

# Extremal $(n, m)$ -Graphs with Respect to Distance–Degree–Based Topological Indices

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## Abstract

In chemical graph theory, distance-degree-based topological indices are expressions of the form  $\sum_{u \neq v} F(\deg(u), \deg(v), d(u, v))$ , where  $F$  is a function,  $\deg(u)$  the degree of  $u$ , and  $d(u, v)$  the distance between  $u$  and  $v$ . Setting  $F$  to be  $(\deg(u) + \deg(v))d(u, v)$ ,  $\deg(u)\deg(v)d(u, v)$ ,  $(\deg(u) + \deg(v))d(u, v)^{-1}$ , and  $\deg(u)\deg(v)d(u, v)^{-1}$ , we get the degree distance index DD, the Gutman index Gut, the additively weighted Harary index  $H_A$ , and the multiplicatively weighted Harary index  $H_M$ , respectively.

Let  $\mathcal{G}_{n,m}$  be the set of connected graphs of order  $n$  and size  $m$ . It is proved that if  $G \in \mathcal{G}_{n,m}$ , where  $4 \leq n \leq m \leq 2n - 4$ , then  $H_A(G) \leq (m(m+5) + 2(n-1)(n-3))/2$  and  $\text{DD}(G) \geq (4m-n)(n-1) - (m-n+1)(m-n+6)$ . The extremal graphs are characterized in both cases and are the same. Similarly, the graphs from  $\mathcal{G}_{n,m}$  with  $m = n + \binom{k}{2} - k$ ,  $2 \leq k \leq n - 1$ , maximizing the multiplicatively weighted Harary index and minimizing the Gutman index are obtained.

## 1 Introduction

In chemical graph theory different graphical invariants are used for establishing correlations of chemical structures with various physical properties, chemical reactivity, or biological activity. Many of these *topological indices*, as they are called in the area, are based on the graph distance, see [31] and references therein. Another large group of topological indices is based on the vertex degree, cf. [13] and references therein. Moreover, several of the indices are based on both, the vertex degree and the graph distance. In this paper we are interested in such indices, specifically the degree distance index [8, 14], Gutman index [14, 25], and a couple of recently introduced weighted Harary indices: the additively weighted Harary index and the multiplicatively weighted Harary index [2, 17]. (The latter two indices form weighted versions of the ordinary Harary index [19, 23].) These four indices are, respectively, defined for connected graphs  $G$  as follows:

$$\begin{aligned} \text{DD}(G) &= \sum_{u \neq v} (\deg(u) + \deg(v))d(u, v), \\ \text{Gut}(G) &= \sum_{u \neq v} \deg(u)\deg(v)d(u, v), \\ H_A(G) &= \sum_{u \neq v} \frac{\deg(u) + \deg(v)}{d(u, v)}, \\ H_M(G) &= \sum_{u \neq v} \frac{\deg(u)\deg(v)}{d(u, v)}. \end{aligned}$$

In the seminal paper [17], the additively weighted Harary index  $H_A$  was called *reciprocal degree distance* because it can be viewed as a reciprocal analogue of the degree distance DD.

Characterizing the extremal graphs from a given class of graphs with respect to some graph invariant is an important direction in extremal graph theory, especially in (extremal) chemical graph theory. For some related (extremality) results on the degree distance index see [1, 9, 18, 26, 28], on the Gutman index see [3, 10–12, 20, 22], and for the weighted Harary indices see [7, 24, 32].

Recall that an  $(n, m)$ -graph is a connected graph of order  $n$  and size  $m$ . Let  $\mathcal{G}_{n,m}$  denote the set of  $(n, m)$ -graphs. In particular,  $\mathcal{G}_{n,n-1}$  is the set of trees,  $\mathcal{G}_{n,n}$  the set of *unicyclic graphs*, and  $\mathcal{G}_{n,n+1}$  the set of *bicyclic graphs* (all of order  $n$ ). Many papers that study the extremality of topological indices concentrate on trees, progress to unicyclic graphs, further progress to bicyclic graphs, and sometimes also to tricyclic graphs. In this paper

we make a more general approach and consider the extremality problem for the above four distance-degree-based indices for all graph from  $\mathcal{G}_{n,m}$ , where  $n - 1 \leq m \leq 2n - 4$ . We proceed as follows. In the next section definitions needed in the paper are listed and several lemmas to be used later proved. In Section 3 we characterize the extremal graphs from  $\mathcal{G}_{n,m}$ ,  $n \leq m \leq 2n - 4$ , maximizing the additively weighted Harary index and minimizing the degree distance, respectively. In Section 4 we consider the maximal graphs with respect to the multiplicatively Harary index and the minimal graphs with respect to the Gutman in the classes  $\mathcal{G}_{n,m}$ ,  $n-1 \leq m \leq n+1$ , while in the final section we characterize the extremal graphs for these two indices for all classes  $\mathcal{G}_{n,m}$  where  $m = n + \binom{k}{2} - k$ ,  $k \geq 2$ .

