i+p-1} \cup U_{s_7, d_7}) \geq m_k(T_{i+p+1, i+p-1} \cup T_{s_7, d_7}) \\ &\geq m_k(T_{i+p+s_7, i+p+d_7-1}) \geq m_k(T_{d+1, d-2}) \end{aligned}$$

or

$$m_k(H) \geq m_k(P_{i+p+1} \cup U_{s_7, d_7}) \geq m_k(P_{i+p+1} \cup T_{s_7, d_7}) \geq m_k(T_{i+p+s_7, i+p+d_7}) \geq m_k(T_{d+1, d-2}).$$

Subcase 2.2 v lies outside any cycle. Then $H \supseteq C_a \cup C_b$.

First, suppose that v lies on $P(G)$ and take $v = x_i$. If $P(G)$ has no common vertices with any cycle, then $H \supseteq C_a \cup C_b \cup P_i \cup P_{d-i}$. Thus

$$m_k(H) \geq m_k(C_a \cup C_b \cup P_i \cup P_{d-i}) \geq m_k(P_3 \cup P_{d-1}) \geq m_k(P_{d+1}) \geq m_k(T_{d+1, d-2}).$$

If $P(G)$ has no common vertices with exactly one cycle, say C_a . Then $H \supseteq C_a \cup P_i \cup G_1$, where $G_1 \in \mathcal{U}(s_1, d_1)$, $d_1 \geq d - i - 1$, $s_1 \geq d_1 + 2$. If $d_1 = 1$, then $i = d - 2$, $G_1 = C_3$, hence

$$m_k(H) \geq m_k(C_a \cup P_i \cup C_3) \geq m_k(P_2 \cup P_i \cup P_3) \geq m_k(P_{i+3}) = m_k(P_{d+1}) \geq m_k(T_{d+1, d-2}).$$

If $d_1 = 2$, then $i \geq d - 3$, $s_1 \geq 4$. Consequently,

$$m_k(H) \geq m_k(C_a \cup P_i \cup G_1) \geq m_k(P_2 \cup P_i \cup T_{s_1, 2}) \geq m_k(T_{i+s_1, i+2}) \geq m_k(T_{d+1, d-2}).$$

If $d_1 \geq 3$, then

$$\begin{aligned} m_k(H) &\geq m_k(C_a \cup P_i \cup G_1) \geq m_k(P_2 \cup P_i \cup U_{s_1, d_1}) \geq m_k(P_2 \cup P_i \cup T_{s_1, d_1}) \\ &\geq m_k(P_{i+1} \cup T_{s_1, d_1}) \geq m_k(T_{s_1+i, d_1+i}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

If $P(G)$ has common vertices with both cycles, then $H \supseteq P_i \cup G_2$ or $G_3 \cup G_4$, where $G_2 \in \mathcal{U}(s_2, d_2)$, $G_3 \in \mathcal{U}(s_3, d_3)$, $G_4 \in \mathcal{U}(s_4, d_4)$. Meanwhile, $d_2 \geq d - i - 1 \geq 3$, $n - 2 - i \geq s_2 \geq d_2 + 3$, $d_3 \geq i - 1 \geq 1$, $s_3 \geq d_3 + 2$, $d_4 \geq d - i - 1 \geq 1$, $s_4 \geq d_4 + 2$.

Suppose that $H \supseteq P_i \cup G_2$. Since $s_2 - d_2 \leq n - 2 - i - (d - i - 1) = n - d - 1 < h$, thus by the induction hypothesis, $G_2 \succ B_{s_2, d_2}$. Then

$$\begin{aligned} m_k(H) &\geq m_k(P_i \cup G_2) \geq m_k(P_i \cup B_{s_2, d_2}) \geq m_k(P_i \cup T_{s_2, d_2}) \\ &\geq m_k(T_{s_2+i-1, d_2+i-1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

Suppose that $H \supseteq G_3 \cup G_4$. If $d_3 = d_4 = 1$, then $n = 8$, $d = 4$, $G_3 = G_4 = C_3$. In this case, it is easy to obtain that $G \succ B_{8, 4}$.

