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Finding the Least Element of the Ordering of Graphs with Respect to their Matching Numbers

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Abstract

Given two graphs G_1 and G_2, the ordering $G_1 \preccurlyeq G_2$ is defined by $m(G_1,k) \leq m(G_2,k)$ for all k, where $m(G_i,k)$ is the number of k-matchings in G_i. The existence of the least element of $\preccurlyeq$ among connected graphs of order n and size m is conjectured. Special cases of $m = n-1, n$, and $n+1$ are known in literature. In this paper, we further affirm the conjecture by finding the least elements for the cases of $n-1 \leq m \leq 2n-3$ and $\frac{n(n-1)}{2} - (n-2) \leq m \leq \frac{n(n-1)}{2}$. As consequences, we determine the graphs with the minimum matching energy, and with the minimum Hosoya index among connected graphs of order n and size m where $n-1 \leq m \leq 2n-3$ and $\frac{n(n-1)}{2} - (n-2) \leq m \leq \frac{n(n-1)}{2}$.

1 Introduction

Let G be a simple graph of order n and size m, it is called an (n,m)-graph. A k-matching of G is a union of k independent edges in G. We denote $m(G,k)$ the number of k-matchings in G. It is consistent to define $m(G,0) = 1$ and $m(G,k) = 0$ for $k < 0$. Note that $m(G,1) = m$. There is a natural ordering with respect to the matching numbers. According to Gutman and Zhang [4], the idea to define such ordering came from theoretical chemistry.

Definition 1.1. For graphs G_1 and G_2, $G_1 \preccurlyeq G_2$ if $m(G_1,k) \leq m(G_2,k)$ holds for all k.

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Definition 1.2. For graphs G_1 and G_2, $G_1 \sim G_2$ if $m(G_1, k) = m(G_2, k)$ holds for all k.

As a binary relation on graphs, $\preccurlyeq$ is reflexive and transitive, but not anti-symmetric because there are non-isomorphic graphs G_1 and G_2 such that $G_1 \sim G_2$. Hence $\preccurlyeq$ is a quasi-order. Note that $\preccurlyeq$ is not a complete ordering because there are incomparable graphs with respect to $\preccurlyeq$. Nonetheless, it is interesting to ask whether the least and the greatest elements exist in a given class of graphs. First let us consider $\mathcal{G}_n$, the collection of connected graphs of order n. Then it is known [3] that

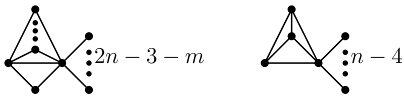
$$S_n \preccurlyeq G \preccurlyeq K_n$$

for all $G \in \mathcal{G}_n$, where S_n is the star graph, and K_n is the complete graph. Hence S_n and K_n are the least and greatest elements in $\mathcal{G}_n$, respectively. Next we consider $\mathcal{G}_{n,m}$, the collection of connected graphs of order n and size m. In particular, for $m = n-1, n, n+1, n+2$, $\mathcal{G}_{n,m}$ is the set of trees, connected unicyclic graphs, connected bicyclic graphs, and connected tricyclic graphs, respectively. In view of the result for $\mathcal{G}_n$, it is tempting to guess the existence of the least and greatest elements in $\mathcal{G}_{n,m}$. From literature [4], we know that the path graph P_n, the cycle graph C_n, and the graph obtained from connecting C_4 and C_{n-4} by an edge is the greatest element in $\mathcal{G}_{n,n-1}$, $\mathcal{G}_{n,n}$, and $\mathcal{G}_{n,n+1}$, respectively. However, Gutman and Cvetković [2] showed that there is NO greatest element in $\mathcal{G}_{n,n+2}$ for $n \geq 12$. Indeed, computer search finds NO greatest element in $\mathcal{G}_{8,19}$. Nonetheless, computer search results show that $\mathcal{G}_{n,m}$ always has a least element for $n \leq 9$. Therefore, we boldly propose the following conjecture about the existence of the least element in $\mathcal{G}_{n,m}$.

Conjecture 1.3. There exists a graph $S_{n,m}$ in $\mathcal{G}_{n,m}$ such that $S_{n,m} \preccurlyeq G$ for all $G \in \mathcal{G}_{n,m}$.

Only the existence of a least element is asserted in Conjecture 1.3. It is even nicer if the structure of $S_{n,m}$ can be described explicitly, and the uniqueness isssue is also addressed. Let E_k be the empty graph of order k. Denote $\vee$ the graph joint of two graphs, and $\cup$ the disjoint union of two graphs. The graphs $F_n^m = (S_{m-n+2} \cup E_{2n-3-m}) \vee E_1$ and $H_n^{n+2} = (C_3 \cup E_{n-4}) \vee E_1$ are shown in Fig. 1.

