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On Extremal Connected Graphs with Respect to the Forgotten Topological Index

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Abstract

In the study of the structure-dependency of the total π-electron from 1972, it is pointed out that it depends on the sums $\sum_{v\in V} d(v)^2$ and $\sum_{v\in V} d(v)^3$, where $d(v)$ is the degree of a vertex v in the underlying molecular graph G. The first sum $\sum_{v\in V} d(v)^2$, which was named the first Zagreb index, is one of the most investigated graph-based topological index. The second sum $\sum_{v\in V} d(v)^3$ has been almost completely neglected except for its potential involvement in the study of the first Zagreb index and the zeroth-order general Randić index. This second sum was named the forgotten index or F-index in short. In this paper, we investigate some properties of the F-index with respect to some new graph transformations, which are used to characterize all extremal graphs having the maximum F-index in the set $\mathcal{G}_{n,m}$ of all connected graphs of order n and size m.

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1 Introduction

In this paper we are concerned with simple undirected connected graphs. Let $G = (V, E)$ be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. Denote by $|V(G)| = n$ and $|E(G)| = m$ the number of vertices and edges of G, respectively. We may assume that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. Then, the degree sequence of G is the non-increasing degree sequence $(d(v_1), d(v_2), \cdots, d(v_n))$. We denote by $d_i = d(v_i)$ the degree of vertex v_i for $i = 1, 2, \ldots, n$. For vertices $u, v \in V(G)$, if u is adjacent to v, then $u \sim v$, if u is not adjacent to v, we write $u \nsim v$. For $e \notin E(G)$, let $G + e$ be a graph which is obtained from G by adding a new edge e. For $e \in E(G)$, let $G - e$ be a graph which is obtained from G by deleting the edge e.

Let $\mathcal{G}_{n,m}$ be the set of all connected graphs of n vertices and m edges. Let $K_n, S_n, \bar{K}_n$ be the complete graph of order n, the star of order n, and the graph consisting n isolated vertices, respectively. Let H_1 and H_2 be two disjoint graphs. Denote by $H_1 \cup H_2$ the disjoint union of H_1 and H_2, where $V(H_1 \cup H_2) = V(H_1) \cup V(H_2)$ and $E(H_1 \cup H_2) = E(H_1) \cup E(H_2)$. Denote by $H_1 \vee H_2$ be the join of H_1 and H_2, obtained by adding all edges between H_1 and H_2, i.e., $V(H_1 \vee H_2) = V(H_1) \cup V(H_2)$, while the edge set of $H_1 \vee H_2$ consists of $E(H_1) \cup E(H_2)$ and edge $\{uv\}$, for every $u \in V(H_1), v \in V(H_2)$.

Topological indices play a significant role in mathematical chemistry, especially in the QSPR/QSAS assessments [20]. Topological indices based on vertex degrees are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activities of chemical compounds, and yielding many chemical applications.

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined as follows:

$$M_1(G) = \sum_{v_i \in V(G)} d^2(v_i) = \sum_{uv \in E(G)} (d(u) + d(v)),$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

The quantity M_1 was first considered in 1972 [12], whereas M_2 was in 1975 [15]. These are the oldest and most thoroughly examined vertex-degree-based topological indices. Details of their theory and applications can be found in the surveys [4–6, 13, 30] and references therein.

Various generalizations of the Zagreb indices have been proposed. Li and Zheng [23] introduced the first general Zagreb index. It is defined as

$$M_\alpha(G) = \sum_{v \in G} d^\alpha(v).$$

where α is an arbitrary real number. It is also known as the general zeroth-order Randić index [17, 22] and variable first Zagreb index [27].

In the study of structure-dependency of the total π-electron energy, the Zagreb index is the most studied topological index. However, there is another crucial term for the study of this energy, which did not attract any attention at all. Furtula and Gutman [10] introduced this topological index as the forgotten topological index, or the forgotten index, or the F-index for simplicity, which is defined as the sum of cubes of vertex degrees of G:

$$F(G) = \sum_{v_i \in V(G)} d^3(v_i) = \sum_{uv \in E(G)} (d^2(u) + d^2(v)).$$

If $\alpha = 3$, the first general Zagreb index $M_\alpha(G)$ equals the forgotten index. For the entropy and acentric factor, Furtula and Gutman [10] showed that the F-index of molecular graphs can be used to predict some chemical properties of molecular structure, and presented several upper and lower bounds for the F-index. De et al. [9] discovered that the F-index of molecular graphs performs better than the Zagreb index in some applications. Che and Chen [8] obtained lower and upper bounds for the F-index in terms of graph irregularity, graph size, and maximum/minimum vertex degrees. Abdo et al. [1] obtained the extremal trees with respect to the F-index. Akhter et al. [3] and Jahanbani [18] determined the extremal graphs with respect to the F-index among the classes of unicyclic graphs and bicyclic graphs, respectively. Jahanbani et. al. [19] presented sharp upper bounds for the F-index of bicyclic graphs in terms of the order and maximum degree.

Let $\mathcal{G}_{n,m}$ be the set of all simple connected graphs of order n and size m. In 2021, Tomescu [32] posed the following conjecture.

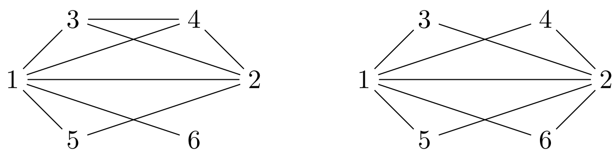
Conjecture 1.1. If $G \in \mathcal{G}_{n,m}$ is a connected graph with $n \geq 6$, $n - 1 \leq m \leq \frac{1}{2}\binom{n-1}{2}$ and $m = nk - \binom{k+1}{2} + a$, where $1 \leq k \leq n-1$ and $0 \leq a < n-k-1$, then

$$F(G) \leq k(n-1)^3 + a(k+1)^3 + (n-k-a-1)k^3 + (k+a)^3.$$

Given two integers $n \leq m$, let k be the largest integer such that $m - n + 1 \geq \sum_{i=1}^{k-1} i$ and $\sum_{i=1}^{k-1} i + (n-1) + \bar{a} = m$. Let

$$L_{n,m} = \begin{cases} (K_k \cup (n-k-1)K_1) \vee K_1, & \text{for } \bar{\mathrm{a}} = 0; \\ (K_{\bar{a}} \vee (K_{k-\bar{a}-1} \cup K_1) \cup (n-k-1)K_1) \vee K_1, & \text{for } \bar{\mathrm{a}} > 0. \end{cases}$$

Let k' be the largest integer such that $m \geq \sum_{i=1}^{k'}(n-i)$ and $\hat{a} = m - \sum_{i=1}^{k'}(n-i)$. We also define $S_{n,m} = K_{k'} \vee (S_{\hat{a}+1} \cup (n-\hat{a}-k'-1)K_1)$. Note that if $m = n(n-1)/2$, then $S_{n,m} = K_n$. For example, $L_{6,9}$ and $S_{6,9}$ are depicted in Figure 1, where $k = 3$, $\bar{a} = 1$; $k' = 2$, $\hat{a} = 0$.



(a) $L_{6,9}$ (b) $S_{6,9}$

Figure 1. $L_{n,m}$ and $S_{n,m}$ with $n = 6$, $m = 9$

In Section 2, we introduce some known results that are useful for our work. In Section 3, we present several new graph transformations that keep the F-index non-increasing. In Section 4, we prove all extremal graphs having the maximum F-index in the set of all connected graphs of order n and size m are $S_{n,m}$ for $n-1 \leq m \leq \frac{1}{4}\binom{n-1}{2}$, which supports the statement of Conjecture 1.1.