## 2 Preliminaries

All graphs considered in this paper are finite, undirected and simple. Let  $G$  be a graph with vertex set  $V(G)$  and edge set  $E(G)$ . For a vertex  $v \in V(G)$ , we denote by  $N_G(v)$  the set of neighbors of  $v$  in  $G$ ,  $\deg_G(v) = |N_G(v)|$  is the degree of  $v$  in  $G$ . For vertices  $u$  and  $v$  of  $G$ , we denote by  $d_G(u, v)$  the distance between  $u$  and  $v$ , that is, the number of edges on a shortest  $u, v$ -path. Notations  $N_G(v)$ ,  $\deg_G(v)$ , and  $d_G(u, v)$  will be simplified to  $N(v)$ ,  $\deg(v)$ , and  $d(u, v)$ , respectively, if  $G$  will be clear from the context. If  $G$  and  $H$  are graphs, then their *join*  $G \oplus H$  is the graph obtained from the disjoint union of  $G$  and  $H$  by adding all edges between  $V(G)$  and  $V(H)$ .

The *first Zagreb index*  $M_1(G)$  and the *second Zagreb index*  $M_2(G)$  of  $G$  are, respectively, defined as follows [15, 16]:

$$M_1(G) = \sum_{v \in V(G)} \deg(v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} \deg(u)\deg(v).$$

The first Zagreb index can be equivalently written as

$$M_1(G) = \sum_{uv \in E(G)} (\deg(u) + \deg(v)). \tag{1}$$

For some recent results on the Zagreb indices see [21, 29, 30].

The *first Zagreb coindex* and the *second Zagreb coindex* of  $G$  are defined as follows [4]:

$$\overline{M}_1(G) = \sum_{\substack{u \neq v \\ uv \notin E(G)}} (\deg(u) + \deg(v)) \quad \text{and} \quad \overline{M}_2(G) = \sum_{\substack{u \neq v \\ uv \notin E(G)}} \deg(u)\deg(v).$$

We continue with some useful lemmas which will play an important role in the proofs of our main results in the subsequent sections. In the following lemma two relations between the Zagreb indices and coindices are recalled.

**Lemma 2.1** [5] *If  $G \in \mathcal{G}_{n,m}$ , then*

- (1)  $\overline{M}_1(G) = 2m(n - 1) - M_1(G)$ ;
- (2)  $\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G)$ .

For any (connected) graph  $G$  we now introduce the following new invariants:

$$M^*(G) = \sum_{xy \in E(G)} (2\deg(x)\deg(y) - \deg(x) - \deg(y)),$$

$$N^*(G) = \sum_{xy \in E(G)} (\deg(x)\deg(y) + \deg(x) + \deg(y)).$$

Note that  $N^*(G) = M_1(G) + M_2(G)$  holds by (1) and by the definition of the second Zagreb index. The next lemma is important for a characterization of the  $(n, m)$ -graphs with maximal  $M^*(G)$ . For any  $n \geq 4$  and  $p, q \geq 1$ , let  $\mathcal{G}_n(p, q)$  denote the class of graphs  $G$  of order  $n$  defined as follows.  $G$  contains a subgraph  $G'$  of order  $n - p - q$  with two vertices  $u$  and  $v$  of degree  $n - p - q - 1$  in  $G'$ , and  $G$  is obtained from  $G'$  by connecting  $u$  and  $v$  to  $p$  and  $q$  new leaves, respectively, so that  $u$  and  $v$  are in  $G$  of degree  $n - q - 1$  and  $n - p - 1$ , respectively.

**Lemma 2.2** *Let  $n \geq 4$  and let  $G$  be a graph from  $\mathcal{G}_{n,m}$  with largest  $M^*(G)$ . If  $G \notin \mathcal{G}_n(p, q)$  ( $p, q \geq 1$ ), then  $\Delta(G) = n - 1$ .*

**Proof.** Suppose on the contrary that  $\Delta(G) < n - 1$ . Let  $u$  be a vertex of  $G$  of degree  $\Delta(G)$ . By the degree assumption and because  $G$  is connected, there exists a vertex  $w$  such that  $d(u, w) = 2$ . Let  $v$  be a common neighbor of  $u$  and  $w$ . Now,  $\{w\} \subseteq N(v) \setminus N(u) \neq \emptyset$ , hence setting  $N(v) \setminus (N(u) \cup \{u\}) = \{v_1, \dots, v_s\}$  we have  $s \geq 1$  (due to  $w$ ).