If $d_3 = 2$, $d_4 = 1$, then $d = 5$, $s_3 \geq 4$, $G_4 = C_3$. We can have

$$m_k(H) \geq m_k(G_3 \cup G_4) \geq m_k(S_{s_3} \cup C_3) \geq m_k(T_{4, 2} \cup P_3) \geq m_k(T_{6, 4}) \geq m_k(T_{d+1, d-2}).$$

If $d_3 \geq 3$, $d_4 = 1$, then $d_3 \geq d - 3$. Accordingly,

$$\begin{aligned} m_k(H) &\geq m_k(G_3 \cup G_4) \geq m_k(U_{s_3, d_3} \cup C_3) \geq m_k(T_{s_3, d_3} \cup P_3) \\ &\geq m_k(T_{s_3+2, d_3+2}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

If $d_3 = 2$, $d_4 = 2$, then $d = 6$, $s_3 \geq 4$, $s_4 \geq 4$. Hence

$$m_k(H) \geq m_k(G_3 \cup G_4) \geq m_k(S_{s_3} \cup S_{s_4}) \geq m_k(T_{4, 2} \cup T_{4, 2}) \geq m_k(T_{7, 4}) = m_k(T_{d+1, d-2}).$$

If $d_3 \geq 3$, $d_4 = 2$, then $d_3 \geq d - 4$, $s_4 \geq 4$. Thus

$$\begin{aligned} m_k(H) &\geq m_k(G_3 \cup G_4) \geq m_k(U_{s_3, d_3} \cup S_{s_4}) \geq m_k(T_{s_3, d_3} \cup T_{s_4, 2}) \\ &\geq m_k(T_{s_3+s_4-1, d_3+2}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

If $d_3 \geq 3$, $d_4 \geq 3$, then $d_3 + d_4 \geq d - 2$. Therefore,

$$\begin{aligned} m_k(H) &\geq m_k(G_3 \cup G_4) \geq m_k(U_{s_3, d_3} \cup U_{s_4, d_4}) \geq m_k(T_{s_3, d_3} \cup T_{s_4, d_4}) \\ &\geq m_k(T_{s_3+s_4-1, d_3+d_4}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

Next, suppose that v lies outside $P(G)$. Then $H \supseteq C_a \cup C_b \cup P(G)$, $C_a \cup G_5$ or G_6 , where $G_5 \in \mathcal{U}(s_5, d)$ with $s_5 \geq d + 2$ and $G_6 \in \mathcal{B}(s_6, d)$ with $d + 3 \leq s_6 \leq n - 2$. It is easy to show as above that $m_k(H) \geq m_k(T_{d+1, d-2})$.

Case 3 Any diametrical path of G contains all pendent vertices.

Let $P(G) = x_0x_1 \cdots x_d$ be any diametrical path of G . Suppose that $y_0y_1 \cdots y_p$ is a path whose internal vertices y_1, y_2, \dots, y_{p-1} all have degree two and y_p is a pendent vertex. Then we call it a pendent path, denoted by (y_0, y_p) .

Subcase 3.1 There are exactly two pendent vertices in G , namely, x_0 and x_d .

Suppose that $\deg_G(x_i), \deg_G(x_l) \geq 3$ such that (x_i, x_0) and (x_l, x_d) are distinct pendent paths. Let $s = l - i$.

If $s = 0$, i.e., $x_i = x_l$. Then $i \geq 3, l \leq d - 3$. Since

$$\begin{aligned} m_k(G) &= m_k(G - x_{i-3}x_{i-2}) + m_{k-1}(G - x_{i-3} - x_{i-2}) \\ &= m_k(G - x_{i-3}x_{i-2} - x_{l+1}x_{l+2}) + m_{k-1}(G - x_{i-3}x_{i-2} - x_{l+1} - x_{l+2}) \\ &\quad + m_{k-1}(G - x_{i-3} - x_{i-2} - x_{l+2}x_{l+3}) + m_{k-2}(G - x_{i-3} - x_{i-2} - x_{l+2} - x_{l+3}) \\ &= m_k(G_1 \cup P_{i-2} \cup P_{d-i-1}) + m_{k-1}(G_3 \cup P_{i-2} \cup P_{d-i-2}) \\ &\quad + m_{k-1}(G_2 \cup P_{i-3} \cup P_{d-i-2}) + m_{k-2}(G_4 \cup P_{i-3} \cup P_{d-i-3}) \end{aligned}$$