2 Preliminaries

A graph $G = (V, E)$ is called a *threshold* graph if G is $\{2K_2, C_4, P_4\}$-free. Threshold graphs have a beautiful structure and possess many important mathematical properties such as being the extreme cases of certain graph properties (see [11, 31]). For more information of threshold graphs, one can see the monograph [26].

Lemma 2.1. [31] Let $G = (V, E)$ be an undirected graph with degree sequence $(d_1, d_2, \ldots, d_n)$. The following statements are equivalent:
(i). G is a threshold graph;
(ii). G can be constructed from the one-vertex graph by repeatedly adding an isolated vertex or a universal (or dominating) vertex (a vertex adjacent to every other vertex);
(iii). every three distinct vertices i, j, k of G satisfy: if $d_i \geq d_j$ and jk is an edge, then ik is an edge.

Lemma 2.2. *[16, Theorem 6.1]* Any threshold graph is uniquely defined by its degree sequence.

Let $D = (d_1, d_2, \ldots, d_n)$ be a non-increasing integer sequence with all elements being integers. The Ferrers matrix (or Ferrers diagram; see e.g. [26, p62]) of D is a $n \times n$ matrix F of $\circ'$s, $\bullet'$s and, $+'$s such that

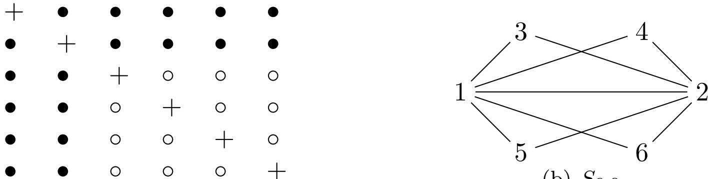
$\star$ all the diagonal entries and no others are $+$;

$\star$ for each i, $i \in [n]$, the number of $\bullet'$s contained in the ith row is d_i;

$\star$ the symbols $\bullet'$s in each row are to the left.

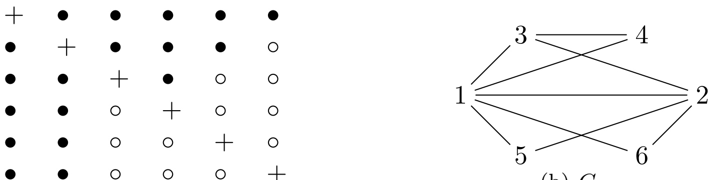
In fact, the Ferrers matrix $FR(G)$ of a threshold graph G is the adjacency matrix of such a graph if we consider the symbol $\circ$ and $+$ as the digit 0, and the symbol $\bullet$ as the digit 1, then the Ferrers matrix of a threshold graph is symmetrical (see Figure 2 as an example and Figure 3 as a counterexample). We only concern and describe the entries below the diagonal of the Ferrers matrix.

Lemma 2.3. [32] Let $x \geq y \geq 1$. If the function $f(x)$ is strictly convex, then $f(x+1) + f(y-1) > f(x) + f(y)$; else if the function $f(x)$ is strictly concave, then $f(x+1) + f(y-1) < f(x) + f(y)$.



(a) Ferrer matrix of $S_{6,9}$ (b) $S_{6,9}$

Figure 2. The Ferrers matrix of a threshold graph is symmetrical



(a) Ferrer matrix of $G_{6,9}$ (b) $G_{6,9}$

Figure 3. The Ferrers matrix of a non-threshold graph is asymmetrical

Ábrego et al. [2] showed the following.

Lemma 2.4. [2] If $\alpha < 0$ or $\alpha > 1$, then all extremal graphs which maximize $M_\alpha(G)$ must be threshold graphs; if $0 < \alpha < 1$, then all extremal graphs which minimizes $M_\alpha(G)$ must be threshold graphs. In particular, all extremal graph having maximum value $F(G)$ are threshold graphs.

Let $\mathcal{G}^*{}_{n,m}$ be the set of all connected threshold graphs of n vertices and m edges. By Lemma 2.4,

$$\max_{G \in \mathcal{G}_{n,m}} F(G) = \max_{G \in \mathcal{G}^*{}_{n,m}} F(G).$$

Hence we focus our attention on the set of the threshold graphs to characterize all extremal graphs which have the maximum F-index.

3 Transformations

In this section, we focus on threshold graphs. First, we introduce some graphic transformations and related properties, which will be used to prove our main results.

Definition 1. Let $d = (d_1, \ldots, d_n)$ be a non-increasing degree sequence of a threshold graph G. Suppose that there are four integers $1 \leq i, j, p, q \leq n$ with $q < j, j + l < i - c$, and $i < p$ such that $d_{q-c} = \cdots = d_q = p + l - 1$, $d_{i-c} = \cdots = d_i = j - 1$, $d_j = \cdots = d_{j+l} = i - c - 2$, $d_p = \cdots = d_{p+l} = q$, where $l \geq 0$ and $c \geq 0$. If the non-increasing degree sequence $d' = (d'_1, \ldots, d'_n)$ of a threshold graph G' is the same as the degree sequence of G except $d'_{q-c} = \cdots = d'_q = p - 2$, $d'_{i-c} = \cdots = d'_i = j + l$, $d'_j = \cdots = d'_{j+l} = i - 1$ and $d'_p = \cdots = d'_{p+l} = q - c - 1$, then we say G' is obtained from G through a transformation (from G to G') with respect to $(q, j, i, p; l + 1, c + 1)$.

For example, there are three concrete transformations from $S_{9,23}$ to $G_{9,23}$ with respect to $(3, 4, 8, 9; 1, 2)$, from $S_{7,12}$ to $L_{7,12}$ with respect to $(2, 3, 5, 6; 2, 1)$, and from $S_{9,22}$ to $L_{9,22}$ with respect to $(3, 4, 7, 8; 1, 2)$ which are depicted in Table 1, 2 and 3 respectively.

Table 1. Transformation from $S_{9,23}$ to $G_{9,23}$ with respect to $(3, 4, 8, 9; 1, 2)$

+	•	•	•	•	•	•	•	•
•	+	•	•	•	•	•	•	•
•	•	+	•	•	•	•	•	•
•	•	•	+	•	•	○	○	○
•	•	•	•	+	○	○	○	○
•	•	•	•	○	+	○	○	○
•	•	•	○	○	○	+	○	○
•	•	•	○	○	○	○	+	○
•	•	•	○	○	○	○	○	+

⇒

+	•	•	•	•	•	•	•	•
•	+	•	•	•	•	•	•	○
•	•	+	•	•	•	•	•	○
•	•	•	+	•	•	•	•	○
•	•	•	•	+	○	○	○	○
•	•	•	•	○	+	○	○	○
•	•	•	•	○	○	+	○	○
•	•	•	•	○	○	○	+	○
•	○	○	○	○	○	○	○	+

Table 2. Transformation from $S_{7,12}$ to $L_{7,12}$ with respect to $(2, 3, 5, 6; 2, 1)$

+	•	•	•	•	•	•
•	+	•	•	•	•	•
•	•	+	•	○	○	○
•	•	•	+	○	○	○
•	•	○	○	+	○	○
•	•	○	○	○	+	○
•	•	○	○	○	○	+

⇒

+	•	•	•	•	•	•
•	+	•	•	•	○	○
•	•	+	•	•	○	○
•	•	•	+	•	○	○
•	•	•	•	+	○	○
•	○	○	○	○	+	○
•	○	○	○	○	○	+