Again, from literature [3, 5], we know that $S_n = F_n^{n-1}$, F_n^n, and F_n^{n+1} is the least element in $\mathcal{G}_{n,n-1}$, $\mathcal{G}_{n,n}$, and $\mathcal{G}_{n,n+1}$, respectively. Let A_n^m be the graph obtained from K_n by deleting the $n(n-1)/2 - m$ edges in K_n which share a common vertex, where



(a) F_n^m (b) H_n^{n+2}

Figure 1: F_n^m and H_n^{n+2}

$n(n-1)/2-(n-2) \leq m \leq n(n-1)/2$. Let $B_n^{n(n-1)/2-3}$ be the graph obtained from K_n by deleting the three edges of C_3 in K_n. In this paper, we give further evidence for Conjecture 1.3 in the following result.

Theorem 1.4. (i) Let $n-1 \leq m \leq 2n-3$. For $G \in \mathcal{G}_{n,m}$,

$$F_n^m \preccurlyeq G.$$

Moreover $G \sim F_n^m$ if and only if $G = F_n^m$, or H_n^{n+2} when $m = n+2$.

(ii) Let $\frac{n(n-1)}{2}-(n-2) \leq m \leq \frac{n(n-1)}{2}$. For $G \in \mathcal{G}_{n,m}$,

$$A_n^m \preccurlyeq G.$$

Moreover $G \sim A_n^m$ if and only if $G = A_n^m$, or $B_n^{n(n-1)/2-3}$ when $m = n(n-1)/2-3$.

We want to mention two immediate applications of Theorem 1.4: one about matching energy and the other about Hosoya index. The matching polynomial of a graph G of order n is defined as

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

The concept of matching energy of a graph is introduced by Gutman and Wagner [3] and it is a quantity of relevalence for chemical applications. The matching energy of G of order n is defined as

$$ME(G) = \sum_{i=1}^{n} |\alpha_i|,$$

where α_1, α_2, $\cdots$, and α_n denote the zeros of $\alpha(G)$. An equivalent definition [3] for the matching energy of a graph G is

$$ME(G) = \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2} \ln\Big[\sum_{k\geq 0} m(G,k)x^{2k}\Big] \mathrm{d}x.$$

This equivalent definition makes comparison of matching energies easier by using the matching ordering. Indeed, from the equivalent definition of matching energy and Theorem 1.4, we have the following result.

Theorem 1.5. (i) For $G \in \mathcal{G}_{n,m}$ with $n-1 \le m \le 2n-3$,

$$ME(F_n^m) \le ME(G).$$

Equality holds if and only if $G = F_n^m$, or H_n^{n+2} when $m = n+2$.

(ii) For $G \in \mathcal{G}_{n,m}$ with $\frac{n(n-1)}{2} - (n-2) \le m \le \frac{n(n-1)}{2}$,

$$ME(A_n^m) \le ME(G).$$

Equality holds if and only if $G = A_n^m$, or $B_n^{n(n-1)/2-3}$ when $m = n(n-1)/2 - 3$.

Theorem 1.5 (i) with $m = n-1, n, n+1$ was proved earlier in [3, 5]. We believe the results in Theorem 1.5 (i) with $n+2 \le m \le 2n-3$ and Theorem 1.5 (ii) are new.

Next we consider the Hosoya index of a graph G which is defined as $Z(G) = \sum_{k \ge 0} m(G,k)$. For more results and techniques on Hosoya index, see [7]. By the definition of Hosoya index and Theorem 1.4, we also have the following result.

Theorem 1.6. (i) For $G \in \mathcal{G}_{n,m}$ with $n-1 \le m \le 2n-3$,

$$Z(F_n^m) \le Z(G).$$

Equality holds if and only if $G = F_n^m$, or H_n^{n+2} when $m = n+2$.

(ii) For $G \in \mathcal{G}_{n,m}$ with $\frac{n(n-1)}{2} - (n-2) \le m \le \frac{n(n-1)}{2}$,

$$Z(A_n^m) \le Z(G).$$

Equality holds if and only if $G = A_n^m$, or $B_n^{n(n-1)/2-3}$ when $m = n(n-1)/2 - 3$.

Theorem 1.6 (i) was proved earlier in [6] using the formula: $Z(G) = Z(G-uv) + Z(G-u-v)$ where uv is an edge with vertices u and v. We believe the results in Theorem 1.6 (ii) are new.

The rest of the paper is organized as follows. In Section 2, we collect some preliminary results for later use. Section 3 is devoted to finding the maximum sum of degree squares for connected graphs, and then we give the proof of Theorem 1.4 in Secion 4.

2 Preliminary results

In this section, we are interested in the sum of squares of entries from a positive integer sequence $\mathbf{a} = (a_1, \cdots, a_n)$. For the sake of convenience, we define $SS(\mathbf{a}) = \sum_{i=1}^{n} a_i^2$.

