**MATCH**
*Communications in Mathematical and in Computer Chemistry*

*MATCH Commun. Math. Comput. Chem.* **91** (2024) 197–234
**ISSN:** 0340–6253
**doi:** 10.46793/match.91-1.197X

# $(n, m)$-Graphs with Maximum Vertex–Degree Function–Index for Convex Functions

**Si-Ao Xu, Baoyindureng Wu***

*College of Mathematics and System Sciences, Xinjiang University, Urumqi, Xinjiang, 830046, P. R. China*

siaoxu24@163.com, baoywu@163.com

(Received September 6, 2023)

**Abstract**

An $(n, m)$-graph is a graph with $n$ vertices and $m$ edges. The vertex-degree function-index $H_f(G)$ of a graph $G$ is defined as $H_f(G) = \sum_{v \in V(G)} f(d(v))$, where $f$ is a real function.

In this paper, we show that if $f(x)$ is strictly convex and strictly monotonically decreasing and satisfies some additional properties, then $H_f(G) \leq (n-k-1)f(0) + f(p) + (k-p)f(k-1) + pf(k)$ for any connected $(n, m)$-graph $G$ with $m = n + k(k-3)/2 + p$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-2$. The unique graph that satisfies the above equality is characterized. As an instance, the function $f(x) = (x+q)^\alpha$ is such a function when $\alpha \leq -t$, $-1 < q \leq 2.038t - 0.038$ and $t \geq 1$ or when $\alpha < 0$, $-1 < q \leq 0$.

We also prove that if $f(x)$ is strictly convex and strictly monotonically decreasing and satisfies some additional properties, then $H_f(G) \leq (n-k-1)f(0) + f(p) + (k-p)f(k-1) + pf(k)$ for any $(n, m)$-graph $G$ with $m = k(k-1)/2 + p$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-1$. The unique graph that satisfies the above equality is characterized. As an instance, the function $f(x) = (x+q)^\alpha$ has the properties as described above when $\alpha \leq -t$ and $0 < q \leq 1.413t + 0.587$ and $t \geq 1$.

*Corresponding author.

# 1 Introduction

In this paper, we only consider simple undirected graphs. For undetermined notations and terminologies, see the book by Bondy and Murty [5]. We use $V(G)$ and $E(G)$ to denote the vertex-set and edge-set of a graph $G$, respectively. Let $G[S]$ denote an induced subgraph of $G$ whose vertex set is $S$ and whose edge set consists of all edges of $G$ which have both end-vertices in $S$. We denote a complete graph with $n$ vertices by $K_n$.

Let $n$ and $m$ be two positive integers with $n \geq 2$ and $1 \leq m \leq n(n-1)/2$. An $(n, m)$-graph is a graph $G = (V(G), E(G))$, where $m = |E(G)|$ and $n = |V(G)|$. Let $\mathcal{G}_c(n, m)$ be the family of all $(n, m)$-graphs $G$ satisfying that $d(v) \in \left\{ \left\lfloor \frac{2m}{n} \right\rfloor, \left\lceil \frac{2m}{n} \right\rceil \right\}$ for all $v \in V(G)$.

In 1972, Gutman and Trinajstić [9] introduced the first Zagreb index:

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

where $d(v)$ denotes the degree of $v$ in $G$. The zeroth-order general Randić index ${}^0R_\alpha(G)$ of a graph $G$, was defined by Li and Zheng in [15] as

$${}^0R_\alpha(G) = \sum_{u \in V} d(v)^\alpha,$$

where $\alpha$ is a real number and $\alpha \notin \{0, 1\}$. In particular, ${}^0R_{-1}(G)$ is called the inverse degree $ID(G)$ of $G$ [8], ${}^0R_2(G)$ is just equal to $M_1(G)$, and ${}^0R_{-\frac{1}{2}}(G)$ in [10] is called the Randić index $R(G)$ of $G$. Some extremal results concerning the zeroth-order general Randić index were deduced in [2, 12–15, 17].