Table 3. Transformation from $S_{9,22}$ to $L_{9,22}$ with respect to $(3,4,7,8;2,2)$

$$
\begin{array}{ccccccccc}
+ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & + & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & + & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & \bullet & + & \bullet & \circ & \circ & \circ & \circ \\
\bullet & \bullet & \bullet & \bullet & + & \circ & \circ & \circ & \circ \\
\bullet & \bullet & \bullet & \circ & \circ & + & \circ & \circ & \circ \\
\bullet & \bullet & \bullet & \circ & \circ & \circ & + & \circ & \circ \\
\bullet & \bullet & \bullet & \circ & \circ & \circ & \circ & + & \circ \\
\bullet & \bullet & \bullet & \circ & \circ & \circ & \circ & \circ & +
\end{array}
\quad \Rightarrow \quad
\begin{array}{ccccccccc}
+ & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & + & \bullet & \bullet & \bullet & \bullet & \bullet & \circ & \circ \\
\bullet & \bullet & + & \bullet & \bullet & \bullet & \bullet & \circ & \circ \\
\bullet & \bullet & \bullet & + & \bullet & \bullet & \bullet & \circ & \circ \\
\bullet & \bullet & \bullet & \bullet & + & \bullet & \bullet & \circ & \circ \\
\bullet & \bullet & \bullet & \bullet & \bullet & + & \circ & \circ & \circ \\
\bullet & \bullet & \bullet & \bullet & \bullet & \circ & + & \circ & \circ \\
\bullet & \circ & \circ & \circ & \circ & \circ & \circ & + & \circ \\
\bullet & \circ & \circ & \circ & \circ & \circ & \circ & \circ & +
\end{array}
$$

Table 4. The differences of the degrees of G and G' in the transformation from G to G' with respect to $(q,j,i,p;l+1,c+1)$

The subscript x of the degree d_x	$q-c,\ \ldots,\ q$	$j,\ \ldots,\ j+l$	$i-c,\ \ldots,\ i$	$p,\ \ldots,\ p+l$
The degree d_x of G	$p+l-1$	$i-c-2$	$j-1$	q
The degree d_x of G'	$p-2$	$i-1$	$j+1$	$q-c-1$

If there is a transformation from G to G' with respect to $(q,j,i,p;l+1,c+1)$, it is easy to see that the differences of the degrees of G and G' as depicted in Table 4.

Furthermore, let $FR(G)=(f_{x,y})_{n\times n}$ and $FR(G')=(f_{x',y'})_{n\times n}$ be two Ferrers matrices of G and G', respectively. Then the corresponding entries of $FR(G)=(f_{x,y})_{n\times n}$ and $FR(G')=(f_{x',y'})_{n\times n}$ are the same except the following entries:

$$
f_{x,y}=\begin{cases} \circ, & \text{if } \mathrm{i-c \le x \le i,\ j \le y \le j+l;} \\ \bullet, & \text{if } \mathrm{p \le x \le p+l,\ q-c \le y \le q;} \end{cases}
$$

and

$$
f_{x',y'}=\begin{cases} \bullet, & \text{if } \mathrm{i-c \le x \le i,\ j \le y \le j+l;} \\ \circ, & \text{if } \mathrm{p \le x \le p+l,\ q-c \le y \le q.} \end{cases}
$$

Theorem 3.1. Let G' be obtained from $G \in \mathcal{G}^*_{n,m}$ through a transformation with respect to $(q,j,i,p;l+1,c+1)$, where $q<j, j+l<i-c,, i<p$, $l \ge 0$, $c \ge 0$. If $i+j \le p+q$, then $F(G) > F(G')$.

Proof. Let $s=p-i-1$, $r=j-i+c+l+1$ and $t=i+j-p-q$. Then

$s \geq 0$, $r \geq 0$, $t \leq 0$, $s+t \geq 0$ and $i \geq 2c+l+r+s+t+4$. Hence

$$\begin{aligned}
\triangle_t : &= F(G)-F(G') \\
&= \left[q^3(l+1)+(c+1)(j-1)^3+(c+1)(l+p-1)^3+(l+1)(-c+i-2)^3\right] \\
&\quad -\left[(c+1)(j+l)^3+(c+1)(p-2)^3+(i-1)^3(l+1)+(l+1)(-c+q-1)^3\right] \\
&= 3c^3l+3c^3+6c^2l^2+3c^2lr+9c^2ls+9c^2lt+18c^2l+3c^2r \\
&\quad +9c^2s+9c^2t+12c^2+3cl^3+3cl^2r+9cl^2s+6cl^2t+18cl^2 \\
&\quad +6clrs+6clrt+12clr+6cls^2+6clst+30cls+3clt^2+30clt+30cl \\
&\quad +6crs+6crt+9cr+6cs^2+6cst+21cs+3ct^2+24ct+15c \\
&\quad -i(6clt+6ct+6lt+6t)+3l^3+3l^2r \\
&\quad +9l^2s+6l^2t+12l^2+6lrs+6lrt+9lr+6ls^2+6lst+21ls+3lt^2 \\
&\quad +21lt+15l+6rs+6rt+6r+6s^2+6st+12s+3t^2+15t+6 \\
&\geq 3c^3l+3c^3+6c^2l^2+3c^2lr+9c^2ls+18c^2l+3c^2r+9c^2s+12c^2 \\
&\quad +3cl^3+3cl^2r+9cl^2s+18cl^2+6clrs+12clr+6cls^2+30cls \\
&\quad +30cl+6crs+9cr+6cs^2+21cs+15c+3l^3+3l^2r+9l^2s+12l^2 \\
&\quad +6lrs+9lr+6ls^2+21ls+15l+6rs+6r+6s^2+12s \\
&\quad -t^2(3cl+3c+3l+3)-t\left(3c^2l+3c^2+12cl+12c+9l+9\right)+6.
\end{aligned}$$

Let $\varphi(t) = -t^2(3cl+3c+3l+3)-t\left(3c^2l+3c^2+12cl+12c+9l+9\right)$. It is easy to see that $\varphi(t) \geq \max\{\varphi(0), \varphi(-s)\}$ for $-s \leq t \leq 0$. Hence

$$\begin{aligned}
\triangle_t \geq\ & 3c^3l+3c^3+6c^2l^2+3c^2lr+9c^2ls+18c^2l+3c^2r+9c^2s+12c^2 \\
& +3cl^3+3cl^2r+9cl^2s+18cl^2+6clrs+12clr+6cls^2+30cls \\
& +30cl+6crs+9cr+6cs^2+21cs+15c+3l^3+3l^2r+9l^2s+12l^2 \\
& +6lrs+9lr+6ls^2+21ls+15l+6rs+6r+6s^2+12s \\
& +\max\{\varphi(0), \varphi(-s)\}+6 \geq 0.
\end{aligned}$$

Thus the proof is complete. ■

Remark 1. If $t = i+j-p-q > 0$, then $F(G)-F(G')$ might be negative. For example, $L_{6,11}$ can be obtained from $S_{6,11}$ with respect to $(2,4,5,6,1,1)$ and $F(S_{6,11})-F(L_{6,11}) < 0$, which is depicted in Table 5.

Corollary 3.2. Let G' be the graph obtained from $G \in \mathcal{G}^*{}_{n,m}$ by transformation $(q,j,i,p;l+1,1)$. If $i+j-p-q \leq 0$, then G' is not an extremal graph having the maximum F-index in the set $\mathcal{G}_{n,m}$.