Let  $G'$  be the graph obtained from  $G$  in the following way:

$$G' = G - \{vv_1, \dots, vv_s\} + \{uv_1, \dots, uv_s\}.$$

(This construction was named the *neighbor-change transformation* in [30].) Let  $A_i = M_i(G') - M_i(G)$  for  $i = 1, 2$ . From the structures of  $G$  and  $G'$ , we have

$$\begin{aligned} A_1 &= \sum_{x \in N(u) \setminus N(v)} (\deg(u) + s + \deg(x)) + \sum_{i=1}^s (\deg(u) + s + \deg(v_i)) \\ &\quad + \sum_{y \in N(u) \cap N(v)} (\deg(u) + s + \deg(v) - s + 2\deg(y)) - \sum_{x \in N(u) \setminus N(v)} (\deg(u) + \deg(x)) \\ &\quad - \sum_{i=1}^s (\deg(v) + \deg(v_i)) - \sum_{y \in N(u) \cap N(v)} (\deg(u) + \deg(v) + 2\deg(y)) \\ &= s \sum_{x \in N(u) \setminus (N(v) \cup \{v\})} 1 + s^2 + s(\deg(u) - \deg(v)), \end{aligned}$$

$$\begin{aligned}
 A_2 &= \sum_{x \in N(u) \setminus (N(v) \cup \{v\})} (\deg(u) + s) \deg(x) \\
 &+ \sum_{i=1}^s (\deg(u) + s) \deg(v_i) + (\deg(u) + s) (\deg(v) - s) \\
 &+ \sum_{y \in N(u) \cap N(v)} (\deg(u) + s + \deg(v) - s) \deg(y) - \sum_{x \in N(u) \setminus (N(v) \cup \{v\})} \deg(u) \deg(x) \\
 &- \sum_{i=1}^s \deg(v) \deg(v_i) - \deg(u) \deg(v) - \sum_{y \in N(u) \cap N(v)} (\deg(u) + \deg(v)) \deg(y) \\
 &= s \sum_{x \in N(u) \setminus (N(v) \cup \{v\})} \deg(x) + s \sum_{i=1}^s \deg(v_i) + (\deg(u) - \deg(v)) \left( \sum_{i=1}^s \deg(v_i) - s \right) - s^2.
 \end{aligned}$$

Setting  $X = M^*(G') - M^*(G)$  and having in mind that  $\deg(u) \geq \deg(v)$  holds by the way the vertex  $u$  was selected, we get:

$$\begin{aligned}
 X &= 2A_2 - A_1 \\
 &= s \sum_{x \in N(u) \setminus (N(v) \cup \{v\})} (2\deg(x) - 1) + (s + \deg(u) - \deg(v)) \left( 2 \sum_{i=1}^s \deg(v_i) - 3s \right) \\
 &\geq 0.
 \end{aligned}$$

with equality holding if and only if every vertex  $x$  in  $N(u) \setminus (N(v) \cup \{v\})$  and  $v_i$  for  $i = 1, 2, \dots, s$  are pendent vertices in  $G$ , i.e.,  $G \in \mathcal{G}_n(p, q)$ , contradicting the choice of  $G$ . Thus we have  $X > 0$ .

Hence we have constructed an  $(n, m)$ -graph  $G'$  with  $M^*(G') > M^*(G)$  which contradicts the choice of  $G$ . □

Using a very similar reasoning as that in the proof of Lemma 2.2 we can obtain the following lemma; hence we omit its proof.

**Lemma 2.3** *If  $n \geq 4$  and  $G$  is a graph from  $\mathcal{G}_{n,m}$  with largest  $N^*(G)$ , then  $\Delta(G) = n - 1$ .*

For  $n \geq 3$  and  $3 \leq n \leq m \leq 2n - 4$  let  $G_{n,m} \in \mathcal{G}_{n,m}$  be the graph shown in Fig. 1. Note that  $G_{n,n}$  is the graph obtained by adding a new edge between two pendent vertices of the star of order  $n$ .

To recall the next lemma, we also need the graph  $G'_{n,n+2} \in \mathcal{G}_{n,n+2}$ ,  $n \geq 4$ , which is shown in Fig. 2.