A more general graph invariant was introduced in [1]:

$${}^0R_{\alpha,q}(G) = \sum_{v \in V} (d(v) + q)^\alpha,$$

where $\alpha$ and $q$ are real numbers and $\alpha \neq 0$ or 1. The invariant ${}^0R_{\alpha,q}(G)$ is a modified form of the zeroth-order general Randić index. In particular,

${}^0R_{\alpha,0}(G) = {}^0R_\alpha(G)$ and ${}^0R_{2,0}(G) = M_1(G)$. In addition,

$$ {}^0R_{-1,1}(G) = \sum_{v \in V} \frac{1}{d(v)+1} $$

are known to be Caro-Wei index of a graph [6, 20]. It is well known that

$$ \alpha(G) \geq {}^0R_{-1,1}(G), $$

where $\alpha(G)$ is the independence number of $G$ for any graph $G$.

Recall some specific graphs defined in [4]. A pineapple with parameters $n, k$ ($k \leq n$), denoted by $PA(n,k)$, is a graph on $n$ vertices consisting of a clique on $k$ vertices and a stable set on the remaining $n-k$ vertices in which each vertex of the stable set is adjacent to a unique and the same vertex of the clique.

A fanned pineapple of type 1 with parameters $n, k, p$ ($n \geq k \geq p$), denoted by $FPA_1(n,k,p)$, is a graph (on $n$ vertices) obtained from a pineapple $PA(n,k)$ by connecting a vertex from the stable set by edges to $p$ vertices of the clique, with $0 \leq p \leq k-2$. $FPA_1(7,4,1)$ is represented in Figure 1.

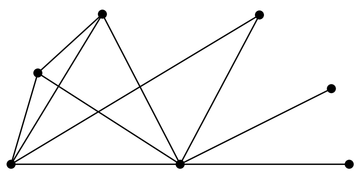

**Figure 1.** $FPA_1(7,4,1)$.

In [12], the authors characterized the connected $(n,m)$-graphs with extremal maximum zeroth-order general Randić index for $\alpha < -1$.

**Theorem 1** (Hu, Li, Shi and Xu [12])**.** *Let $\alpha \leq -1$ be a real number, and $n, m, k, p$ be nonnegative integers satisfying $m = n + k(k-3)/2 + p$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-2$. If $G$ is a connected $(n,m)$-graph, then*

$$ {}^0R_\alpha(G) \leq (n-k-1) \cdot 1^\alpha + (p+1)^\alpha + (k-p-1)(k-1)^\alpha + p \cdot k^\alpha + (n-1)^\alpha, $$

*the equality holds if and only if* $G = FPA_1(n, k, p)$.

Li and Shi [14], independently Pavlović, Lazić and Aleksić [17] extended the above result to the case when $\alpha < 0$.

**Theorem 2** (Li and Shi [14], Pavlović, Lazić and Aleksić [17]). *Let* $\alpha < 0$ *be a real number, and* $n, m, k, p$ *be nonnegative integers satisfying* $m = n + k(k-3)/2 + p$, *where* $2 \le k \le n-1$ *and* $0 \le p \le k-2$. *If* $G$ *is a connected* $(n, m)$*-graph, then*

$$\begin{aligned} {}^0R_\alpha(G) \le\, & (n-k-1)\cdot 1^\alpha + (p+1)^\alpha + (k-p-1)(k-1)^\alpha \\ & + p \cdot k^\alpha + (n-1)^\alpha, \end{aligned}$$

*the equality holds if and only if* $G = FPA_1(n, k, p)$.

In [21], Yao, Liu, Belardo and Yang introduced the vertex-degree function-index $H_f(G)$ of a graph $G$ with a real-valued function $f(x)$ as follows:

$$H_f(G) = \sum_{v \in V(G)} f(d(v)).$$

Some properties about the vertex-degree function-index have been studied, see [3, 7, 11, 18, 19, 21, 22].

Recently, Ali, Gutman, Saber and Alanazi [3] gave the following lower bound for $H_f(G)$ of a connected $(n, m)$-graph $G$ with $n \ge 4$ and $n+1 \le m \le \frac{3n}{2}$ under the condition that $f(G)$ is convex.