Table 5. Transformation$(2,4,5,6,1,1)$ from $S_{6,11}$ to $L_{6,11}$ with $t=1$

$$\begin{array}{cccccc} + & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & + & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & + & \bullet & \bullet & \circ \\ \bullet & \bullet & \bullet & + & \circ & \circ \\ \bullet & \bullet & \bullet & \boxed{\circ} & + & \circ \\ \bullet & \boxed{\bullet} & \circ & \circ & \circ & + \end{array} \quad F(S_{6,11}) = 376 \Rightarrow F(L_{6,11}) = 382 \quad \begin{array}{cccccc} + & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & + & \bullet & \bullet & \bullet & \circ \\ \bullet & \bullet & + & \bullet & \bullet & \circ \\ \bullet & \bullet & \bullet & + & \bullet & \circ \\ \bullet & \bullet & \bullet & \boxed{\bullet} & + & \circ \\ \bullet & \boxed{\circ} & \circ & \circ & \circ & + \end{array}$$

Corollary 3.3. Let G' be the graph obtained from $G \in \mathcal{G}^*{}_{n,m}$ by transformation $(q,j,i,p;1,c+1)$. If $i+j-p-q \le 0$, then G' is not an extremal graph having the maximum F-index in the set $\mathcal{G}_{n,m}$.

Definition 2. Let $G \in \mathcal{G}^*{}_{n,m}$ be a connected threshold graph with non-increasing degree sequence $d=(d_1,\ldots,d_n)$. Let $d_{n_0} = d_n$, $a_0 = \|\{i : d_i = d_{n_0}\}\|$, $b_0 = \|\{i : d_i = d_{n_0}+1\}\|$, $c_0 = \min\{d_i - d_{n_0} - 1 : d_i - d_{n_0} - 1 > 0\}$, $\theta_0 = n_0 + d_{n_0} + 1$. Generally, assume that a_{k-1}, b_{k-1}, c_{k-1} and n_{k-1} are defined. Let $n_k = n_{k-1} - a_{k-1} - b_{k-1}$, $a_k = \|\{i : d_i = d_{n_k}\}\|$, $b_k = \|\{i : d_i = d_{n_k}+1\}\|$, $c_k = \min\{d_i - d_{n_k} - 1 : d_i > d_{n_k}+1\}$, $\theta_k = n_k + d_{n_k} + 1$. Clearly, $c_k = d_{n_{k+1}} - d_{n_k} - 1$.

For example, there is a graph $G_{13,56}$ with $n_0 = 13$, $a_0 = 1$, $b_0 = 1$, $c_0 = 3$ and $n_1 = 11$, $a_1 = 1$, $b_1 = 0$, $c_1 = 2$, which is depicted in Table 6.

Now we present an algorithm which determines whether a threshold graph G can be obtained from another graph H by a transformation depicted in Corollary 3.2, or 3.3.

Algorithm 1: Determine an (n, m)-graph G with degree sequence $d = (d_1, \ldots, d_n)$ can or cannot be obtained from a graph H by the transformation depicted in Corollary 3.2, or 3.3

Data: a graph $G \in \mathcal{G}_{n,m}$

Result: Determine the a (n, m)-graph G with degree sequence $d = (d_1, \ldots, d_n)$ can or cannot be obtained from another graph H by a transformation depicted in Corollaries 3.2, or 3.3.

Set $d_0 = d_n$, $a = a_0 = \|\{i : d_i = d_0\}\|$, $b = b_0 = \|\{i : d_i = d_0 + 1\}\|$, $n_0 = n$, $n_1 = n_0 - a - b$, $c = c_0 = d_{n_1} - d_{n_0} - 1$;

while $(b \leq 1$ *and* $n_1 \geq d_0)$ *or* $(b > 1$ *and* $n_1 \geq d_0 + 1)$ **do**

    if $c \leq a + b$ **then**

        Output G can be obtained from a graph by the transformation depicted in Corollary 3.2, or 3.3;

        End;

    else

        Set $d_0 = d_{n_1}$, $a = \|\{i : d_i = d_0\}\|$, $b = \|\{i : d_i = d_0 + 1\}\|$, $n_0 = n_1$, $n_1 = n_0 - a - b$, $c = d_{n_1} - d_{n_0} - 1$;

        if $(b_0 = 0$ *and* $b > 0$ *and* $a + b \geq c_0 + 1)$ *or* $(b_0 > 0$ *and* $b = 0$ *and* $a + b \geq c_0 - 1)$ *or* $(b_0 = 0$ *and* $b = 0$ *and* $a + b \geq c_0)$ *or* $(b_0 > 0$ *and* $b > 0$ *and* $a + b \geq c_0)$ **then**

            Output G can be obtained from a graph by the transformation depicted in Corollaries 3.2, or 3.3;

            End;

        else

            Set $c_0 = c$, $b_0 = b$;

        end

    end

end

Output G can not be obtained from a graph by the transformation depicted in Corollary 3.2, or 3.3;

In order to prove the correctness of the above algorithm, let

$$\phi_k = \begin{cases} n_k - a_k - b_k - d_{n_k} - 1, & \text{if} \quad \mathrm{b_k} > 1; \\ n_k - a_k - b_k - d_{n_k}, & \text{if} \quad \mathrm{b_k} = 0 \quad \text{or} \quad \mathrm{b_k} = 1 \end{cases}$$

for $k = 0, 1, 2, \ldots$.

Table 6. $G_{13,56}$

+	●	●	●	●	●	●	●	●	●	●	●	●
●	+	●	●	●	●	●	●	●	●	●	●	●
●	●	+	●	●	●	●	●	●	●	●	●	○
●	●	●	+	●	●	●	●	●	●	●	○	○
●	●	●	●	+	●	●	●	●	●	●	○	○
●	●	●	●	●	+	●	●	●	●	●	○	○
●	●	●	●	●	●	+	●	●	●	○	○	○
●	●	●	●	●	●	●	+	●	●	○	○	○
●	●	●	●	●	●	●	●	+	●	○	○	○
●	●	●	●	●	●	●	●	●	+	○	○	○
●	●	●	●	●	●	○	○	○	○	+	○	○
●	●	●	○	○	○	○	○	○	○	○	+	○
●	●	○	○	○	○	○	○	○	○	○	○	+

Lemma 3.4. For $G \in \mathcal{G}^*{}_{n,m}$, $m > n-1$, assume G is the extremal graph in $\mathcal{G}^*{}_{n,m}$ with the maximum F-index, k is a positive integer, then
(i). If $\phi_k > 0$, then $c_k > a_k + b_k$;
(ii). If $\phi_k > 0$, then

$$\begin{cases} c_k + 1 > a_{k+1} + b_{k+1}, & \text{if} \quad \mathrm{b_k = 0} \quad \text{and} \quad \mathrm{b_{k+1} > 0}; \\ c_k - 1 > a_{k+1} + b_{k+1}, & \text{if} \quad \mathrm{b_k > 0} \quad \text{and} \quad \mathrm{b_{k+1} = 0}; \\ c_k > a_{k+1} + b_{k+1}, & \text{others.} \end{cases}$$

(iii). If $\phi_k > 0$, then $\theta_k \geq \theta_{k-1} + 2 \geq \theta_0 + 2k$.

Proof. (i).