and

$$\begin{aligned} m_k(B_{n,d}) &= m_k(B_{n-d+3,3} \cup P_{d-3}) + m_{k-1}(S_{n-d+2} \cup P_{d-4}) \\ &= m_k(B_{n-d+3,3} \cup P_{i-2} \cup P_{d-i-1}) + m_{k-1}(B_{n-d+3,3} \cup P_{i-3} \cup P_{d-i-2}) \\ &\quad + m_{k-1}(S_{n-d+2} \cup P_{i-2} \cup P_{d-i-2}) + m_{k-2}(S_{n-d+2} \cup P_{i-3} \cup P_{d-i-3}), \end{aligned}$$

it suffices to prove that $G_1, G_2 \succ B_{n-d+3,3}$ and $G_3, G_4 \succ S_{n-d+2}$, where $G_1 = G - (x_{i-3}, x_0) - (x_{l+2}, x_d) \in \mathcal{B}(n-d+3, d_1)$, $G_2 = G - (x_{i-2}, x_0) - (x_{l+3}, x_d) \in \mathcal{B}(n-d+3, d_2)$, $G_3 = G - (x_{i-3}, x_0) - (x_{l+1}, x_d)$, $G_4 = G - (x_{i-2}, x_0) - (x_{l+2}, x_d)$, $d_1 \geq 4, d_2 \geq 4$. Since $n-d+3-d_1 \leq n-d-1 < h$, $n-d+3-d_2 \leq n-d-1 < h$. Then by the induction hypothesis, $G_1 \succ B_{n-d+3, d_1} \succ B_{n-d+3,3}$, $G_2 \succ B_{n-d+3, d_2} \succ B_{n-d+3,3}$. In addition, both G_3 and G_4 are bicyclic graphs with $n-d+2$ vertices, consequently, we have $G_3, G_4 \succ S_{n-d+2}$.

If $s = 1$ or $s = 2$, then by similar arguments as above, we have the desired result.

If $s \geq 3$, it is easy to obtain that $i \geq 2$ and $l \leq d - 2$. Then

$$\begin{aligned} m_k(G) &= m_k(G - x_{i-2}x_{i-1}) + m_{k-1}(G - x_{i-2} - x_{i-1}) \\ &= m_k(G - x_{i-2}x_{i-1} - x_{l+1}x_{l+2}) + m_{k-1}(G - x_{i-2}x_{i-1} - x_{l+1} - x_{l+2}) \\ &\quad + m_{k-1}(G - x_{i-2} - x_{i-1} - x_{l+1}x_{l+2}) + m_{k-2}(G - x_{i-2} - x_{i-1} - x_{l+1} - x_{l+2}) \\ &= m_k(G_5 \cup P_{i-1} \cup P_{d-l-1}) + m_{k-1}(G_7 \cup P_{i-1} \cup P_{d-l-2}) \\ &\quad + m_{k-1}(G_6 \cup P_{i-2} \cup P_{d-l-1}) + m_{k-2}(G_8 \cup P_{i-2} \cup P_{d-l-2}), \end{aligned}$$

$$\begin{aligned}
m_k(B_{n,d}) &= m_k(B_{n-d+l+1,l+1} \cup P_{d-l-1}) + m_{k-1}(B_{n-d+l,l} \cup P_{d-l-2}) \\
&= m_k(B_{n-d+s+2,s+2} \cup P_{i-1} \cup P_{d-l-1}) + m_{k-1}(B_{n-d+s+1,s+1} \cup P_{i-2} \cup P_{d-l-1}) \\
&\quad + m_{k-1}(B_{n-d+s+1,s+1} \cup P_{i-1} \cup P_{d-l-2}) + m_{k-2}(B_{n-d+s,s} \cup P_{i-2} \cup P_{d-l-2}).
\end{aligned}$$

Hence it suffices to show that $G_5 \succ B_{n-d+s+2,s+2}$, $G_6, G_7 \succ B_{n-d+s+1,s+1}$, $G_8 \succ B_{n-d+s,s}$.

Let $d_j = d(G_j)$, and $n_j = |V(G_j)|$, where $j = 5, 6, 7, 8$. Then $d_j \geq 4$. If $n_j - d_j < h$ holds for all $j \in \{5, 6, 7, 8\}$, then by the induction hypothesis and previous Lemmas, we have the desired results. Otherwise, there exists at least a $j \in \{5, 6, 7, 8\}$ such that $n_j - d_j = h$. When $j = 5$, $G_5 \in \mathcal{B}(n-d+s+2, s+2)$. If there exists some diametrical path $P(G_5)$ such that x_{i-1} or x_{l+1} lies outside $P(G_5)$, the proof is similar with Case 2, thus $G_5 \succ B_{n-d+s+2,s+2}$. Otherwise, $G_5 - x_{i-1} \in \mathcal{B}(n-d+s+1, s+1)$, then by Lemma 4.3, $G_5 \succ B_{n-d+s+1,s+2}$. We also have $G_5 - x_{i-1} - x_i \succeq U_{n-d+s,s} \succ T_{n-d+s,s} \succ T_{s+3,s}$. Therefore, $G_5 \succ B_{n-d+s+2,s+2}$.