**Theorem 3** (Ali, Gutman, Saber and Alanazi [3]). *Let* $G$ *be a connected* $(n, m)$*-graph, where* $n$ *and* $m$ *be two integers with* $n \ge 4$, $n+1 \le m \le \frac{3n}{2}$, *and let* $k = \lfloor 2m/n \rfloor$ *and* $r = 2m - kn$. *If* $f(x)$ *is a strictly convex function, then it holds that*

$$H_f(G) \ge r f(k+1) + (n-r) f(k),$$

*and the equality holds if and only if* $G$ *is connected and* $G \in \mathcal{G}_c(n, m)$.

Hu, Li and Peng [11] proved that the same lower bound holds among all $(n, m)$-graphs or all connected $(n, m)$-graphs.

**Theorem 4** (Hu, Li and Peng [11]). *Let $G$ be an $(n,m)$-graph, where $n$ and $m$ be two integers with $n \geq 2$ and $n-1 \leq m \leq n(n-1)/2$, and let $k = \lfloor 2m/n \rfloor$ and $r = 2m - kn$. If $f(x)$ is a strictly convex function, then it holds that*

$$H_f(G) \geq rf(k+1) + (n-r)f(k),$$

*and the equality holds if and only if $G \in \mathcal{G}_c(n,m)$.*

**Theorem 5** (Hu, Li and Peng [11]). *Let $G$ be a connected $(n,m)$-graph, where $n$ and $m$ be two integers with $n \geq 2$ and $n-1 \leq m \leq n(n-1)/2$, and let $k = \lfloor 2m/n \rfloor$ and $r = 2m-kn$. If $f(x)$ is a strictly convex function, then it holds that*

$$H_f(G) \geq rf(k+1) + (n-r)f(k),$$

*and the equality holds if and only if $G$ is connected and $G \in \mathcal{G}_c(n,m)$.*

Tomescu [18,19] established sharp upper bound for $H_f(G)$ of an $(n,m)$-graph $G$ with $m \leq \frac{3n}{2}$ under the restriction that $f$ is a strictly convex, $f(x)$ is differentiable and its derivative is strictly convex.

**Lemma 1** (Tomescu [19]). *If $G$ is an $(n,m)$-graph that maximizes (minimizes) $H_f(G)$ for a strictly convex (concave) function $f(x)$, then $G$ has at most one nontrivial connected component $C$, and $C$ has a vertex of degree $|V(C)|-1$.*

**Lemma 2** (Tomescu [19]). *In the set of connected $(n,m)$-graphs $G$ having $m \geq n-1$, the graph which maximizes (minimizes) $H_f(G)$ for a strictly convex (concave) function $f(x)$, $G$ has a vertex $v$ with degree $n-1$.*

**Theorem 6** (Tomescu [18]). *Let $f(x)$ be a strictly convex function having the property that $f(x)$ is differentiable and its derivative is strictly convex, and let $n$ and $m$ be two integers with $n \geq 2$ and $1 \leq m \leq n-1$. If $G$ is an $(n,m)$-graph, then $H_f(G) \leq f(m) + mf(1) + (n-m-1)f(0)$, with equality if and only if $G = S_{m+1} \cup (n-m-1)K_1$.*

**Theorem 7** (Tomescu [18]). *Let $f(x)$ be a strictly convex function having the property that $f(x)$ is differentiable and its derivative is strictly convex,* *and let $n$ and $m$ be two integers with $n \geq 3$, $n \leq m \leq 2n-3$. If $G$ is a connected $(n,m)$-graph, then*

$$H_f(G) \leq f(n-1) + f(m-n+2) + (m-n+1)f(2) + (2n-m-3)f(1),$$

*with equality if and only if $G = K_1 \vee (K_{1,m-n+1} \cup (2n-m-3)K_1)$.*

It can be found that Tomescu's result does not apply when the function $f(x) = (x+q)^{\alpha}$, where $\alpha < 0$ and $q > 0$, because the function $f(x)$ is strictly convex but its derivative is strictly concave. Therefore it is necessary to find a new method to study it.

In this paper, we will further study the maximum values of $H_f(G)$ among all connected $(n,m)$-graphs as well as on all $(n,m)$-graphs, provided that the function $f(x)$ satisfies the conditions of some or all of the following conditions:

(i) $f(x)$ is a strictly convex function in the range where $H_f(G)$ can be defined.