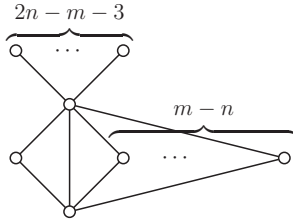


Figure 1: The graph  $G_{n,m}$

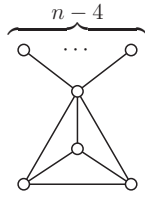


Figure 2: The graph  $G'_{n,n+2}$

**Lemma 2.4** [30] *If  $G \in \mathcal{G}_{n,m}$ ,  $4 \leq n \leq m \leq 2n - 4$ , then*

$$M_1(G) \leq n(n - 1) + (m - n + 1)(m - n + 6)$$

*with equality holding if and only if  $G \cong G_{n,m}$  for  $n \leq m \leq n + 1$  or  $n + 3 \leq m \leq 2n - 4$ ; and  $G \cong G_{n,m}$  or  $G'_{n,n+2}$  for  $m = n + 2$ .*

### 3 Degree distance index and additive Harary index

The first main result of this section bounds from the above the  $H_A$  index as follows:

**Theorem 3.1** *If  $G \in \mathcal{G}_{n,m}$ ,  $4 \leq n \leq m \leq 2n - 4$ , then*

$$H_A(G) \leq \frac{m(m + 5) + 2(n - 1)(n - 3)}{2},$$

*where the equality holds if and only if  $G \cong G_{n,m}$  for  $n \leq m \leq n + 1$  or  $n + 3 \leq m \leq 2n - 4$ ; and  $G \cong G_{n,m}$  or  $G'_{n,n+2}$  for  $m = n + 2$ .*

**Proof.** By the definition of  $H_A$ , Eq. (1), Lemma 2.1 (1), and Lemma 2.4, we have

$$\begin{aligned} H_A(G) &= \sum_{uv \in E(G)} [\deg(u) + \deg(v)] + \sum_{uv \notin E(G), u \neq v} \frac{\deg(u) + \deg(v)}{d(u, v)} \\ &\leq M_1(G) + \frac{1}{2} \overline{M}_1(G) \\ &= m(n-1) + \frac{1}{2} M_1(G) \\ &\leq \frac{(2m+n)(n-1)}{2} + \frac{(m-n+1)(m-n+6)}{2} \\ &= \frac{m(m+5) + 2(n-1)(n-3)}{2}, \end{aligned}$$

where both equalities hold if and only if any two nonadjacent vertices are at distance 2, and  $G$  is as stated in Lemma 2.4. □

The case  $m = n$  of Theorem 3.1 was independently solved in [24] using a significantly more involved approach.

We next characterize the extremal graphs from  $\mathcal{G}_{n,m}$  minimizing the degree distance.

**Theorem 3.2** *If  $G \in \mathcal{G}_{n,m}$ ,  $4 \leq n \leq m \leq 2n - 4$ , then*

$$DD(G) \geq (4m - n)(n - 1) - (m - n + 1)(m - n + 6),$$

where the equality holds if and only if  $G \cong G_{n,m}$  for  $n \leq m \leq n+1$  or  $n+3 \leq m \leq 2n-4$ ; and  $G \cong G_{n,m}$  or  $G'_{n,n+2}$  for  $m = n+2$ .

**Proof.** We apply the definition of the DD index, Eq. (1), Lemma 2.1 (1), and Lemma 2.4, to obtain:

$$\begin{aligned} DD(G) &= \sum_{uv \in E(G)} [\deg(u) + \deg(v)] + \sum_{uv \notin E(G)} (\deg(u) + \deg(v))d(u, v) \\ &\geq M_1(G) + 2\overline{M}_1(G) \\ &= 4m(n-1) - M_1(G) \\ &\geq (4m - n)(n - 1) - (m - n + 1)(m - n + 6). \end{aligned}$$

Both equalities hold if and only if any two nonadjacent vertices are at distance 2, and  $G$  is as stated in Lemma 2.4. □

By selecting  $m = n$  or  $m = n + 1$  in Theorem 3.2 we get the following two earlier results.

**Corollary 3.3** [18,26] *If  $G$  is a unicyclic graph of order  $n \geq 3$ , then*

$$DD(G) \geq 3n^2 - 3n - 6,$$

*with equality holding if and only if  $G \cong G_{n,n}$ .*

**Corollary 3.4** [26] *If  $G$  is a bicyclic graph of order  $n \geq 4$ , then*

$$DD(G) \geq 3n^2 + n - 18,$$

*with equality holding if and only if  $G \cong G_{n,n+1}$ .*

To conclude the section we recall that the structure of extremal graphs minimizing DD for  $n - 1 \leq m \leq n + 4$  was determined, by other means, by Tomescu in [27].

## 4 $H_M$ and Gutman index in $\mathcal{G}_{n,m}$ , $n - 1 \leq m \leq n + 1$

We now turn to the maximal graphs from  $\mathcal{G}_{n,m}$  with respect to the multiplicatively Harary index and the minimal graphs with respect to the Gutman index. In this section we restrict to the case  $\mathcal{G}_{n,m}$ ,  $n - 1 \leq m \leq n + 1$ , and follow with a more general case in the next section. We begin with a lemma on the structure of extremal graphs from  $\mathcal{G}_{n,m}$  maximizing the value of  $H_M$ .