Lemma 2.1. Let $\mathbf{a} = (a_1, \cdots, a_n)$ be a positive integer sequence such that $U \geq a_i \geq L$ for $1 \leq i \leq n$ and $\sum_{i=1}^{n} a_i = C$. If $\mathbf{a}$ has two entries different from U and L then there is another positive integer sequence $\mathbf{b} = (b_1, \cdots, b_n)$ such that $U \geq b_i \geq L$ for $1 \leq i \leq n$, $\sum_{i=1}^{n} b_i = C$, and $SS(\mathbf{b}) > SS(\mathbf{a})$.

Proof: Let the two entries be $U > a_r \geq a_s > L$. Then $U \geq a_r + 1 > a_s - 1 \geq L$. Define $\mathbf{b} = \mathbf{a}$ except $b_r = a_r + 1$, $b_s = a_s - 1$. Hence $U \geq b_i \geq L$ for $1 \leq i \leq n$, $\sum_{i=1}^{n} b_i = C$, and $SS(\mathbf{b}) - SS(\mathbf{a}) = b_r^2 + b_s^2 - a_r^2 - a_s^2 = (a_r+1)^2 + (a_s-1)^2 - a_r^2 - a_s^2 = 2(a_r - a_s + 1) > 0$. ■

Given $n \geq 2$ and $n - 1 \leq m \leq 2n - 3$, consider positive integer sequences of the form:

$$\mathbf{a} = (n-1, h, a_3, \cdots, a_{h+1}, \underbrace{1 \cdots 1}_{n-h-1})$$

where $n - 1 \geq h \geq a_3 \geq \cdots \geq a_{h+1} \geq 2$ and $a_3 + \cdots + a_{h+1} = 2(m - n + 1)$. Let $\mathcal{A}$ be the set of all non-increasing positive integer sequences of the form defined above. Clearly, $\mathcal{A}$ is finite and nonempty, and so the maximum value

$$M = \max\{SS(\mathbf{a}) : \mathbf{a} \in \mathcal{A}\}$$

exists. We are interested in finding the sequence(s) attaining such maximum value.

Corollary 2.2. Let $\mathbf{a} \in \mathcal{A}$. If $SS(\mathbf{a}) = M$ then $\mathbf{a}$ is of the form

$$(n-1, h, \underbrace{h \cdots h, a, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1})$$

where $h \geq a \geq 2$.

Proof: Let $\mathbf{a} = (n-1, h, a_3, \cdots, a_{h+1}, \underbrace{1 \cdots 1}_{n-h-1})$ be a sequence in $\mathcal{A}$ such that $SS(\mathbf{a}) = M$. Note that $h \geq a_3 \geq \cdots \geq a_{h+1} \geq 2$, and $a_3 + \cdots + a_{h+1} = 2(m - n + 1)$. Among $\{a_3, \cdots, a_{h+1}\}$, there is at most one integer a_k different from h and 2, otherwise Lemma 2.1 guarantees the existence of $\mathbf{b} \in \mathcal{A}$ with $SS(\mathbf{b}) > SS(\mathbf{a}) = M$, a contradiction. Hence $\mathbf{a}$ is of the desired form. ■

Example 2.3. Let $m = n+2$. By Corollary 2.2, M is attained at $\mathbf{a}$ of the form:

$$(n-1, h, \underbrace{h \cdots h, a, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1}).$$

Note that $2(h-1) \leq 6 = 2(m-n+1) = h + \cdots + h + a + 2 \cdots + 2 \leq h(h-1)$ and so $3 \leq h \leq 4$. Hence

$$h = 3 \quad \Rightarrow \quad \mathbf{a} = (n-1, 3, 3, 3, \underbrace{1 \cdots 1}_{n-4}),$$
$$h = 4 \quad \Rightarrow \quad \mathbf{a} = (n-1, 4, 2, 2, 2, \underbrace{1 \cdots 1}_{n-5}).$$

However, $SS((n-1, 3, 3, 3, \underbrace{1 \cdots 1}_{n-4})) = SS((n-1, 4, 2, 2, 2, \underbrace{1 \cdots 1}_{n-5}))$. Consequently, both sequences attain the maximum M. ■

Example 2.4. Let $m = n+3$. Then, by Corollary 2.2, M is attained at $\mathbf{a}$ of the form:

$$(n-1, h, \underbrace{h \cdots h, a, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1}).$$

Note that $2(h-1) \leq 8 = 2(m-n+1) = h + \cdots + h + a + 2 \cdots + 2 \leq h(h-1)$ and so $4 \leq h \leq 5$. Hence

$$h = 4 \quad \Rightarrow \quad \mathbf{a} = (n-1, 4, 4, 2, 2, \underbrace{1 \cdots 1}_{n-5}),$$
$$h = 5 \quad \Rightarrow \quad \mathbf{a} = (n-1, 5, 2, 2, 2, 2, \underbrace{1 \cdots 1}_{n-6}).$$

However, $SS((n-1, 4, 4, 2, 2, \underbrace{1 \cdots 1}_{n-5})) = SS((n-1, 5, 2, 2, 2, 2, \underbrace{1 \cdots 1}_{n-6}))$. Consequently, both sequences attain the maximum M. ■

Lemma 2.5. Let $\mathbf{a} = (n-1, h, \underbrace{h \cdots h, a, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1}) \in \mathcal{A}$.