(ii) $f(x)$ is a strictly monotonically decreasing in the range where $H_f(G)$ can be defined.

(iii) $(n-p-j-3)f(p+1) - (n-p+j-3)f(p+j+1) + j(n-p-j-1)f(n-2) - j(n-p-j-3)f(n-1) > 0$ for each $p \in \{0,1,\ldots,n-4\}$ and for each $j \in \{1,\ldots,n-p-4\}$.

(iv) $f(1) + (2r-2)f(r+1) - (2r-1)f(r) \geq 0$ for $r \geq 2$.

(v) $f(1)+(2r-2)f(r+1)-(2r-1)f(r) \geq 0$ for $r \geq 3$ and $f(1)-2f(2)+f(4) \geq 0$.

(vi) $f(1)+(2r-2)f(r+1)-(2r-1)f(r) \geq 0$ for $r \geq 4$, $f(1)-2f(2)+f(4) \geq 0$ and $f(1) - 4f(3) + 2f(4) + f(5) \geq 0$.

(vii) $f(0) + 2f(2) - 3f(1) \geq 0$ and $f(0) - f(1) - 2f(2) + 2f(3) \geq 0$.

We say that a function $f(x)$ satisfies condition $(i)$ if the $i$-th term of the above holds for $f(x)$.

The proposition below reveals the implication between conditions (iv), (v) and (vi).

**Proposition 8.** *Let $f(x)$ be a function that satisfies condition (i). If $f(x)$ satisfies condition (iv), then it necessarily satisfies condition (v). Additionally, the satisfaction of condition (v), implies that condition (vi) is necessarily fulfilled.*

*Proof.* By observation, it is sufficient to prove $f(1)-2f(2)+f(4) \geq f(1)+2f(3)-3f(2)$ and $f(1)-4f(3)+2f(4)+f(5) \geq f(1)+4f(4)-5f(3) \geq 0$ and in turn only need to show that $f(2)+f(4) \geq 2f(3)$ and $f(3)+f(5) \geq 2f(4)$, and the fact it holds follows from Corollary 2, and so the proposition is proved. ∎

To state our main results, two types of graphs are defined below. Let $\overline{PA}(n,k)$ be a graph denoted as follows: a graph with $n$ vertices, composed of a clique on $k$ vertices and a stable set on the other $n-k$ vertices. Let $\overline{FPA_1}(n,k,p)$ be defined as a graph which contains $n$ vertices, constructed from $\overline{PA}(n,k)$ by joining a vertex from the stable set with $p$ vertices of the clique by edges, with $0 \leq p \leq k-1$.

**Theorem 9.** *Assume that a function $f(x)$ satisfy conditions (i), (ii), (iii), and at least one of the conditions (iv), (v) and (vi). Let $n, m, k, p$ be integers satisfying that $m = n + k(k-3)/2 + p$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-2$. If $G$ is a connected $(n,m)$-graph, then*

$$\begin{aligned} H_f(G) \leq (n-k-1)f(1) + f(p+1) \\ + (k-p-1)f(k-1) + pf(k) + f(n-1), \end{aligned} \tag{1}$$

*the equality holds if and only if $G = FPA_1(n,k,p)$.*

**Theorem 10.** *Assume that a function $f(x)$ satisfy conditions (i), (ii), (iii), (vii) and at least one of the conditions (iv), (v) and (vi). Let $n, m, k, p$ be integers satisfying that $m = k(k-1)/2 + p$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-1$. If $G$ is an $(n,m)$-graph, then*

$$H_f(G) \leq (n-k-1)f(0) + f(p) + (k-p)f(k-1) + pf(k), \tag{2}$$

*the equality holds if and only if $G = \overline{FPA_1}(n,k,p)$.*

We will show by Lemmas 16–23 in Section 2 that the function $f(x) = (x+q)^\alpha$ satisfies the assumption in Theorem 9 when $t \geq 1$, $\alpha \leq -t$ and $-1 < q \leq 2.038t - 0.038$, or $\alpha < 0$ and $-1 < q \leq 0$. Furthermore, the function $f(x) = (x+q)^\alpha$ satisfies the conditions of Theorem 10 for $t \geq 1$, $\alpha \leq -t$ and $0 < q \leq 1.413t + 0.587$. Therefore, it is straightforward to obtain the following theorems.