**Lemma 4.1** *If  $G$  is a graph from  $\mathcal{G}_{n,m}$  with largest  $H_M(G)$ , then  $\Delta(G) = n - 1$ .*

**Proof.** From the definitions of  $H_M$  and  $M^*(G)$ , and by Lemma 2.1 (2), we have

$$\begin{aligned} H_M(G) &\leq \sum_{xy \in E(G)} \deg(x)\deg(y) + \sum_{xy \notin E(G)} \frac{\deg(x)\deg(y)}{2} \\ &= M_2(G) + \frac{1}{2}\overline{M}_2(G) \\ &= m^2 + \frac{1}{4}M^*(G). \end{aligned}$$

Hence  $H_M(G)$  attains its maximum only if, in  $G$ , any two nonadjacent vertices are at distance 2 and  $M^*(G)$  reaches its maximal value. Then our result follows immediately from Lemma 2.2. □

From Lemma 4.1, the following corollary can be easily deduced.



**Corollary 4.2** [7] *For any tree of order  $n$ , the star  $S_n$  has uniquely the maximal  $H_M$  with  $H_M(S_n) = (n - 1)(5n - 6)/4$ ; for any  $(n, n)$ -graph, the graph  $G_{n,n}$  has uniquely the maximal  $H_M$  with  $H_M(G_{n,n}) = (5n^2 + n)/4$ .*

Using Lemma 4.1 we can extend Corollary 4.2 to bicyclic graphs as follows.

**Theorem 4.3** *If  $G \in \mathcal{G}_{n,n+1}$ ,  $n \geq 4$ , then*

$$H_M(G) \leq \frac{5n^2 + 13n + 8}{4}$$

*with equality holding if and only if  $G \cong G_{n,n+1}$ .*

**Proof.** From Lemma 4.1, the maximal value of  $H_M(G)$  for any  $(n, n + 1)$ -graph  $G$  is possibly attained at  $G_{n,n+1}$  or another graph, denoted by  $G'_{n,n+1}$ , which is obtained by adding two independent edges into the star  $S_n$ . By the definition of  $H_M$ , we have

$$\begin{aligned} H_M(G_{n,n+1}) &= M_2(G_{n,n+1}) + \frac{1}{2}\overline{M}_2(G_{n,n+1}) \\ &= n^2 + 2n + 9 + \frac{1}{2} \left[ \binom{n-4}{2} + 3(n-4) + 4(n-4) + 4 \right], \end{aligned}$$

and

$$\begin{aligned} H_M(G'_{n,n+1}) &= M_2(G'_{n,n+1}) + \frac{1}{2}\overline{M}_2(G'_{n,n+1}) \\ &= n^2 + 2n + 5 + \frac{1}{2} \left[ \binom{n-5}{2} + 8(n-5) + 16 \right]. \end{aligned}$$

Clearly,  $H_M(G_{n,n+1}) > H_M(G'_{n,n+1})$ . □

From the definitions of the Gutman index and  $N^*(G)$ , and using Lemma 2.1 (2), we infer:

$$\begin{aligned} \text{Gut}(G) &\geq \sum_{xy \in E(G)} \text{deg}(x)\text{deg}(y) + \sum_{xy \notin E(G)} 2 \text{deg}(x)\text{deg}(y) \\ &= M_2(G) + 2\overline{M}_2(G) \\ &= 4m^2 - N^*(G). \end{aligned}$$

Thus, for any graph  $G \in \mathcal{G}_{n,m}$ , we have

$$\text{Gut}(G) \geq 4m^2 - N^*(G). \tag{2}$$

Moreover, the above equality holds if and only if any two non-adjacent vertices in  $G$  are at distance 2. In view of Lemma 2.3, we conclude that a graph  $G \in \mathcal{G}_{n,m}$  has the minimal Gutman index only if  $\Delta(G) = n - 1$ . Then the following result can be easily deduced.

**Corollary 4.4** [10, 14] *For any tree of order  $n$ , the star  $S_n$  has uniquely the minimal Gutman index with  $\text{Gut}(S_n) = 2n^2 - 5n + 3$ ; for any unicyclic graph of order  $n \geq 3$ , the graph  $G_{n,n}$  has uniquely the minimal Gutman index with  $\text{Gut}(G_{n,n}) = 2n^2 + n - 9$ .*

By a similar reasoning as that in the proof of Theorem 4.3, we can obtain the following result that we state without a proof.