By Definition 2, $n_{k+1} = n_k - a_k - b_k$ and $c_k = d_{n_{k+1}} - d_{n_k} - 1$. Obviously, if $b_k = 0$ or $b_k = 1$, $d_{n_{k+1}} < n_{k+1}$. It remains to show that $d_{n_{k+1}} < n_{k+1}$ for $b_k > 1$. If $d_{n_{k+1}} \geq n_{k+1}$, then $d_{n_{k+1}+1} \geq n_{k+1}$. By Definition 2, we have $d_{n_{k+1}+1} \leq d_{n_k} + 1$. So $d_{n_k} + 1 \geq n_{k+1}$, a contradiction. So we have $d_{n_{k+1}} < n_{k+1}$. If $a_k + b_k \geq c_k$, then there exists a graph $G_1 \in \mathcal{G}_{n,m}$, G can be obtained from G_1 by transformation $(d_{n_k} + 1, d_{n_{k+1}} - \widehat{l} + 1, n_{k+1}, n_k - a_k + 1; \widehat{l}, 1)$, $\widehat{l} = min(c_k, a_k)$, $t = d_{n_{k+1}} - \widehat{l} + 1 + n_{k+1} - (n_k - a_k + 1 + d_{n_k} + 1) = d_{n_{k+1}} - d_{n_k} - 1 + n_{k+1} - n_k + a_k - \widehat{l} = c_k - \widehat{l} - b_k \leq c_k - a_k - b_k \leq 0$, by Theorem 3.1, $F(G_1) > F(G)$, a contradiction.

(ii). Clearly $a_k \geq 1$, $a_{k+1} \geq 1$.

- $b_k = 0$:
  - $b_{k+1} = 0$:
    If $c_k \leq a_{k+1} + b_{k+1}$, then we have $G_1 \in \mathcal{G}_{n,m}$, G can be obtained from G_1 by transformation $(d_{n_k} + \widehat{c}, d_{n_{k+1}}, n_{k+1}, n_{k+1} + 1; 1, \widehat{c})$, $\widehat{c} = min(c_k, a_{k+1}) = c_k$, $t = d_{n_{k+1}} + n_{k+1} - (d_{n_k} + \widehat{c} + n_{k+1} + 1) = c_k - \widehat{c} \leq 0$, by Theorem 3.1, $F(G_1) > F(G)$, a contradiction.
  - $b_{k+1} > 0$:
    If $c_k + 1 \leq a_{k+1} + b_{k+1}$, then we have $G_1 \in \mathcal{G}_{n,m}$, G can be obtained from G_1 by transformation $(d_{n_k} + \widetilde{c}, d_{n_{k+1}} + 1, n_{k+1} - a_{k+1}, n_{k+1} + 1; 1, \widetilde{c})$, $\widetilde{c} = min(c_k, b_{k+1})$, $t = d_{n_{k+1}} + 1 + n_{k+1} - a_{k+1} - (d_{n_k} + \widetilde{c} + n_{k+1} + 1) = c_k + 1 - \widetilde{c} - a_{k+1} \leq 0$, by Theorem 3.1, $F(G_1) > F(G)$, a contradiction.

- $b_k > 0$:
  - $b_{k+1} = 0$:
    If $c_k - 1 \leq a_{k+1} + b_{k+1}$, then we have $G_1 \in \mathcal{G}_{n,m}$, G can be obtained from G_1 by transformation $(d_{n_k} + \overline{c} + 1, d_{n_{k+1}}, n_{k+1}, n_{k+1} + 1; 1, \overline{c})$, $\overline{c} = min(c_k - 1, a_{k+1}) = c_k - 1$, $t = d_{n_{k+1}} + n_{k+1} - (d_{n_k} + \overline{c} + 1 + n_{k+1} + 1) = c_k - \overline{c} - 1 \leq 0$, by Theorem 3.1, $F(G_1) > F(G)$, a contradiction.
  - $b_{k+1} > 0$:
    If $c_k \leq a_{k+1} + b_{k+1}$, then we have $G_1 \in \mathcal{G}_{n,m}$, G can be obtained from G_1 by transformation $(d_{n_k} + \acute{c} + 1, d_{n_{k+1}} + 1, n_{k+1} - a_{k+1}, n_{k+1} + 1; 1, \acute{c})$, $\acute{c} = min(c_k, b_{k+1})$, $t = d_{n_{k+1}} + 1 + n_{k+1} - a_{k+1} - (d_{n_k} + \acute{c} + 1 + n_{k+1} + 1) = c_k - \acute{c} - a_{k+1} \leq 0$, by Theorem 3.1, $F(G_1) > F(G)$, a contradiction.

(iii). Clearly, $n_{k+1} + d_{n_{k+1}} > n_k + d_{n_k} + 1$, then $\theta_{k+1} > \theta_k + 1$. So we have $\theta_{k+1} \geq \theta_k + 2$. By repeating this inequality, we obtain $\theta_{k+1} \geq \theta_0 + 2k$. ■

Corollary 3.5. Let $G \in \mathcal{G}_{n,m}$ with degree sequence $d = (d_1, \ldots, d_n)$ have the maximum F-index in $\mathcal{G}_{n,m}$. If the entry (x, y) of the Ferrers matrix

$FR(G) = (f_{x,y})$ with $x > y$ satisfies $y \geq 3$, $f_{x,y} = \bullet$, $f_{x+1,y-1} = \circ$, $f_{x+1,y} = \circ$ and $f_{x,y+1} = \circ$ or $+$, then $x + y \geq n + d_n + 2$.

4 Main results

In this section, using graph transformations, we characterize all extremal graphs having the maximum F-index in the set of all connected graphs of order n with size m for some n and m.

Theorem 4.1. Let $n - 1 < m \leq 2n - 3$. If $G \in \mathcal{G}_{n,m}$ has the maximum F-index in $\mathcal{G}_{n,m}$, then $G = S_{n,m}$. Moreover, the degree sequence of G is $(n-1, d_2, 2, 2, \ldots, 2, 1, \ldots, 1)$.

Proof. Let the non-increasing degree sequence of the extremal graph G is $(d_1, \ldots, d_n)$ with $d_1 \geq d_2 \geq \ldots \geq d_n$. If $G \neq S_{n,m}$, then $i := \max\{x : d_x > 2\} > d_i$. Let $l = d_i - 2$ and $p = \min\{x : d_x = 1\}$, then by $n - 1 < m \leq 2n - 3$, we have $i \leq p - 1$ and $l \leq n - p + 1$. Moreover, $d_k = 2$ for $i < k < p$, $d_2 = p - 2$. Hence there is a threshold graph G', G can be obtained from G' by a transformation $(2, 3, i, p; l, 1)$ with $t = 3 + i - 2 - p = i + 1 - p \leq 0$. By Theorem 3.1, we have $F(G') > F(G)$, which is a contradiction. So the assertion holds. ∎