**Theorem 11.** *Let $f(x) = (x+q)^\alpha$, where $\alpha \leq -t$, $-1 < q \leq 2.038t - 0.038$ and $t \geq 1$. Let $n, m, k, p$ be integers satisfying that $m = n + k(k-3)/2 + p$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-2$. If $G$ is a connected $(n,m)$-graph, then*

$$
\begin{aligned}
{}^0R_{\alpha,q}(G) \leq\, & (n-k-1)(1+q)^\alpha + (p+1+q)^\alpha \\
& + (k-p-1)(k-1+q)^\alpha + p(k+q)^\alpha + (n-1+q)^\alpha,
\end{aligned}
$$

*the equality holds if and only if $G = FPA_1(n,k,p)$.*

**Theorem 12.** *Let $f(x) = (x+q)^\alpha$, where $\alpha < 0$, $-1 < q \leq 0$. Let $n, m, k, p$ be integers satisfying that $m = n + k(k-3)/2 + p$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-2$. If $G$ is a connected $(n,m)$-graph, then*

$$
\begin{aligned}
{}^0R_{\alpha,q}(G) \leq\, & (n-k-1)(1+q)^\alpha + (p+1+q)^\alpha \\
& + (k-p-1)(k-1+q)^\alpha + p(k+q)^\alpha + (n-1+q)^\alpha,
\end{aligned}
$$

*the equality holds if and only if $G = FPA_1(n,k,p)$.*

**Theorem 13.** *Let $f(x) = (x+q)^\alpha$, where $\alpha \leq -t$ and $0 < q \leq 1.413t + 0.587$ and $t \geq 1$. Let $n, m, k, p$ be integers satisfying that $m = n + k(k-3)/2 + p$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-2$. If $G$ is an $(n,m)$-graph, then*

$$
\begin{aligned}
{}^0R_{\alpha,q}(G) \leq\, & (n-k-1)\cdot q^\alpha + (p+q)^\alpha \\
& + (k-p)(k-1+q)^\alpha + p\cdot(k+q)^\alpha,
\end{aligned}
$$

*the equality holds if and only if $G = \overline{FPA}_1(n,k,p)$.*

When $t = 1, \alpha = -1$ and $q = 1$, Theorem 13 implies the following corollary.

**Corollary 1.** *Let $f(x) = \frac{1}{x+1}$. Let $n, m, k, p$ be integers satisfying that $m = n + k(k-3)/2 + p$, where $2 \le k \le n-1$ and $0 \le p \le k-2$. If $G$ is an $(n,m)$-graph, then*

$$H_f(G) \le (n-k-1) + \frac{1}{p+1} + \frac{k-p}{k} + \frac{p}{k+1},$$

*the equality holds if and only if $G = \overline{FPA}_1(n,k,p)$.*

Our results extend those obtained by Hu et al. in [12] and Li et al. in [14] on the case of the maximum value of the zeroth-order general Randić index for $\alpha \le -1$ and $\alpha < 0$, respectively. Theorem 11 can deduce Theorem 1 and Theorem 12 can deduce Theorem 2. Moreover, Theorem 13 obtained sharp upper bounds among all $(n,m)$-graphs, which is not studied in previous works [12], [14], and [17].

# 2 Proof of main results

Firstly, we introduce some useful lemmas. Let $n_i$ be the number of vertices of degree $i$ in a graph $G$.

**Lemma 3** (Tomescu [19])**.** *Let $x \ge y \ge 1$. If $f(x)$ is a strictly convex function, then $f(x+1) + f(y-1) > f(x) + f(y)$.*

**Corollary 2.** *If $f(x)$ is a strictly convex function, then $f(s-1)+f(s+1) > 2f(s)$ for any real number $s > 1$.*

**Lemma 4.** *Let $r$, $s$ and $t$ be real numbers such that $0 < r \le s \le t$. If $f(x)$ is a convex function, then*

$$(t-r)f(s) \le (t-s)f(r) + (s-r)f(t),$$

*with equality if and only if $s = r$ or $t$.*

*Proof.* If $s = r$ or $s = t$, it is obvious that the equality holds. Set $g(s) = (t-s)f(r) + (s-r)f(t) - (t-r)f(s)$. By a simple computation, $\frac{\partial^2 g}{\partial s^2} = -(t-r)\frac{\partial^2 f}{\partial s^2} \le 0$ and the upper inequality follows because the function $g$ is concave. ∎