**Theorem 4.5** *If  $G \in \mathcal{G}_{n,n+1}$ ,  $n \geq 4$ , then*

$$\text{Gut}(G) \geq 2n^2 + 7n - 19$$

*with equality holding if and only if  $G \cong G_{n,n+1}$ .*

### 5 The cases $m = n + \binom{k}{2} - k$ , $4 \leq k \leq n - 1$

In this section we will determine the maximal and the minimal graphs from  $\mathcal{G}_{n,m}$ , where  $m = n + \binom{k}{2} - k$ ,  $4 \leq k \leq n - 1$ , with respect to the multiplicatively weighted Harary index and the Gutman index, respectively. For this sake we first introduce a family of graphs and a certain function as follows.

Let  $K_k^{n-k}$  be the graph obtained from the complete graph  $K_k$  by attaching  $n - k$  pendent vertices to one vertex of  $K_k$ . Clearly,  $K_2^{n-2}$  is the star  $S_n$  of order  $n$  and  $K_3^{n-3}$  is the graph obtained by inserting a new edge between two pendent vertices of  $S_n$ . Moreover, from Fig. 2 we find out that  $K_4^{n-4} \cong G'_{n,n+2}$ .

If  $a$  and  $b$  are positive numbers and  $G$  is a graph, then set

$$f_{a,b}(G) = \sum_{xy \in E(G)} [a \deg(x)\deg(y) + b(\deg(x) + \deg(y))].$$

**Lemma 5.1** *If  $G$  is an  $(n, \binom{k}{2})$ -graph,  $4 \leq k \leq n - 1$ , then*

$$f_{a,b}(G) \leq \frac{ak - a + 2b}{2} k(k - 1)^2$$

*with equality holding if and only if  $G \cong K_k \cup (n - k)K_1$ .*

**Proof.** By the definition of  $f_{a,b}(G)$  and the expression (1) for the first Zagreb index,

$$\begin{aligned} f_{a,b}(G) &= \sum_{uv \in E(G)} [a \deg(u)\deg(v) + b(\deg(u) + \deg(v))] \\ &\leq \sum_{uv \in E(G)} \left[ \frac{a}{2} (\deg(u)^2 + \deg(v)^2) + b(\deg(u) + \deg(v)) \right] \\ &= \sum_{u \in V(G)} \left[ \frac{a}{2} \deg(u)^3 + b \deg(u)^2 \right]. \end{aligned} \tag{3}$$

The equality in (3) holds if and only if  $\deg(u) = \deg(v)$  for any edge  $uv \in E(G)$ . Setting  $h(G) = \sum_{u \in V(G)} \left[ \frac{a}{2} \deg(u)^3 + b \deg(u)^2 \right]$  it suffices to determine the maximum of  $h(G)$ . We distinguish the following two cases.

**Case 1.** The  $\binom{k}{2}$  edges of  $G$  induce a single connected component.

In this case the equality in (3) holds if and only if  $G \cong G^* \cup (n - s)K_1$  where  $G^*$  is a connected regular graph of order  $s$ . Moreover,  $f_{a,b}(G^*) = f_{a,b}(G)$ . Then the degree of  $G^*$  is  $k(k - 1)/s$ , and

$$\begin{aligned} f_{a,b}(G^*) &= s \left[ \frac{a}{2} \left( \frac{k(k - 1)}{s} \right)^3 + b \left( \frac{k(k - 1)}{s} \right)^2 \right] \\ &= \frac{a k^3 (k - 1)^3}{2 s^2} + b \frac{k^2 (k - 1)^2}{s}. \end{aligned}$$

Clearly,  $f_{a,b}(G^*)$  will reach its maximum when  $s$  is as small as possible. Taking into account that  $G^*$  is a regular graph with  $\binom{k}{2}$  edges, we find that the minimum value of  $s$  is  $k$ . Thus we have

$$\begin{aligned} f_{a,b}(G^*) &= \frac{a k^3 (k - 1)^3}{2 s^2} + b \frac{k^2 (k - 1)^2}{s} \\ &\leq \frac{a k^3 (k - 1)^3}{2 k^2} + b \frac{k^2 (k - 1)^2}{k} \\ &= \frac{ak - a + 2b}{2} k(k - 1)^2. \end{aligned}$$

The above equality holds if and only if  $s = k$ , that is, if and only if  $G^* \cong K_k \cup (n - k)K_1$ . This finishes the proof of the “only if” part in this case.