When $j = 7$, $G_7 \in \mathcal{B}(n-d+s+1, s+1)$. If x_{i-1} lies on all diametrical paths of G_7 , then by Lemma 4.3, $G_7 \succ B_{n-d+s+1,s+2} \succ B_{n-d+s+1,s+1}$. Otherwise, in the same way as in Case 2, we can also obtain $G_7 \succ B_{n-d+s+1,s+1}$.

Similarly, when $j = 6$, we can have $G_6 \succ B_{n-d+s+1,s+1}$.

When $j = 8$, $G_8 \in \mathcal{B}(n-d+s, s)$. Since G_8 contains no pendent vertices, then by Lemmas 2.11 and 4.2, $G_8 \succ B_{n-d+s,s+1} \succ B_{n-d+s,s}$.

Subcase 3.2 There is only one pendent vertex in G , say x_0 .

Since there are two vertex-disjoint cycles in G , $\deg_G(x_d) = 2$. Suppose that x_l is the vertex such that $\deg_G(x_l) \geq 3$ and $\deg_G(x_i) = 2$ for $l+1 \leq i \leq d$. It is easy to check that $l \leq d-2$. Then $G - x_{d-1}x_d \in \mathcal{U}(n, d_9)$, where $d_9 \geq d$, and $G - x_{d-1} - x_d \in \mathcal{U}(n-2, d_{10})$, where $d_{10} \geq d-1$. Hence,

$$\begin{aligned}
m_k(G) &= m_k(G - x_{d-1}x_d) + m_{k-1}(G - x_{d-1} - x_d) \\
&\geq m_k(U_{n,d_9}) + m_{k-1}(U_{n-2,d_{10}}) \\
&\geq m_k(U_{n,d}) + m_{k-1}(U_{n-2,d-1}) \\
&\geq m_k(U_{n,d}) + m_{k-1}(T_{n-2,d-1}) \\
&\geq m_k(U_{n,d}) + m_{k-1}(P_{d-3} \cup S_{n-d+1}) \\
&= m_k(B_{n,d}).
\end{aligned}$$

In particular, $m_2(G) > m_2(B_{n,d})$. Thus, $G \succ B_{n,d}$.

Therefore, we complete the proof. ■

Theorem 4.5 *Let $G \in \mathcal{B}(n, d)$ with $n \geq 8$, $3 \leq d \leq n-3$ and $G \neq B_{n,d}$. If there is no vertex-disjoint cycles in G , then $G \succ B_{n,d}$.*

Proof. We will prove this theorem by induction on $n-d$.

By Lemma 4.1, the result holds for $n-d = 3$. Let $h \geq 4$ and suppose that the result holds for $n-d < h$. Now assume that $n-d = h$, let $G \in \mathcal{B}(n, d)$ and $G \neq B_{n,d}$.

Case 1 If G contains no pendent vertices.

Then by Lemmas 2.11 and 4.2, $G \succ B_{n,d+1} \succ B_{n,d}$.

Case 2 If there exists a pendent vertex outside some diametrical path $P(G) = x_0x_1 \dots x_d$.

Let u be a pendent vertex outside $P(G)$ and v be its unique neighbor. Then $G - u \in \mathcal{B}(n-1, d)$. If $G - u = B_{n-1,d}$, then it can be checked that $G - u - v \succ T_{d+1,d-2}$. And thus from (*), we can obtain that $G \succ B_{n,d}$. Otherwise, by the induction hypothesis, we have $G - u \succ B_{n-1,d}$. Let $H = G - u - v$, in order to prove the result, we only need to show that $m_k(H) \geq m_k(T_{d+1,d-2})$. We choose C_a, C_b as above in G , and if there exists the third cycle, denote it by C_c .

Subcase 2.1 When v lies on some cycle, say C_a .