**Lemma 5.** *Let $a$, $b$ be real numbers such that $a \geq b \geq 0$. If $f(x)$ is a convex function, then*

$$f(a+y) - f(a) \geq y(f(b+1) - f(b)) \tag{3}$$

*for any positive integer $y$.*

*Proof.* Since $f(x)$ is a convex function, $f(x+1) - f(x)$ is an increasing function. Thus, $f(a+y) - f(a) = (f(a+1) - f(a)) + (f(a+2) - f(a+1)) + \cdots + (f(a+y) - f(a+y-1)) \geq y(f(b+1) - f(b))$. ■

**Lemma 6** (Pavlović [16])**.** *Let $G$ be a graph with $n$ vertex and $m$ edges, where $m < \binom{n}{2}$. If $n_1 \neq 0$, then $n_{n-1} \leq 1$. If $n_1 = n_2 = \cdots = n_{i-1} = 0$, $n_i \neq 0$, then $n_{n-1} \leq i$.*

**Lemma 7** (Pavlović [16])**.** *Let $G$ be a graph with $n$ vertex and $m$ edges, where $m < \binom{n}{2}$. If $n_{n-1} = 1$, $n_1 = l$, where $2 \leq l \leq n-3$, then $n_{n-l} = n_{n-l+1} = \cdots = n_{n-3} = n_{n-2} = 0$.*

**Lemma 8.** *Let $a, b, c, d, e$ and $x$ all be positive numbers. Let $g(x) = \frac{\ln\left(\frac{b+ax}{c+ax}\right)}{\ln\left(\frac{d+ax}{e+ax}\right)}$. Then $\lim\limits_{x\to+\infty} g(x) = \frac{b-c}{d-e}$. If $b > c = d > e$, then $g(x)$ is monotonically increasing. If $d > b > c = e$, then $g(x)$ is monotonically decreasing.*

*Proof.* Since $\ln(1+x) = x + o(x)$ for $x \in (-1, 1]$, we have

$$\lim_{x\to+\infty} g(x) = \lim_{x\to+\infty} \frac{\frac{b-c}{c+ax} + o\left(\frac{b-c}{c+ax}\right)}{\frac{d-e}{e+ax} + o\left(\frac{d-e}{e+ax}\right)} = \frac{b-c}{d-e}.$$

By a simple calculation, $\frac{\mathrm{d}g}{\mathrm{d}x} = \frac{a\ln\left(\frac{b+ax}{c+ax}\right)(d-e)}{\ln^2\left(\frac{d+ax}{e+ax}\right)(d+ax)(e+ax)} - \frac{a(b-c)}{\ln\left(\frac{d+ax}{e+ax}\right)(b+ax)(c+ax)}$. Set $h(x) = a\ln\left(\frac{b+ax}{c+ax}\right)(d-e) - \frac{a\ln\left(\frac{d+ax}{e+ax}\right)(b-c)(d+ax)(e+ax)}{(b+ax)(c+ax)}$.

If $b > c = d > e$, then $\frac{\mathrm{d}h}{\mathrm{d}x} = -\frac{a^2\ln\left(\frac{c+ax}{e+ax}\right)(b-c)(b-e)}{(b+ax)^2} < 0$. Since $\lim\limits_{x\to+\infty} h(x) = 0$, the inequality $h(x) > 0$ holds on the interval $(0, +\infty)$. Therefore, $\frac{\mathrm{d}g}{\mathrm{d}x} > 0$ is valid on the interval $(0, +\infty)$ and $g(x)$ is monotonically increasing.

If $d > b > c = e$, then $\frac{\mathrm{d}h}{\mathrm{d}x} = -\frac{a^2\ln\left(\frac{d+ax}{c+ax}\right)(b-c)(b-d)}{(b+ax)^2} > 0$. Since $\lim\limits_{x\to+\infty} h(x) = 0$, the inequality $h(x) < 0$ holds on the interval $(0, +\infty)$.