Table 7. Transformations on $G_{13,22}$

$F(S_{13,22}) = 3544$												
+	•	•	•	•	•	•	•	•	•	•	•	•
•	+	•	•	•	•	•	•	•	•	•	•	•
•	•	+	○	○	○	○	○	○	○	○	○	○
•	•	○	+	○	○	○	○	○	○	○	○	○
•	•	○	○	+	○	○	○	○	○	○	○	○
•	•	○	○	○	+	○	○	○	○	○	○	○
•	•	○	○	○	○	+	○	○	○	○	○	○
•	•	○	○	○	○	○	+	○	○	○	○	○
•	•	○	○	○	○	○	○	+	○	○	○	○
•	•	○	○	○	○	○	○	○	+	○	○	○
•	•	○	○	○	○	○	○	○	○	+	○	○
•	•	○	○	○	○	○	○	○	○	○	+	○
•	•	○	○	○	○	○	○	○	○	○	○	+
$\Downarrow$ 3178												
+	•	•	•	•	•	•	•	•	•	•	•	•
•	+	•	•	•	•	•	•	•	•	•	•	○
•	•	+	•	○	○	○	○	○	○	○	○	○
•	•	•	+	○	○	○	○	○	○	○	○	○
•	•	○	○	+	○	○	○	○	○	○	○	○
•	•	○	○	○	+	○	○	○	○	○	○	○
•	•	○	○	○	○	+	○	○	○	○	○	○
•	•	○	○	○	○	○	+	○	○	○	○	○
•	•	○	○	○	○	○	○	+	○	○	○	○
•	•	○	○	○	○	○	○	○	+	○	○	○
•	•	○	○	○	○	○	○	○	○	+	○	○
•	•	○	○	○	○	○	○	○	○	○	+	○
•	○	○	○	○	○	○	○	○	○	○	○	+
$\Downarrow$ 2692												
+	•	•	•	•	•	•	•	•	•	•	•	•
•	+	•	•	•	•	•	•	•	•	○	○	○
•	•	+	•	•	○	○	○	○	○	○	○	○
•	•	•	+	•	○	○	○	○	○	○	○	○
•	•	•	•	+	○	○	○	○	○	○	○	○
•	•	○	○	○	+	○	○	○	○	○	○	○
•	•	○	○	○	○	+	○	○	○	○	○	○
•	•	○	○	○	○	○	+	○	○	○	○	○
•	•	○	○	○	○	○	○	+	○	○	○	○
•	•	○	○	○	○	○	○	○	+	○	○	○
•	○	○	○	○	○	○	○	○	○	+	○	○
•	○	○	○	○	○	○	○	○	○	○	+	○
•	○	○	○	○	○	○	○	○	○	○	○	+
$\Downarrow$ 2458												
+	•	•	•	•	•	•	•	•	•	•	•	•
•	+	•	•	•	•	•	○	○	○	○	○	○
•	•	+	•	•	•	○	○	○	○	○	○	○
•	•	•	+	•	•	○	○	○	○	○	○	○
•	•	•	•	+	•	○	○	○	○	○	○	○
•	•	•	•	•	+	○	○	○	○	○	○	○
•	•	○	○	○	○	+	○	○	○	○	○	○
•	○	○	○	○	○	○	+	○	○	○	○	○
•	○	○	○	○	○	○	○	+	○	○	○	○
•	○	○	○	○	○	○	○	○	+	○	○	○
•	○	○	○	○	○	○	○	○	○	+	○	○
•	○	○	○	○	○	○	○	○	○	○	+	○
•	○	○	○	○	○	○	○	○	○	○	○	+

Remark 2. For example, if $n = 13$ and $m = 22$ with $n - 1 < m \leq 2n - 3$, it is easy to see that each threshold graph can be obtained from $S_{n,m}$ by transformations with respect to $(q, j, i, p, l + 1, c + 1)$ (see Table 7).

Theorem 4.2. Let n and m be two integers where $2n-3 < m \leq 3n-6$. If $G \in \mathcal{G}_{n,m}$ with degree sequence $d = (d_1, \ldots, d_n)$ has the maximum F-index, then $G = S_{n,m}$ except $(n, m) = (6, 11)$.

Proof. Let $a = \|\{i : d_i = 1\}\| \geq 0$, $b = \|\{i : d_i = 2\}\| \geq 0$, $c = \min\{d_i - 3 : d_i - 3 \geq 0, i > 3\} \geq 0$. By $m \leq 3n-6$, we have $2a + b \geq c(c+1)/2$. Clearly, by Corollary 3.2, if $a+b \geq c+1$, $a > 0$, then there exists a threshold graph $G_1 \in \mathcal{G}_{n,m}$ such that G can be obtained from G_1 by a transformation $(2, 3+c-\widetilde{l}+1, n-a-b, n-a+1, \widetilde{l}, 1)$, where $\widetilde{l} = \min(a, c)$, which is a contradiction. If $a + b \geq c$ and $a = 0$, then there exists a threshold graph $G_1 \in \mathcal{G}_{n,m}$ and G can be obtained from G_1 by a transformation $(3, 4, n-a-b, n-a-b+1, \widetilde{l}, 1)$, where $\widetilde{l} = \min(b, c) = c$, which is a contradiction. Hence $a + b < c + 1$ and $b < c$. Therefore $a + c + 1 > 2a + b + > c(c+1)/2$, which implies that $c < 1/2 + \sqrt{(8a+9)/4}$. So

$$a - 1 < c - b \leq c < 1/2 + \sqrt{(8a+9)/4}, \tag{1}$$

which implies that $0 \leq a < 5$.

- $a = 0$. It is easy to see that the assertion holds by similar proof of Theorem 4.1.

- $a = 1$. By (1), $0 < c < 2.56$, which implies that either $c = 1$ or $c = 2$. If $c = 1$, then $(n, m) = (6, 11)$ and $F(S_{6,11}) < F(L_{6,11})$. If $c = 2$, then $b = 1$ and $(n, m) = (8, 18)$. It is easy to see that $S_{n,m}$ has the maximum F-index in $\mathcal{G}_{8,18}$.

- $a = 2, 3$. The proof is similar to Case $a = 1$.

- $a \geq 4$. Then $c > 3$. On the other hand, by (1), $c < 3.7$, which is a contradiction. ■

Theorem 4.3. Let n, m be two integers with $3n-6 < m \leq 4n-10$. If $G \in \mathcal{G}_{n,m}$, with degree sequence $d = (d_1, \ldots, d_n)$, has the maximum F-index in $\mathcal{G}_{n,m}$, then $G = S_{n,m}$, except for $(n, m) = (7, 16), (7, 17), (8, 22)$.

We skip the proof here. The argument is similar to that of Theorem 4.2. By Theorem 4.1, 4.2, 4.3, we have the following result.

Corollary 4.4. Let n, m be two integers with $m = nk - \frac{k(k+1)}{2} + a$, where $n \geq 6$, $1 \leq k \leq 3$ and $1 \leq a \leq n-k-1$. If $G \in \mathcal{G}_{n,m}$, then

$$F(G) \leq \begin{cases} 382, & \text{if n=6,m=11;} \\ 842, & \text{if n=7,m=16;} \\ 940, & \text{if n=7,m=17;} \\ 1640, & \text{if n=8,m=22.} \\ k(n-1)^3+a(k+1)^3+(n-k-a-1)k^3+(k+a)^3, & \text{otherwise.} \end{cases}$$

Theorem 4.5. Let k, n, m be three positive integers with $kn-k(k+1)/2 < m \leq (k+1)n-(k+2)(k+1)/2$, where $\tau = \lfloor \frac{(2k-1)+\sqrt{(12k^2-20k+1)}}{2} \rfloor$ and $n > 2(\tau + k)$. If a threshold graph G has the maximum F-index in $\mathcal{G}_{n,m}$, then $G = S_{n,m}$.

Proof. Let $a := \|\{i : d_i = 1\}\| \geq 0$,

$$g = \begin{cases} 0, & \text{if } \mathrm{d_{k+2} \leq k+1;} \\ \min\{d_i - k - 1 : d_i - k - 1 > 0\}. & \text{if } \mathrm{d_{k+2} > k+1.} \end{cases}$$

- $d_{k+2} \leq k+1$:

  If G is not $S_{n,m}$, let $q = \min\{x : d_x < n-1\}$, $q = d_q + 2$, $j = k+1$, $i = d_j + 1$. Clearly, $i + j - p - q \leq 0$, by Corollary 3.3, G is not the extremal graph, a contradiction.