First, suppose that $v = u_0$ or u_t , then H contains no cycles. If v lies outside $P(G)$, then $H \supseteq P(G)$. Thus $m_k(H) \geq m_k(P(G)) = m_k(P_{d+1}) \geq m_k(T_{d+1,d-2})$. If v lies on $P(G)$, say $v = x_i$.

(1) If C_a and C_b have exactly one common vertex, then $H \supseteq P_2 \cup P_2 \cup P_i \cup P_{d-i}, P_2 \cup P_i \cup P_{d-i+1}, P_2 \cup P_{i+1} \cup P_{d-i}, P_{i+1} \cup P_{d-i+1}, P_2 \cup P_i \cup T_1, P_2 \cup P_{d-i} \cup T_2, P_{i+1} \cup T_1, P_{d-i+1} \cup T_2$ or $T_1 \cup T_2$, where $T_1 \in \mathcal{T}(d-i+1, d-i-1)$ and $T_2 \in \mathcal{T}(i+1, i-1)$.

If $H \supseteq P_2 \cup P_2 \cup P_i \cup P_{d-i}, P_2 \cup P_i \cup P_{d-i+1}, P_2 \cup P_{i+1} \cup P_{d-i}$ or $P_{i+1} \cup P_{d-i+1}$, then $m_k(H) \geq m_k(P_{d+1}) \geq m_k(T_{d+1,d-2})$;

If $H \supseteq P_2 \cup P_i \cup T_1$, then $m_k(H) \geq m_k(P_{i+1} \cup T_1) \geq m_k(P_{i+1} \cup T_{d-i+1,d-i-1}) \geq m_k(T_{d+1,d-1}) \geq m_k(T_{d+1,d-2})$; Similarly, if $H \supseteq P_2 \cup P_{d-i} \cup T_2$, we also have $m_k(H) \geq m_k(T_{d+1,d-2})$;

If $H \supseteq T_1 \cup T_2$, then $m_k(H) \geq m_k(T_1 \cup T_2) \geq m_k(T_{d-i+1,d-i-1} \cup T_{i+1,i-1}) \geq m_k(T_{d+1,d-2})$;

If $H \supseteq P_{i+1} \cup T_1$ or $H \supseteq P_{d-i+1} \cup T_2$, then $m_k(H) \geq m_k(T_1 \cup T_2) \geq m_k(T_{d+1,d-2})$.

(2) If C_a and C_b have at least two common vertices, then $H \supseteq P_3 \cup P_i \cup P_{d-i}, P_i \cup P_{d-i+2}, P(G), P_i \cup T_3$ or $P_i \cup T_4$, where $T_3 \in \mathcal{T}(d-i+2, d-i-1)$ and $T_4 \in \mathcal{T}(d-i+2, d-i)$.

If $H \supseteq P_3 \cup P_i \cup P_{d-i}, P_i \cup P_{d-i+2}$ or $P(G)$, then $m_k(H) \geq m_k(P_{d+1}) \geq m_k(T_{d+1,d-2})$;

If $H \supseteq P_i \cup T_3$, then $m_k(H) \geq m_k(P_i \cup T_3) \geq m_k(P_i \cup T_{d-i+2,d-i-1}) \geq m_k(T_{d+1,d-2})$;

If $H \supseteq P_i \cup T_4$, then $m_k(H) \geq m_k(P_i \cup T_4) \geq m_k(P_i \cup T_{d-i+2,d-i}) \geq m_k(T_{d+1,d-1}) \geq m_k(T_{d+1,d-2})$.

Next, suppose that $v \neq u_0$ and $v \neq u_t$. If v lies outside $P(G)$, then $H \supseteq P(G)$, similarly, we have $m_k(H) \geq m_k(T_{d+1,d-2})$. So suppose that v lies on $P(G)$. Then $P(G)$ and C_a have common vertices, say x_i, \dots, x_{i+p} , where $p \geq 0$.