If $6 \leq a$, or $5 = a < h$, or $4 = a < h$ then $SS(\mathbf{a}) < M$.

Proof: Case 1: $a = 2k+2$ for some $k \geq 1$.

Because $m \leq 2n-3$, we have $2k+2+2(h-2) \leq 2(m-n+1) \leq 2(n-2)$, and so $k \leq n-h-1$. Then

$$\mathbf{a}' = (n-1, h+k, \underbrace{h \cdots h, 2, 2 \cdots 2}_{h-1}, \underbrace{2 \cdots 2}_{k}, \underbrace{1 \cdots 1}_{n-h-1-k}) \in \mathcal{A}$$

Moreover,

$$\begin{aligned} SS(\mathbf{a}') - SS(\mathbf{a}) &= (h+k)^2 + (k+1)4 - h^2 - (2k+2)^2 - k \\ &= k(2h - 3k - 5) \\ &\geq k(2(2k+2) - 3k - 5) \\ &= k(k-1) \end{aligned}$$

and so $SS(\mathbf{a}) < SS(\mathbf{a}') \leq M$ if $k \geq 2$ or $h > 4 = a$.

Case 2: $a = 2k + 3$ for some $k \geq 1$.

By parity, there is at least an h in the list $\underbrace{h \cdots h, a, 2 \cdots 2}_{h-1}$ because a is odd and their sum is even. Because $m \leq 2n - 3$, we have $2k + 3 + 2(h-3) + 3 \leq 2(m - n + 1) \leq 2(n-2)$, and so $k + 1 \leq n - h - 1$. Then

$$\mathbf{a}' = (n-1, h+k+1, \underbrace{h \cdots h-1, 2, 2 \cdots 2}_{h-1}, \underbrace{2 \cdots 2}_{k+1}, \underbrace{1 \cdots 1}_{n-h-2-k}) \in \mathcal{A}$$

Moreover,

$$\begin{aligned} SS(\mathbf{a}') - SS(\mathbf{a}) &= (h+k+1)^2 + (h-1)^2 + (k+2)4 - 2h^2 - (2k+3)^2 - k - 1 \\ &= k(2h - 3k - 7) \\ &\geq k(2(2k+3) - 3k - 5) \\ &= k(k-1) \end{aligned}$$

and so $SS(\mathbf{a}) < SS(\mathbf{a}') \leq M$ if $k \geq 2$ or $h > 5 = a$. ∎

Lemma 2.6. Let $\mathbf{a} = (n-1, h, \underbrace{h \cdots h, a, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1}) \in \mathcal{A}$. If $h = a = 5$ then $SS(\mathbf{a}) < M$.

Proof: Since $h = a = 5$ is odd, by parity, $\mathbf{a}$ can only be

$$(n-1, 5, 5, 5, 5, 5, \underbrace{1 \cdots 1}_{n-6}) \text{ or } (n-1, 5, 5, 5, 2, 2, \underbrace{1 \cdots 1}_{n-6}).$$

Note that $SS((n-1, 5, 5, 5, 5, 5, \underbrace{1 \cdots 1}_{n-6})) = SS((n-1, 7, 5, 5, 4, 2, 2, 2, \underbrace{1 \cdots 1}_{n-8})) < M$ by Corollary 2.2, and

$$SS((n-1, 5, 5, 5, 2, 2, \underbrace{1 \cdots 1}_{n-6})) = SS((n-1, 7, 4, 2, 2, 2, 2, 2, \underbrace{1 \cdots 1}_{n-8})) < M$$

by Lemma 2.5. In both cases, $SS(\mathbf{a}) < M$. ∎

Lemma 2.7. Let $\mathbf{a} = (n-1, h, \underbrace{h \cdots h, a, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1}) \in \mathcal{A}$. If $h > a = 3$ then $SS(\mathbf{a}) < M$.

Proof: Since $a = 3$ is odd, by parity, there must be at least two h in $\mathbf{a}$ and h must be odd too.

Case 1: $h = 5$.