- $d_{k+2} > k+1$:

  If G is not $S_{n,m}$, then $g + k - 1 > a$ since G is an extremal graph. Further, we have $g + k - 2 \geq a$. Obviously $kn - k(k+1)/2 < m \leq (k+1)n - (k+2)(k+1)/2$, so $ka \geq \frac{g(g+1)}{2}$, it follows that $k(g+k-2) \geq \frac{g(g+1)}{2}$, we have $g \leq \tau = \frac{(2k-1)+\sqrt{(2k-1)^2+4(2k^2-4k))}}{2}$. It can be easily observed that $n \leq 2(\tau + k)$, a contradiction. ■

The relation between the parameters k, τ and the order of the graph n is shown in Table 8.

Before introducing our last theorem, we state a simple lemma.

Lemma 4.6. Let $G \in \mathcal{G}^*{}_{n,m}$, $a = \|\{i : d_i = d_n\}\|$, if $d_n = 1$, then the maximum size of G is

$$\mu_n := n - 1 + \frac{(n-a-2)(n-a-1)}{2}.$$

Table 8. The relation of k, τ and n

k	τ	n
1	0	2
2	3	10
3	6	18
4	8	24
5	11	32
6	14	40
7	17	48
8	19	54
9	22	62
10	25	70

Now, let

$$z_n = \begin{cases} \frac{n+3}{2}, & \text{if} \quad \text{n} \quad \text{is} \quad \text{odd;} \\ \frac{n+2}{2}, & \text{if} \quad \text{n} \quad \text{is} \quad \text{even.} \end{cases}$$

Letting $a = z_n$ in Lemma 4.6, we have

$$\mu_n = \begin{cases} \frac{n^2+8n-9}{8}, & \text{if} \quad \text{n} \quad \text{is} \quad \text{odd;} \\ \frac{n^2+6n-8}{8}, & \text{if} \quad \text{n} \quad \text{is} \quad \text{even.} \end{cases}$$

Theorem 4.7. Let n, m be two positive integers with $m \leq \mu_n$. If a threshold graph G in $\mathcal{G}_{n,m}$ has the maximum F-index, then $G = S_{n,m}$, and any threshold graph can be obtained from $S_{n,m}$ by some transformations depicted in Section 3.

Proof. Assume that G in $\mathcal{G}_{n,m}$ has the maximum F-index, By Lemma 3.4 and Corollary 3.5, the entries (x, y) of $FR(G)$ with $x > y$, $y \geq 3$ and $x + y \geq n + 3$ are described as follows: $f_{x,y} = \bullet$, $f_{x+1,y-1} = \circ$, $f_{x+1,y} = \circ$ and $f_{x,y+1} = \circ$ or $+$.

Denote $d' = d_{z_n}$, $\widetilde{a} = \max\{i : d_i = d'\}$, $\widetilde{i} = \min\{i : d_i = d'\}$. Clearly $z_n + z_n - 1 \leq n + 2$, $d' < z_n$. We consider the following two cases.

- $\|\{i : d_i = d' - 1\}\| = 0$. Since $\widetilde{a} + d' \geq n + 3$, we have $\widetilde{a} + d' \geq 2z_n$, which implies that $\widetilde{a} - z_n \geq z_n - d'$. By Lemma 3.4, we have $d' > \widetilde{a} - z_n$. Obviously $\|\{(x, y) : f_{x,y} = \circ, x > y, y > d', x \leq$

$z_n\}\| < \|\{(x,y) : f_{x,y} = \bullet, x > y, y \leq d', i > z_n\}\|$, then $m > \mu_n$, a contradiction.

- $\|\{i : d_i = d' - 1\}\| > 0$. Let $a' = \|\{i : d_i = d' - 1\}\|$, then $\widetilde{a} + a' + d' - 1 \geq n + 3$, so $\widetilde{a} + a' - z_n \geq z_n - d' + 1$. It is easy to see that $\|\{(x,y) : f_{x,y} = \circ, x > y, y > d', x \leq z_n\}\| < \|\{(x,y) : f_{x,y} = \bullet, x > y, y \leq d' - 1, x > z_n\}\|$. Then $m > \mu_n$, a contradiction.

Therefore, the proof is completed. ■

5 Concluding remarks

In addition to the results established in this paper, we also list some computational results. They should help us to gain some insights regarding the quality of the bounds obtained in the previous sections. It is worth noting that, if $n \leq 11$, the results in Theorem 4.7 is better than Conjecture 1.1. For example, see Table 9.

For small n, such as $6 \leq n \leq 16$, through computer search, we consider all connected threshold graphs in $\mathcal{G}^*{}_{n,m}$ to find all extremal graph with maximum F-index. For example, see Table 12 for the case of $n = 12$. For fixed n, if $m = n, n+1, n+2, \frac{n(n-1)}{2} - 1, \frac{n(n-1)}{2} - 2, \frac{n(n-1)}{2} - 3$, all extremal graphs which attain maximum F-index are $S_{n,m}$. For $n < 12$, all extremal graphs are either $S_{n,m}$ or $L_{n,m}$, but for $n \geq 12$, extremal graphs may not be $S_{n,m}$ or $L_{n,m}$. With the help of computer, the known results for the case $6 \leq n \leq 16$ are summarized in Tables 10 and 11.

Table 9. Comparation of the upper bound of m in Theorem 4.7 and Conjecture 1.1

n	Theorem 4.7: μ_n	Conjecture 1.1
6	8	5
7	12	7
8	13	10
9	18	14
10	19	18
11	25	22
12	26	27
13	33	33
14	34	39
15	42	45
16	43	52
17	52	60
18	53	68
19	63	76

Table 10. The minimum size m of G which has the maximum F-index and G isn't $S_{n,m}$

n	m	degree sequence	F-index
6	11	5, 4, 4, 4, 4, 1	382
7	16	6, 5, 5, 5, 5, 5, 1	842
8	22	7, 6, 6, 6, 6, 6, 6, 1	1640
9	28	8, 7, 7, 7, 7, 7, 6, 6, 1	2660
10	36	9, 8, 8, 8, 8, 8, 8, 7, 7, 1	4488
11	44	10, 9, 9, 9, 9, 9, 9, 8, 8, 7, 1	6742
12	49	11, 11, 9, 9, 9, 9, 9, 9, 9, 9, 2, 2	8510
13	59	12, 12, 10, 10, 10, 10, 10, 10, 10, 10, 10, 2, 2	12472
14	68	13, 11, 11, 11, 11, 11, 11, 11, 11, 11, 11, 11, 1, 1	16840
15	79	14, 12, 12, 12, 12, 12, 12, 12, 12, 12, 12, 11, 11, 1, 1	22688
16	93	15, 13, 13, 13, 13, 13, 13, 13, 13, 13, 13, 13, 13, 13, 1, 1	31938