(1) If $p = 0$, then $i \geq 1$ and $H \supseteq P_i \cup P_{d-i} \cup C_s$, where $s = b$ or c . It

follows that

$$\begin{aligned} m_k(H) &\geq m_k(P_i \cup P_{d-i} \cup C_s) \geq m_k(P_i \cup P_{d-i} \cup S_s) \geq m_k(P_i \cup P_{d-i} \cup P_3) \\ &\geq m_k(P_{d+1}) \geq m_k(T_{d+1,d-2}). \end{aligned}$$

(2) If $p \geq 1$. When $v \neq x_i$ and $v \neq x_{i+p}$, then $H \supseteq G_1$, where $G_1 \in \mathcal{U}(s_1, d_1)$, $d_1 \geq d$ and $s_1 \geq d_1 + 2$. Thus

$$m_k(H) \geq m_k(G_1) \geq m_k(U_{s_1, d_1}) \geq m_k(T_{s_1, d_1}) \geq m_k(T_{s_1, d}) \geq m_k(T_{d+1, d-2}).$$

When $v = x_i$ or x_{i+p} , say $v = x_i$ ($i \geq 1$), then $H \supseteq P_i \cup G_2$, where $G_2 \in \mathcal{U}(s_2, d_2)$, $d_2 \geq d - i - 1 \geq 2$ ($d - i - 1 \geq 1$, for $d - i - 1 = 1$, clearly $m_k(H) \geq m_k(T_{i+3, i})$) and $s_2 \geq d - i + 2$; or $H \supseteq P_i \cup G_3$, where $G_3 \in \mathcal{U}(s_3, d_3)$, $d_3 \geq d - i \geq 2$ and $s_3 \geq d_3 + 2$; or $H \supseteq P_i \cup G'$, where G' is the graph obtained by attaching a path P_{d-i-2} to a vertex of $C_b = C_3$.

Suppose that $H \supseteq P_i \cup G_2$. If $d_2 = 2$, then $i = d - 3$ and $s_2 \geq 5$. Hence,

$$m_k(H) \geq m_k(P_i \cup G_2) \geq m_k(P_i \cup S_{s_2}) \geq m_k(P_i \cup T_{5,2}) \geq m_k(T_{i+4, i+1}) = m_k(T_{d+1, d-2}).$$

If $d_2 \geq 3$, then

$$\begin{aligned} m_k(H) &\geq m_k(P_i \cup G_2) \geq m_k(P_i \cup U_{s_2, d_2}) \geq m_k(P_i \cup T_{s_2, d_2}) \\ &\geq m_k(T_{i+s_2-1, i+d_2-1}) \geq m_k(T_{d+1, d-1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

Suppose that $H \supseteq P_i \cup G_3$. If $d_3 = 2$, then $i = d - 2$ and $s_3 \geq 4$. Thus

$$\begin{aligned} m_k(H) &\geq m_k(P_i \cup G_3) \geq m_k(P_i \cup S_{s_3}) \geq m_k(P_i \cup T_{4,2}) \\ &\geq m_k(T_{d+1, d-1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

If $d_3 \geq 3$, then

$$\begin{aligned} m_k(H) &\geq m_k(P_i \cup G_3) \geq m_k(P_i \cup U_{s_3, d_3}) \geq m_k(P_i \cup T_{s_3, d_3}) \\ &\geq m_k(T_{i+s_3-1, i+d_3-1}) \geq m_k(T_{d+1, d-1}) \geq m_k(T_{d+1, d-2}). \end{aligned}$$

Suppose that $H \supseteq P_i \cup G'$. If $d - i - 2 = 0$, then $i = d - 2$ and $H \supseteq P_i \cup C_3$.

Therefore,

$$m_k(H) \geq m_k(P_i \cup G') \geq m_k(P_i \cup T_{4,2}) \geq m_k(T_{i+3, i+1}) = m_k(T_{d+1, d-1}) \geq m_k(T_{d+1, d-2}).$$

If $d - i - 2 \geq 1$, choose an edge $u_0 u_1$ of G' in C_3 such that both u_0 and u_1 have degree 2. Then

$$\begin{aligned} m_k(H) &\geq m_k(P_i \cup G') \\ &= m_k(P_i \cup G' - u_0 u_1) + m_{k-1}(P_i \cup G' - u_0 - u_1) \\ &= m_k(P_i \cup T_{d-i+1, d-i-1}) + m_{k-1}(P_i \cup P_{d-i-1}) \\ &\geq m_k(T_{d, d-2}) + m_{k-1}(P_{d-3}) \\ &= m_k(T_{d+1, d-2}). \end{aligned}$$

Subcase 2.2 When v lies outside any cycle.

In this case, H contains two cycles C_a and C_b with at least one common vertex. Let $C_a \cdot C_b$ denote the subgraph of G induced by $V(C_a) \cup V(C_b)$.

First, suppose that v lies on $P(G)$, say $v = x_i$.