**Case 2.** The  $\binom{k}{2}$  edges of  $G$  induce at least two non-trivial connected components.

By the argument above Case 1, when  $f_{a,b}(G)$  reaches its maximum, the  $\binom{k}{2}$  edges induce a regular subgraph with  $t \geq 2$  nontrivial connected components. Hence  $G = G_0 \cup (n - s)K_1$ , where  $G_0 = \cup_{i=1}^t G_i$  is the disjoint union of connected non-trivial regular graphs. Let  $G_i$ ,  $1 \leq i \leq t$ , be a  $p_i$ -regular graph of order  $s_i$  and size  $m_i$ , such that  $\sum_{i=1}^t m_i = \binom{k}{2}$ . Then we have  $s_i = 2m_i/p_i$ . Therefore, in this case it suffices to prove the following inequality:

$$\sum_{i=1}^t \frac{2m_i}{p_i} \left( \frac{a}{2} p_i^3 + b p_i^2 \right) < \frac{ak - a + 2b}{2} k(k - 1)^2,$$

that is,

$$\sum_{i=1}^t \left( \frac{a}{2} p_i^2 + b p_i \right) m_i < \frac{ak - a + 2b}{2} (k - 1) \sum_{i=1}^t m_i. \tag{4}$$

Since  $p_i < k - 1$  for  $1 \leq i \leq t$  with  $2 \leq t \leq k - 2$ , we have the following inequality:

$$\frac{a}{2}p_i^2 + bp_i < \frac{ak - a + 2b}{2}(k - 1).$$

Thus the inequality (4) holds immediately. This finishes the proof of the “only if” part in this case.

To complete the proof we can easily check that  $f_{a,b}(G) = \frac{ak-a+2b}{2}k(k-1)^2$  when  $G \cong K_k \cup (n-k)K_1$ , which completes the proof of this lemma.  $\square$

We are now ready for the first main result of this section.

**Theorem 5.2** *If  $G$  is an  $(n, n + \binom{k}{2} - k)$ -graph,  $n \geq 5$ ,  $4 \leq k \leq n - 1$ , then*

$$H_M(G) \leq \frac{(2n + k^2 - 3k)(n + k^2 - 3k + 1)}{2} + \frac{(n - k)(n + k - 3)}{4}$$

*with equality holding if and only if  $G \cong K_k^{n-k}$ .*

**Proof.** By Lemma 4.1 and its proof, it suffices to find an  $(n, m)$ -graph  $G$  with  $\Delta(G) = n - 1$  and maximum value of  $M^*(G)$ . Therefore  $G = K_1 \oplus G^*$ , where  $G^*$  is an  $(n - 1, \binom{k-1}{2})$ -graph. Let  $d_1 \geq \dots \geq d_n$  be the degree sequence of  $G$  and let  $d_1^* \geq \dots \geq d_{n-1}^*$  be the degree sequence of  $G^*$ . Clearly,  $d_1 = n - 1$  and  $d_i = d_{i-1}^* + 1$  for  $2 \leq i \leq n$ . Thus, by Lemma 5.1 (for  $a = 2$  and  $b = 1$ ),

$$\begin{aligned} M^*(G) &= \sum_{v_i v_j \in E(G)} (2d_i d_j - d_i - d_j) \\ &= \sum_{v_i v_j \in E(G)} (2d_1 d_j - d_1 - d_j) + \sum_{v_i v_j \in E(G), 2 \leq i < j \leq n} (2d_i d_j - d_i - d_j) \\ &= (2n - 3) \sum_{i=2}^n d_i - (n - 1)^2 + \sum_{v_i v_j \in E(G^*)} [2(d_i^* + 1)(d_j^* + 1) - d_i^* - d_j^* - 2] \\ &= (2n - 3) \left( k^2 + n - 3k + 1 \right) - (n - 1)^2 + f_{2,1}(G^*) \\ &\leq (2n - 3) \left( k^2 + n - 3k + 1 \right) - (n - 1)^2 + (k - 1)^2 (k - 2)^2 \\ &= [2n - 3 + (k - 1)(k - 2)](k - 1)(k - 2) + (n - 2)(n - 1) \end{aligned}$$

with equality holding if and only if  $G^* \cong K_{k-1} \cup (n-k)K_1$ . Thus we have

$$\begin{aligned} H_M(G) &\leq \left[ n + \binom{k}{2} - k \right]^2 + \frac{1}{4}M^*(G) \\ &\leq \frac{[2n + k(k-3)]^2}{4} + \frac{[2n-3 + (k-1)(k-2)](k-1)(k-2)}{4} + \frac{(n-2)(n-1)}{4} \\ &= \frac{(2n + k^2 - 3k)(n + k^2 - 3k + 1)}{2} + \frac{(n-2)(n-1) - (k-1)(k-2)}{4} \\ &= \frac{(2n + k^2 - 3k)(n + k^2 - 3k + 1)}{2} + \frac{(n-k)(n+k-3)}{4}. \end{aligned}$$

Both the above equalities hold if and only if  $G \cong K_1 \oplus (K_{k-1} \cup (n-k)K_1) = K_k^{n-k}$ , finishing the proof of this theorem.  $\square$

Using Corollary 4.2 we can extend Theorem 5.2 from  $k \geq 4$  to  $k \geq 2$ :

**Theorem 5.3** *If  $G$  is an  $(n, n + \binom{k}{2} - k)$ -graph,  $n \geq 5$ ,  $2 \leq k \leq n - 1$ , then*

$$H_M(G) \leq \frac{(2n + k^2 - 3k)(n + k^2 - 3k + 1)}{2} + \frac{(n-k)(n+k-3)}{4}$$

*with equality holding if and only if  $G \cong K_k^{n-k}$ .*

We now turn to the Gutman index and prove the following result in parallel to Theorem 5.2.