Table 11. Extremal graph with maximal F-index

n	$S_{n,m}$	$L_{n,m}$	Other
6	$m \neq 11$	$m = 11$	
7	$m \neq 16, 17$	$m = 16, 17$	
8	$m \neq 22, 23, 24$	m=22,23,24	
9	$m < 28$ or $m > 32$	$28 \leq m \leq 32$	
10	$m < 36$ or $m > 41$	$36 \leq m \leq 41$	
11	$m < 44$ or $m > 51$	$44 \leq m \leq 51$	
12	$m < 49$ or $m > 62$ or $m = 50, 51, 52$	$54 \leq m \leq 62$	m=49,53
13	$m < 59$ or $m > 74$ or $m = 62, 63$	$65 \leq m \leq 74$	$m = 59, 60, 61, 64$
14	$m < 68$ or $m > 87$ or m=70	$m = 68, 69, 74, 75$ or $77 \leq m \leq 87$	m=71,72,73,76
15	$m < 79$ or $m > 101$	$m = 79, 80, 81, 87, 88$ or $90 \leq m \leq 101$	m=82,83,84,85,86,89
16	$m < 93$ or $m > 116$	$m = 93, 94, 100, 101, 102$ or $104 \leq m \leq 116$	m=95,96,97,98,99,103

Table 12. Extremal graph with maximal F-index when $n = 12$

n	m	degree sequence	Extremal graph	F-index
12	12	11, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1	$S_{n,m}$	1356
12	13	11, 3, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1	$S_{n,m}$	1382
12	14	11, 4, 2, 2, 2, 1, 1, 1, 1, 1, 1, 1	$S_{n,m}$	1426
12	15	11, 5, 2, 2, 2, 2, 1, 1, 1, 1, 1, 1	$S_{n,m}$	1494
12	16	11, 6, 2, 2, 2, 2, 2, 1, 1, 1, 1, 1	$S_{n,m}$	1592
12	17	11, 7, 2, 2, 2, 2, 2, 2, 1, 1, 1, 1	$S_{n,m}$	1726
12	18	11, 8, 2, 2, 2, 2, 2, 2, 2, 1, 1, 1	$S_{n,m}$	1902
12	19	11, 9, 2, 2, 2, 2, 2, 2, 2, 2, 1, 1	$S_{n,m}$	2126
12	20	11, 10, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1	$S_{n,m}$	2404
12	21	11, 11, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2	$S_{n,m}$	2742
12	22	11, 11, 3, 3, 2, 2, 2, 2, 2, 2, 2, 2	$S_{n,m}$	2780
12	23	11, 11, 4, 3, 3, 2, 2, 2, 2, 2, 2, 2	$S_{n,m}$	2836
12	24	11, 11, 5, 3, 3, 3, 2, 2, 2, 2, 2, 2	$S_{n,m}$	2916
12	25	11, 11, 6, 3, 3, 3, 3, 2, 2, 2, 2, 2	$S_{n,m}$	3026
12	26	11, 11, 7, 3, 3, 3, 3, 3, 2, 2, 2, 2	$S_{n,m}$	3172
12	27	11, 11, 8, 3, 3, 3, 3, 3, 3, 2, 2, 2	$S_{n,m}$	3360
12	28	11, 11, 9, 3, 3, 3, 3, 3, 3, 3, 2, 2	$S_{n,m}$	3596
12	29	11, 11, 10, 3, 3, 3, 3, 3, 3, 3, 3, 2	$S_{n,m}$	3886
12	30	11, 11, 11, 3, 3, 3, 3, 3, 3, 3, 3, 3	$S_{n,m}$	4236
12	31	11, 11, 11, 4, 4, 3, 3, 3, 3, 3, 3, 3	$S_{n,m}$	4310
12	32	11, 11, 11, 5, 4, 4, 3, 3, 3, 3, 3, 3	$S_{n,m}$	4408
12	33	11, 11, 11, 6, 4, 4, 4, 3, 3, 3, 3, 3	$S_{n,m}$	4536
12	34	11, 11, 11, 7, 4, 4, 4, 4, 3, 3, 3, 3	$S_{n,m}$	4700
12	35	11, 11, 11, 8, 4, 4, 4, 4, 4, 3, 3, 3	$S_{n,m}$	4906
12	36	11, 11, 11, 9, 4, 4, 4, 4, 4, 4, 3, 3	$S_{n,m}$	5160
12	37	11, 11, 11, 10, 4, 4, 4, 4, 4, 4, 4, 3	$S_{n,m}$	5468
12	38	11, 11, 11, 11, 4, 4, 4, 4, 4, 4, 4, 4	$S_{n,m}$	5836
12	39	11, 11, 11, 11, 5, 5, 4, 4, 4, 4, 4, 4	$S_{n,m}$	5958
12	40	11, 11, 11, 11, 6, 5, 5, 4, 4, 4, 4, 4	$S_{n,m}$	6110
12	41	11, 11, 11, 11, 7, 5, 5, 5, 4, 4, 4, 4	$S_{n,m}$	6298
12	42	11, 11, 11, 11, 8, 5, 5, 5, 5, 4, 4, 4	$S_{n,m}$	6528
12	43	11, 11, 11, 11, 9, 5, 5, 5, 5, 5, 4, 4	$S_{n,m}$	6806
12	44	11, 11, 11, 11, 10, 5, 5, 5, 5, 5, 5, 4	$S_{n,m}$	7138
12	45	11, 11, 11, 11, 11, 5, 5, 5, 5, 5, 5, 5	$S_{n,m}$	7530
12	46	11, 11, 11, 11, 11, 6, 6, 5, 5, 5, 5, 5	$S_{n,m}$	7712
12	47	11, 11, 11, 11, 11, 7, 6, 6, 5, 5, 5, 5	$S_{n,m}$	7930
12	48	11, 11, 11, 11, 11, 8, 6, 6, 6, 5, 5, 5	$S_{n,m}$	8190
12	49	11, 11, 9, 9, 9, 9, 9, 9, 9, 9, 2, 2	Other	8510
12	50	11, 11, 11, 11, 11, 10, 6, 6, 6, 6, 6, 5	$S_{n,m}$	8860
12	51	11, 11, 11, 11, 11, 11, 6, 6, 6, 6, 6, 6	$S_{n,m}$	9282
12	52	11, 11, 11, 11, 11, 11, 7, 7, 6, 6, 6, 6	$S_{n,m}$	9536
12	53	11, 10, 10, 10, 10, 10, 10, 10, 8, 8, 8, 1	Other	9868
12	54	11, 10, 10, 10, 10, 10, 10, 10, 9, 9, 8, 1	$L_{n,m}$	10302
12	55	11, 10, 10, 10, 10, 10, 10, 10, 10, 9, 9, 1	$L_{n,m}$	10790
12	56	11, 10, 10, 10, 10, 10, 10, 10, 10, 10, 10, 1	$L_{n,m}$	11332
12	57	11, 11, 10, 10, 10, 10, 10, 10, 10, 10, 10, 2	$L_{n,m}$	11670
12	58	11, 11, 11, 10, 10, 10, 10, 10, 10, 10, 10, 3	$L_{n,m}$	12020
12	59	11, 11, 11, 11, 10, 10, 10, 10, 10, 10, 10, 4	$L_{n,m}$	12388
12	60	11, 11, 11, 11, 11, 10, 10, 10, 10, 10, 10, 5	$L_{n,m}$	12780
12	61	11, 11, 11, 11, 11, 11, 10, 10, 10, 10, 10, 6	$L_{n,m}$	13202
12	62	11, 11, 11, 11, 11, 11, 11, 10, 10, 10, 10, 7	$L_{n,m}$	13660
12	63	11, 11, 11, 11, 11, 11, 11, 11, 11, 9, 9, 9	$S_{n,m}$	14166
12	64	11, 11, 11, 11, 11, 11, 11, 11, 11, 10, 10, 9	$S_{n,m}$	14708
12	65	11, 11, 11, 11, 11, 11, 11, 11, 11, 11, 10, 10	$S_{n,m}$	15310

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