We have $\mathbf{a} = (n-1, 5, 5, 3, 2, 2, \underbrace{1 \cdots 1}_{n-6})$. Note that $SS((n-1, 5, 5, 3, 2, 2, \underbrace{1 \cdots 1}_{n-6})) = SS((n-1, 6, 4, 2, 2, 2, 2, \underbrace{1 \cdots 1}_{n-7})) < M$ by Lemma 2.5.

Case 2: $h \geq 7$.

(i) $\mathbf{a}$ has exactly two h, i.e., $\mathbf{a} = (n-1, h, \underbrace{h, 3, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1}))$. Then $SS((n-1, h, \underbrace{h, 3, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1})) = SS((n-1, h+1, \underbrace{h-1, 2 \cdots 2}_{h}, \underbrace{1 \cdots 1}_{n-h-2})) < M$ by Lemma 2.5.

or (ii) $\mathbf{a}$ has more than two h, i.e., $\mathbf{a} = (n-1, h, \underbrace{h \cdots h, h, h, 3, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1}))$. Then

$$
\begin{aligned}
& SS((n-1, h, \underbrace{h \cdots h, h, h, 3, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1})) \\
= \; & SS((n-1, h+1, \underbrace{h \cdots h, h, h-1, 2 \cdots 2}_{h}, \underbrace{1 \cdots 1}_{n-h-2})) < M
\end{aligned}
$$

by Corollary 2.2. ■

Lemma 2.8. Let $\mathbf{a} = (n-1, h, \underbrace{h \cdots h, a, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1}) \in \mathcal{A}$. If $h = a = 4$ then $SS(\mathbf{a}) = M$ if and only if $\mathbf{a} = (n-1, 4, 4, 2, 2, \underbrace{1 \cdots 1}_{n-5}))$.

Proof: Since $h = a = 4$, $\mathbf{a}$ can only be

$$
(n-1, 4, 4, 2, 2, \underbrace{1 \cdots 1}_{n-5}), \quad (n-1, 4, 4, 4, 2, \underbrace{1 \cdots 1}_{n-5}), \quad (n-1, 4, 4, 4, 4, \underbrace{1 \cdots 1}_{n-5}).
$$

Note that $SS((n-1, 4, 4, 2, 2, \underbrace{1 \cdots 1}_{n-5})) = SS((n-1, 5, 2, 2, 2, 2 \underbrace{1 \cdots 1}_{n-6})) = M$ by Example 2.4, $SS((n-1, 4, 4, 4, 2, \underbrace{1 \cdots 1}_{n-5})) = SS((n-1, 5, 4, 2, 2, 2 \underbrace{1 \cdots 1}_{n-6})) < M$ by Lemma 2.5, and $SS((n-1, 4, 4, 4, 4, \underbrace{1 \cdots 1}_{n-5})) = SS((n-1, 5, 4, 4, 2, 2, \underbrace{1 \cdots 1}_{n-6})) < M$ by Corollary 2.2. In all cases, $SS(\mathbf{a}) = M$ if and only if $\mathbf{a} = (n-1, 4, 4, 2, 2, \underbrace{1 \cdots 1}_{n-5}))$.

■

Lemma 2.9. Let $\mathbf{a} = (n-1, h, \underbrace{h \cdots h, a, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1}) \in \mathcal{A}$. If $h = a = 3$ then $\mathbf{a} = (n-1, 3, 3, 3, \underbrace{1 \cdots 1}_{n-4})$ and $SS(\mathbf{a}) = M$.

Proof: $\mathbf{a}$ must be $(n-1, 3, 3, 3, \underbrace{1 \cdots 1}_{n-4})$. Note that $SS((n-1, 3, 3, 3, \underbrace{1 \cdots 1}_{n-4})) = SS((n-1, 4, 2, 2, 2, \underbrace{1 \cdots 1}_{n-5})) = M$, by Example 2.3. ■

Lemma 2.10. If $M = SS(\mathbf{a})$ then

(i) $\mathbf{a} = (n-1, m-n+2, \underbrace{2, \cdots, 2}_{m-n+1}, \underbrace{1, \cdots, 1}_{2n-3-m})$ with any $n-1 \le m \le 2n-3$, or

(ii) $\mathbf{a} = (n-1, 4, 4, 2, 2, \underbrace{1 \cdots 1}_{n-5})$ with $m = n+3$, or

(iii) $\mathbf{a} = (n-1, 3, 3, 3, \underbrace{1 \cdots 1}_{n-4})$ with $m = n+2$.

Proof: Since the set $\mathcal{A}$ is finite, M is attained at some $\mathbf{a} \in \mathcal{A}$.

Case 1: When $a_3 = 2$, then $a_3 = \cdots = a_{h+1} = 2$, and so $2(h-1) = 2(m-n+1)$, i.e., $h = m-n+2$. Hence $\mathbf{a}$ has the form in (i).