If vertices on $P(G)$ lie outside any cycle, then $H \supseteq C_a \cdot C_b \cup P_i \cup P_{d-i}$. Thus,

$$m_k(H) \geq m_k(C_a \cdot C_b \cup P_i \cup P_{d-i}) \geq m_k(P_3 \cup P_i \cup P_{d-i}) \geq m_k(P_{d+1}) \geq m_k(T_{d+1, d-2}).$$

Otherwise, $H \supseteq P_i \cup G_1$, where $G_1 \in \mathcal{B}(s_1, d_1)$, $d_1 \geq \max\{d - i - 1, 2\}$ and $d_1 + 2 \leq s_1 \leq n - 2 - i$.

Suppose that $s_1 \geq d_1 + 3$. If $d_1 = 2$, then $i \geq d - 3$ and $s_1 \geq 5$. Thus we have

$$m_k(H) \geq m_k(P_i \cup G_1) \geq m_k(P_i \cup S_{s_1}) \geq m_k(P_i \cup T_{5,2}) \geq m_k(T_{i+4, i+1}) \geq m_k(T_{d+1, d-2}).$$

If $d_1 \geq 3$, then $d - i - 1 \leq d_1$, which deduces that $s_1 - d_1 \leq n - 2 - i - (d - i - 1) = n - d - 1 < h$. By the induction hypothesis, $G_1 \succ B_{s_1, d_1}$, therefore,

$$m_k(H) \geq m_k(P_i \cup G_1) \geq m_k(P_i \cup B_{s_1, d_1}) \geq m_k(P_i \cup T_{s_1, d_1}) \geq m_k(T_{d+1, d-2}).$$

Now suppose that $s_1 = d_1 + 2$. In this case, G_1 is obtained by attaching respectively paths P_l ($0 \leq l \leq d_1 - 2$) and P_{d_1-l-2} to the two non-adjacent vertices in $K_4 - e$. If $d_1 = 2$, then $i \geq d - 3$. It can be easily checked that $m_k(K_4 - e) \geq m_k(T_{5,2})$. Thus $m_k(H) \geq m_k(P_i \cup (K_4 - e)) \geq m_k(P_i \cup T_{5,2}) \geq m_k(T_{d+1, d-2})$. If $d_1 \geq 3$, choose an edge $u_0 u_1$ of G_1 such that u_0 and u_1 are both of degree 3 in $K_4 - e$. Then we get

$$\begin{aligned} m_k(H) &\geq m_k(P_i \cup G_1) \\ &= m_k(P_i \cup G_1 - u_0 u_1) + m_{k-1}(P_i \cup G_1 - u_0 - u_1) \\ &\geq m_k(P_i \cup U_{s_1, d_1}) + m_{k-1}(P_i \cup P_{l+1} \cup P_{d_1-l-1}) \\ &\geq m_k(P_i \cup T_{s_1, d_1}) + m_{k-1}(P_i \cup P_{d_1-1}) \\ &\geq m_k(P_i \cup T_{d-i+1, d-i-1}) + m_{k-1}(P_i \cup P_{d-i-2}) \\ &\geq m_k(T_{d, d-2}) + m_{k-1}(P_{d-3}) \\ &= m_k(T_{d+1, d-2}). \end{aligned}$$

Next, suppose that v lies outside $P(G)$.

In this case, $H \supseteq G_2$ or $H \supseteq C_a \cdot C_b \cup P(G)$, where $G_2 \in \mathcal{B}(s, d)$ with $d + 2 \leq s \leq n - 2$. It is easy to verify that $m_k(H) \geq m_k(T_{d+1, d-2})$.

Case 3 If any diametrical path of G contains all pendent vertices in G .

We can obtain that $G \succ B_{n, d}$ by similar arguments as those in Case 3 of Theorem 2.

Consequently, the proof is complete. \blacksquare

Combining Theorems 4.4 and 4.5, we obtain the following main result of this section.

Theorem 4.6 Let $G \in \mathcal{B}(n, d)$ with $n \geq 8$, $3 \leq d \leq n - 3$ and $G \neq B_{n,d}$. Then $ME(G) > ME(B_{n,d})$.

Proof. According to Theorems 4.4 and 4.5, we have known that $G \succ B_{n,d}$. And then using the increasing property (namely, $G_1 \succ G_2 \implies ME(G_1) > ME(G_2)$), we get the result we want. ■

We will conclude this section by discussing the case $d = n - 2$. Since any graph G in $\mathcal{B}(n, n - 2)$ is of the form B_n^s (as shown in Figure 9), where $0 \leq s \leq \lfloor n/2 \rfloor - 2$. Through simple analysis, we get the following result.