Therefore, $\frac{\mathrm{d}g}{\mathrm{d}x} < 0$ is valid on the interval $(0, +\infty)$ and $g(x)$ is monotonically decreasing. ■

**Lemma 9.** *Let $a, b, c$ and $x$ all be positive numbers. Let $g(x) = x \ln\left(\frac{b+ax}{c+ax}\right)$ and $h(x) = \left(\frac{b+ax}{c+ax}\right)^x$. Then $\lim_{x\to+\infty} g(x) = \frac{b-c}{a}$ and $\lim_{x\to+\infty} h(x) = e^{\frac{b-c}{a}}$. If $b > c$, then $g(x)$ and $h(x)$ are monotonically increasing, while $\frac{\mathrm{d}g}{\mathrm{d}x}$ is positive and monotonically decreasing. If $c > b$, then $g(x)$ and $h(x)$ are monotonically decreasing, while $\frac{\mathrm{d}h}{\mathrm{d}x}$ is negative and monotonically increasing.*

*Proof.* Since $\ln(1 + x) = x + o(x)$ for $x \in (-1, 1]$, we have

$$\lim_{x\to+\infty} g(x) = \lim_{x\to+\infty} x\left(\frac{b-c}{c+ax} + o\left(\frac{b-c}{c+ax}\right)\right) = \frac{b-c}{a}.$$

By a simple calculation, $\frac{\mathrm{d}g}{\mathrm{d}x} = \ln\left(\frac{b+ax}{c+ax}\right) - \frac{ax(b-c)}{(b+ax)(c+ax)}$, $\frac{\mathrm{d}^2g}{\mathrm{d}x^2} = -\frac{a(b-c)(2bc+abx+acx)}{(b+ax)^2(c+ax)^2}$, $\frac{\mathrm{d}h}{\mathrm{d}x} = e^{g(x)}\frac{\mathrm{d}g}{\mathrm{d}x}$, and $\frac{\mathrm{d}^2h}{\mathrm{d}x^2} = e^{g(x)}\left((\frac{\mathrm{d}g}{\mathrm{d}x})^2 + \frac{\mathrm{d}^2g}{\mathrm{d}x^2}\right)$.

If $b > c$, then $\frac{\mathrm{d}^2g}{\mathrm{d}x^2} < 0$. Since $\lim_{x\to+\infty} \frac{\mathrm{d}g}{\mathrm{d}x} = 0$, $\frac{\mathrm{d}g}{\mathrm{d}x} > 0$. Thus, $g(x)$ and $h(x)$ are monotonically increasing, whereas $\frac{\mathrm{d}g}{\mathrm{d}x}$ is positive and monotonically decreasing.

If $c > b$, then $\frac{\mathrm{d}^2g}{\mathrm{d}x^2} > 0$ and $\frac{\mathrm{d}^2h}{\mathrm{d}x^2} > 0$. Since $\lim_{x\to+\infty} \frac{\mathrm{d}g}{\mathrm{d}x} = 0$, $\frac{\mathrm{d}g}{\mathrm{d}x} < 0$. Thus, $g(x)$ and $h(x)$ are monotonically decreasing, while $\frac{\mathrm{d}h}{\mathrm{d}x}$ is negative and monotonically increasing. ■

**Lemma 10.** *Let $g(x) = (x + 1)\ln(\frac{b+ax}{c+ax})$, where $a > 0$, $b > c > 0$ and $2a^2 - ab - ac < 0$. If $ab + ac - 2bc < 0$, then $g(x) \geq g(1)$ for any $x \geq 1$. When $ab + ac - 2bc > 0$, if $\frac{\mathrm{d}g}{\mathrm{d}x}$ has no root on the interval $(1, \infty)$, then $g(x) \geq g(1)$ for any $x \geq 1$; otherwise, $\frac{\mathrm{d}g}{\mathrm{d}x}$ has a unique root $x_1$ on the interval $(1, \infty)$, we have $g(x) \geq g(x_1)$ for any $x \geq 1$.*