Case 2: When $a_3 \ge 3$, then, by Corollary 2.2, $\mathbf{a}$ is of the form

$$\mathbf{a} = (n-1, h, \underbrace{h \cdots h, a, 2 \cdots 2}_{h-1}, \underbrace{1 \cdots 1}_{n-h-1})$$

where $3 \le a \le h$. By Lemmas 2.5, 2.6, and 2.7, $h = a = 4$ or $h = a = 3$. Hence the conclusion in (ii) and (iii) follows from Lemmas 2.8 and 2.9, respectively. ■

Therefore we obtain the following result about the maximum sum of squares of sequences in $\mathcal{A}$.

Theorem 2.11. For $\mathbf{a} \in \mathcal{A}$,

$$SS(\mathbf{a}) \le SS((n-1, m-n+2, \underbrace{2, \cdots, 2}_{m-n+1}, \underbrace{1, \cdots, 1}_{2n-3-m})).$$

Equality holds if and only if $\mathbf{a} = (n-1, m-n+2, \underbrace{2, \cdots, 2}_{m-n+1}, \underbrace{1, \cdots, 1}_{2n-3-m})$ or $(n-1, 4, 4, 2, 2, \underbrace{1 \cdots 1}_{n-5})$, or $(n-1, 3, 3, 3, \underbrace{1 \cdots 1}_{n-4})$.

Remark 2.12. The sequence $(n-1, m-n+2, \underbrace{2, \cdots, 2}_{m-n+1}, \underbrace{1, \cdots, 1}_{2n-3-m})$ is the degree sequence of the unique connected graph F_n^m. The sequence $(n-1, 3, 3, 3, \underbrace{1 \cdots 1}_{n-4})$ is the degree sequence of the unique connected graph H_n^{n+2}. But, the sequence $(n-1, 4, 4, 2, 2, \underbrace{1 \cdots 1}_{n-5})$ is NOT graphical.

3 Maximum sum of degree squares

The sums of degrees of (n, m)-graphs are always a constant $(= 2m)$, but the sums of degree squares of (n, m)-graphs vary. It is interesting to know the possible range of such sums, and the graphs achieving the maximum and minimum value. Graphs with the minimum sum of degree squares among general (not necessarily connected) (n, m)-graphs have a difference of at most one between their maximum and minimum degrees. Such graphs always exist and indeed can be taken to be connected provided $m \geq n - 1$, and so the corresponding results for general and connected (n, m)-graphs are the same. Graphs with the maximum sum of degree squares among general (n, m)-graphs are known but harder to describe, see [1] for a comprehensive discussion. However, the corresponding result for connected (n, m)-graphs cannot be found in literature. In this section, we are looking for graphs with the maximum sum of degree squares among connected (n, m)-graphs for $n - 1 \leq m \leq 2n - 3$. The problem is reduced to finding the maximum sum of squares of entries of a specific type of positive integer sequences, which is resolved in Section 2. Denote $\mathbf{d}(G) = (d_1, \cdots, d_n)$ the non-increasing sequence of degrees of a graph $G \in \mathcal{G}_{n,m}$. Then $1 \leq d_i \leq n - 1$ for $1 \leq i \leq n$, and $\sum_{i=1}^{n} d_i = 2m$. We are looking for the graph $G_0 \in \mathcal{G}_{n,m}$ such that

$$SS(\mathbf{d}(G_0)) = \max \{SS(\mathbf{d}(G)) : G \in \mathcal{G}_{n,m}\}.$$

Let $N(u)$ be the set of neighbors of a vertex u, and $deg(u) = |N(u)|$ be the degree of u.

Lemma 3.1. $\mathbf{d}(G_0) \in \mathcal{A}$.

Proof. Let $\mathbf{d}(G_0) = (a_1, a_2, \cdots, a_n)$ with $n - 1 \geq a_1 \geq \cdots \geq a_n \geq 1$. Label the vertices $\{u_1, \cdots, u_n\}$ of G_0 such that $deg(u_i) = a_i$ for $1 \leq i \leq n$.

Claim 1. $a_1 = n - 1$.

Otherwise, $a_1 = |N(u_1)| < n - 1$. Then there exists a vertex $u_k \notin N(u_1) \cup \{u_1\}$. By connectedness of G_0, u_k is adjacent to a vertex $u_j \in N(u_1)$ with $a_j = deg(u_j) \geq 2$. Let G_0' be the graph obtained from G_0 by first deleting the edge $u_k u_j$ and then adding the edge $u_1 u_k$. Then $G_0' \in \mathcal{G}_{n,m}$ and

$$SS(\mathbf{d}(G_0')) - SS(\mathbf{d}(G_0)) = (a_1 + 1)^2 + (a_j - 1)^2 - a_1^2 - a_j^2 = 2(a_1 - a_j + 1) > 0$$

because $a_1 \geq a_j$. Hence $SS(\mathbf{d}(G_0')) > SS(\mathbf{d}(G_0))$, contradicting the maximality of G_0.