**Theorem 5.4** *If  $G$  is an  $(n, n + \binom{k}{2} - k)$ -graph,  $n \geq 5$ ,  $4 \leq k \leq n - 1$ , then*

$$\text{Gut}(G) \geq 2n^2 + n - 1 + (3n + k^2 - 3k)(k^2 - 3k) - \frac{k+1}{2}(k-1)^2(k-2)$$

*with equality holding if and only if  $G \cong K_k^{n-k}$ .*

**Proof.** In view of the inequality (2) and Lemma 2.3, we find that the minimum Gutman index of the graphs from  $\mathcal{G}_{n,m}$  is attained at a graph  $G \in \mathcal{G}_{n,m}$  with  $\Delta(G) = n - 1$  and maximum  $N^*(G)$ . By an analogous argument as that in the proof of Theorem 5.2,  $G$  must be of the form  $K_1 \oplus G^*$  where  $G^*$  is an  $(n - 1, \binom{k-1}{2})$ -graph. Let  $d_1 \geq \dots \geq d_n$  be the degree sequence of  $G$ , and let  $d_1^* \geq \dots \geq d_{n-1}^*$  be the degree sequence of  $G^*$ . Then  $d_1 = n - 1$  and  $d_i = d_{i-1}^* + 1$ ,  $2 \leq i \leq n$ . Applying Lemma 5.1 (for  $a = 1$  and  $b = 2$ ), we

get:

$$\begin{aligned}
 \text{Gut}(G) &\geq 4m^2 - N^*(G) \\
 &= 4m^2 - \sum_{v_i v_j \in E(G)} (d_i d_j + d_i + d_j) \\
 &= 4m^2 - \sum_{v_i v_j \in E(G)} (d_i d_j + d_1 + d_j) - \sum_{v_i v_j \in E(G), 2 \leq i < j \leq n} (d_i d_j + d_i + d_j) \\
 &= 4m^2 - n \sum_{i=2}^n d_i - (n-1)^2 - \sum_{v_i v_j \in E(G^*)} [(d_i^* + 1)(d_j^* + 1) + d_i^* + d_j^* + 2] \\
 &= 4m^2 - n[2m - (n-1)] - 3[m - (n-1)] - (n-1)^2 - f_{1,2}(G^*) \\
 &= 4m^2 - n(k^2 - 3k + n + 1) - \frac{3}{2}(k^2 - 3k + 2) - (n-1)^2 - f_{1,2}(G^*) \\
 &\geq (2n + k^2 - 3k)^2 - n(k^2 - 3k + n + 1) - \frac{3}{2}(k^2 - 3k + 2) - (n-1)^2 \\
 &\quad - \frac{k+2}{2}(k-1)(k-2)^2 \\
 &= 2n^2 + n - 1 + (3n + k^2 - 3k)(k^2 - 3k) - \frac{k+1}{2}(k-1)^2(k-2).
 \end{aligned}$$

The above equalities hold if and only if any two non-adjacent vertices in  $G$  have the distance 2 and  $G^* \cong K_{k-1} \cup (n-k)K_1$ , i.e.,  $G \cong K_1 \oplus (K_{k-1} \cup (n-k)K_1) = K_k^{n-k}$ , which completes the proof of this theorem.  $\square$

Theorem 5.3 can also be extended from  $k \geq 4$  to  $k \geq 2$  after using Corollary 4.4:

**Theorem 5.5** *If  $G$  is an  $(n, n + \binom{k}{2} - k)$ -graph,  $n \geq 5$ ,  $4 \leq k \leq n - 1$ , then*

$$\text{Gut}(G) \geq 2n^2 + n - 1 + (3n + k^2 - 3k)(k^2 - 3k) - \frac{k+1}{2}(k-1)^2(k-2)$$

*with equality holding if and only if  $G \cong K_k^{n-k}$ .*

Setting  $k = 3$  in Theorem 5.5 (and checking the cases  $n = 3, 4$  separately) we obtain:

**Corollary 5.6** [7, Theorem 8] *If  $G$  is a unicyclic graph of order  $n \geq 3$ , then*

$$H_M(G) \leq \frac{n(5n+1)}{4}$$

*with equality holding if and only if  $G \cong K_3^{n-3}$ .*

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