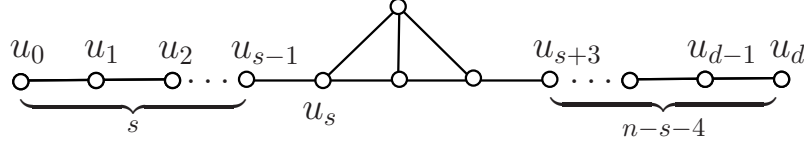


Figure 9: Graph B_n^s with $0 \leq s \leq \lfloor n/2 \rfloor - 2$.

Theorem 4.7 Let $G \in \mathcal{B}(n, n - 2)$ with $n \geq 6$ and $G \neq B_n^1$, then $ME(G) > ME(B_n^1)$.

Proof. Since $G \in \mathcal{B}(n, n - 2)$ and $G \neq B_n^1$, then G is B_n^s , where $s = 0, 2, \dots, \lfloor n/2 \rfloor - 2$.

Case 1 $G = B_n^0$.

Then $G - u_d = B_n^0 - u_d = B_n^1 - u_0$ and $G - u_{d-1} - u_d = B_n^0 - u_{d-1} - u_d \succ B_n^1 - u_0 - u_1$. Thus we have $G = B_n^0 \succ B_n^1$ by Lemma 2.8.

Case 2 $G = B_n^s (s = 2, \dots, \lfloor n/2 \rfloor - 2)$.

Then

$$\begin{aligned} m_k(G = B_n^s) &= m_k(B_n^s - u_{s-2}u_{s-1}) + m_{k-1}(B_n^s - u_{s-2} - u_{s-1}) \\ &= m_k(P_{s-1} \cup B_{n-s+1}^1) + m_{k-1}(P_{s-2} \cup B_{n-s}^0), \end{aligned}$$

together with

$$\begin{aligned} m_k(B_n^1) &= m_k(B_n^1 - u_{d-s+1}u_{d-s+2}) + m_{k-1}(B_n^1 - u_{d-s+1} - u_{d-s+2}) \\ &= m_k(P_{s-1} \cup B_{n-s+1}^1) + m_{k-1}(P_{s-2} \cup B_{n-s}^1). \end{aligned}$$

By Case 1, we have got that $B_{n-s}^0 \succ B_{n-s}^1$, then $m_{k-1}(P_{s-2} \cup B_{n-s}^0) \geq m_{k-1}(P_{s-2} \cup B_{n-s}^1)$ and $m_2(P_{s-2} \cup B_{n-s}^0) > m_2(P_{s-2} \cup B_{n-s}^1)$. Thus $G = B_n^s \succ B_n^1$.

Therefore, we always have $G \succ B_n^1$. And then $ME(G) > ME(B_n^1)$. ■

5 Summary

In [25, 35], the authors introduced the concept of “set-complexity”, based on a context-dependent measure of information, and used this concept to describe the complexity of gene interaction networks. The binary graphs and edge-colored graphs are studied and the relation between complexity and structure of these graphs is examined in detail. In contrast, we put the emphasis on analyzing properties of spectra-based entropies and study interrelations thereof.

In this paper, we characterize the graphs with minimal matching energy among all unicyclic and bicyclic graphs with a given diameter d . With respect to matching energy of graphs, $U_{n,d}$ and $B_{n,d}$ are two extremal graphs in $\mathcal{U}(n, d)$ and $\mathcal{B}(n, d)$ respectively. Moreover, both of them are interesting and have the similar extremum property in other aspects. For example, among all unicyclic graphs of a given diameter, $U_{n,d}$ is the extremal graph on graph energy [29]. Besides, it is also the underling graph of the extremal graph on skew energy [38]. In addition, $B_{n,d}$ has the minimal energy in one class of bicyclic graphs with a given diameter [39]. From this point, we guess that this two graphs may also be the extremal graphs on some other parameters of graphs. Studying the properties of this two graphs will be one of the future work of us. An important question is how general the bounds are. Obviously, the proof techniques use structural properties of the graphs under consideration and it may be intricate to extend the techniques when using more general graphs. On the other hand, the roots of graph polynomials could be used to characterize graphs structurally. This will be one of the future work. For more results, we refer to [11, 28].

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