Claim 2. Each vertex in $N(u_1) \setminus \{N(u_2) \cup \{u_2\}\}$ has degree one.
Otherwise, there exists a vertex $u_k \in N(u_1) \setminus \{N(u_2) \cup \{u_2\}\}$ with $deg(u_k) \geq 2$. Hence u_k is adjacent to a vertex $u_j \neq u_1, u_2$ with $a_j = deg(u_j) \geq 2$. Let G_0' be the graph obtained from G_0 by first deleting the edge $u_k u_j$ and then adding the edge $u_k u_2$. Then $G_0' \in \mathcal{G}_{n,m}$ and

$$SS(\mathbf{d}(G_0')) - SS(\mathbf{d}(G_0)) = (a_2+1)^2 + (a_j-1)^2 - a_2^2 - a_j^2 = 2(a_2 - a_j + 1) > 0$$

because $a_2 \geq a_j$. Hence $SS(\mathbf{d}(G_0')) > SS(\mathbf{d}(G_0))$, contradicting the maximality of G_0.

Let $a_2 = |N(u_2)| = h$. By Claims 1 and 2, there are $|N(u_1) \setminus \{N(u_2) \cup \{u_2\}\}| = n-1-h$ vertices with degree one. Thus, $\mathbf{d}(G_0) = (n-1, h, a_3 \cdots a_{h+1}, \underbrace{1 \cdots 1}_{n-h-1})$ and so $2m = (n-1)+h+a_3+\cdots+a_{h+1}+(n-h-1)$, i.e., $a_3+\cdots+a_{h+1} = 2(m-n+1)$. Consequently, $\mathbf{d}(G_0) \in \mathcal{A}$. ■

Let us recall the graphs $F_n^m = (S_{m-n+2} \cup E_{2n-3-m}) \vee E_1$ and $H_n^{n+2} = (C_3 \cup E_{n-4}) \vee E_1$.

Theorem 3.2. For $G \in \mathcal{G}_{n,m}$,

$$SS(\mathbf{d}(G)) \leq SS(\mathbf{d}(F_n^m)).$$

Equality holds if and only if $G = F_n^m$, or H_n^{n+2} when $m = n+2$.

Proof. Let $G_0 \in \mathcal{G}_{n,m}$ be such that $SS(\mathbf{d}(G_0)) = \max\{SS(\mathbf{d}(G)) : G \in \mathcal{G}_{n,m}\}$. By Lemma 3.1, $d(G_0) \in \mathcal{A}$. Hence, by Theorem 2.11 and Remark 2.12, $SS(\mathbf{d}(G_0)) \leq SS(\mathbf{d}(F_n^m))$, and so

$$SS(\mathbf{d}(G)) \leq SS(\mathbf{d}(G_0)) \leq SS(\mathbf{d}(F_n^m))$$

for any $G \in \mathcal{G}_{n,m}$.

If $SS(\mathbf{d}(G)) = SS(\mathbf{d}(F_n^m))$ then we can take $G = G_0$, and $SS(\mathbf{d}(G_0)) = SS(\mathbf{d}(F_n^m))$ if and only if $\mathbf{d}(G_0) = \mathbf{d}(F_n^m)$ or $\mathbf{d}(H_n^{n+2})$ when $m = n+2$, by Theorem 2.11. Hence, Remark 2.12 asserts that $G_0 = F_n^m$, or H_n^{n+2} when $m = n+2$. ■

4 Proof of Theorem 1.4

Now we restate Theorem 1.4 in two parts and give their proofs separately.

Theorem 1.4(i). For $G \in \mathcal{G}_{n,m}$ with $n-1 \leq m \leq 2n-3$,

(a) $F_n^m \preccurlyeq G$

(b) $G \sim F_n^m$ if and only if $G = F_n^m$ or H_n^{n+2} when $m = n+2$.

Proof: (a) Since $F_n^m, G \in \mathcal{G}_{n,m}$, we have $m(F_n^m, 1) = m(G, 1) = m$. Next, we observe that, for $G \in \mathcal{G}_{n,m}$ with the degree sequence $\mathbf{d}(G) = (d_1, \cdots, d_n)$,

$$m(G,2) \quad = \quad \binom{m}{2} - \sum_{i=1}^{n} \binom{d_i}{2} = \binom{m}{2} + m - \frac{1}{2} SS(\mathbf{d}(G)).$$

because of $2m = \sum_{i=1}^{n} d_i$ and the definition of SS. Hence $m(F_n^m, 2) \leq m(G, 2)$ because $SS(\mathbf{d}(F_n^m)) \geq SS(\mathbf{d}(G))$ by Theorem 3.2. Finally, $m(F_n^m, k) = 0 \leq m(G, k)$ for $k \geq 3$. Consequently, $F_n^m \preccurlyeq G$.

(b) Case 1: $m \neq n+2$.

If $G \neq F_n^m$ then $SS(d(G)) < SS(d(F_n^m))$ by Theorem 3.2, and so $m(G, 2) > m(F_n^m, 2)$. Consequently, $F_n^m \not\sim G$.

Case 2: $m = n+2$.

Note that $m(F_n^{n+2}, k) = m(H_n^{n+2}, k)$ for all k. If $G \neq F_n^{n+2}, H_n^{n+2}$ then $SS(d(G)) < SS(d(F_n^{n+2}))$ by Theorem 3.2, and so $m(G, 2) > m(F_n^{n+2}, 2)$. Consequently, $F_n^{n+2} \not\sim G$. ■

The following well-known formula (1) is useful for the proof of Theorem 1.4 (ii).
Let $e = uv$ be an edge of G and k a positive integer. Then

$$m(G,k) = m(G-e,k) + m(G-u-v,k-1). \tag{1}$$

Theorem 1.4 (ii) Let $\frac{n(n-1)}{2} - (n-2) \leq m \leq \frac{n(n-1)}{2}$. For $G \in \mathcal{G}_{n,m}$,

(a) $A_n^m \preccurlyeq G$.

(b) $G \sim A_n^m$ if and only if $G = A_n^m$, or $B_n^{n(n-1)/2-3}$ when $m = n(n-1)/2 - 3$.

Proof: For $m = n(n-1)/2$ and $m = n(n-1)/2 - 1$, there is only one graph in $\mathcal{G}_{n,m}$, and so the conclusion is obvious.

From now on, we consider $n(n-1)/2 - (n-2) \leq m \leq n(n-1)/2 - 2$. Let $r = n(n-1)/2 - m$, and so $2 \leq r \leq n-2$.

(a) Note that A_n^m is the graph obtained from K_n by deleting r edges which share a common vertex. Let these r edges of K_n be $e'_1, \cdots, e'_r$ with $e'_y = uw_y$, where $1 \leq y \leq r$. Then $A_n^m = K_n - e'_1 - \cdots - e'_r$.

Repeatedly using (1) r times, we obtain

$$\begin{aligned} m(K_n, k) &= m(A_n^m, k) + \sum_{y=1}^{r} m(K_n - u - w_y, k-1) \\ &= m(A_n^m, k) + rm(K_{n-2}, k-1). \end{aligned} \tag{2}$$

Note that $G \in \mathcal{G}_{n,m}$ can be viewed as the graph obtained from K_n by deleting the r edges in K_n. Let these r edges of K_n be $e_1, \cdots, e_r$ with $e_x = u_x v_x$, where $1 \leq x \leq r$. Then $G = K_n - e_1 - \cdots - e_r$.

Repeatedly using (1) r times, we get

$$m(K_n, k) = m(G, k) + \sum_{x=0}^{r-1} m(K_n - e_1 - \cdots - e_x - u_{x+1} - v_{x+1}, k-1). \tag{3}$$

For a fixed x with $0 \leq x \leq r-1$, obviously, $K_n - e_1 - \cdots - e_x - u_{x+1} - v_{x+1}$ is K_{n-2} or a proper subgraph of K_{n-2}. Hence

$$m(K_n, k) \leq m(G, k) + rm(K_{n-2}, k-1). \tag{4}$$

Therefore, by (2) and (4), we have $m(A_n^m, k) \leq m(G, k)$ for all k.

(b) Recall that $B_n^{n(n-1)/2-3}$ is the graph obtained from K_n by deleting the three edges of C_3 in K_n. If $G = B_n^{n(n-1)/2-3}$ when $r = 3$, then we can verify that $K_n - e_1 - \cdots - e_x - u_{x+1} - v_{x+1}$ is K_{n-2} for all $x = 0, 1, 2$. Thus, by (2) and (3), we obtain $A_n^m \sim B_n^{n(n-1)/2-3}$.

If $G \neq A_n^m$ and $G \neq B_n^{n(n-1)/2-3}$ when $r = 3$, then there exist two independent edges among $\{e_1, \cdots, e_r\}$. Namely, there exists a fixed x with $1 \leq x \leq r-1$ such that $K_n - e_1 - \cdots - e_x - u_{x+1} - v_{x+1}$ is a proper subgraph of K_{n-2}. Hence,

$$m(K_n - e_1 - \cdots - e_x - u_{x+1} - v_{x+1}, 1) < m(K_{n-2}, 1). \tag{5}$$

It follows from (2)–(5) that

$$m(A_n^m, 2) < m(G, 2).$$

Hence $G \not\sim A_n^m$. ∎

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