*Proof.* Since $\frac{\mathrm{d}g}{\mathrm{d}x} = \ln\left(\frac{b+ax}{c+ax}\right) - \frac{a(b-c)(x+1)}{(b+ax)(c+ax)}$ and $\frac{\mathrm{d}^2g}{\mathrm{d}x^2} = \frac{a(b-c)\left((2a^2-ab-ac)x+ab+ac-2bc\right)}{(b+ax)^2(c+ax)^2}$, $\frac{\mathrm{d}^2g}{\mathrm{d}x^2} < 0$ if $x > -\frac{ab+ac-2bc}{2a^2-ab-ac}$ and $\frac{\mathrm{d}^2g}{\mathrm{d}x^2} > 0$ if $x < -\frac{ab+ac-2bc}{2a^2-ab-ac}$. Since $\lim_{x\to+\infty} \frac{\mathrm{d}g}{\mathrm{d}x} = 0$, $\frac{\mathrm{d}g}{\mathrm{d}x} > 0$ on the interval $(-\frac{ab+ac-2bc}{2a^2-ab-ac}, +\infty)$.

If $ab+ac-2bc<0$, then $-\frac{ab+ac-2bc}{2a^2-ab-ac}<0$, so $g(x)\geq g(1)$ for any $x\geq 1$. When $ab+ac-2bc>0$, we have $-\frac{ab+ac-2bc}{2a^2-ab-ac}>0$. If $\frac{\mathrm{d}g}{\mathrm{d}x}$ has no root in $(1,\infty)$, then $\frac{\mathrm{d}g}{\mathrm{d}x}>0$ on the interval $(1,\infty)$ and $g(x)\geq g(1)$ for any $x\geq 1$. Otherwise, $\frac{\mathrm{d}g}{\mathrm{d}x}$ has a unique root $x_1$ in $(1,\infty)$, $\frac{\mathrm{d}g}{\mathrm{d}x}<0$ on the interval $(1,x_1)$ and $\frac{\mathrm{d}g}{\mathrm{d}x}>0$ on the interval $(x_1,\infty)$. Thus, $g(x)\geq g(x_1)$ for any $x\geq 1$. ■

**Lemma 11.** *Let* $g(x)=\frac{\ln\left(\frac{b+ax}{c+ax}\right)}{\ln\left(\frac{c+ax}{d+ax}\right)}\left(\frac{d+ax}{b+ax}\right)^x$, *where* $a,b,c$ *and* $d$ *be real numbers with* $a>0$, $b>c>d>0$. *For any* $x\geq 1$, $g(x)\leq\frac{(b-c)(a+d)}{(c-d)(a+b)}$.

*Proof.* Let $h_1(x)=\frac{\ln\left(\frac{b+ax}{c+ax}\right)}{\ln\left(\frac{c+ax}{d+ax}\right)}$ and $h_2(x)=\left(\frac{d+ax}{b+ax}\right)^x$. By Lemmas 8 and 9, $\lim\limits_{x\to+\infty}h_1(x)=\frac{b-c}{c-d}$, the function $h_1(x)$ is monotonically increasing and the function $h_2(x)$ is monotonically decreasing. Thus, $g(x)=h_1(x)\cdot h_2(x)\leq h_1(\infty)\cdot h_2(1)=\frac{b-c}{c-d}\cdot\frac{a+d}{a+b}=\frac{(b-c)(a+d)}{(c-d)(a+b)}$. ■

For convenience, we call a graph $G$ a *maximum connected* $(n,m)$*-graph* if it has the maximum vertex-degree function-index among all connected $(n,m)$-graphs, and respectively, a *maximum* $(n,m)$*-graph* if it has the maximum vertex-degree function-index among all $(n,m)$-graphs.

Next, we are going to prove Theorem 9 that the fanned pineapple of type 1 graph has the maximum $H_f$-value among $(n,m)$-connected graphs. This implies that the maximum connected $(n,m)$-graph should have $n_1=n-k-1, n_{p+1}=1, n_{k-1}=k-1-p, n_k=p$ and $n_{n-1}=1$.

Theorem 9 describes the solution of the following problem $(P)$ :

$$\max n_1\cdot f(1)+n_2\cdot f(2)+\cdots+n_{n-1}\cdot f(n-1)$$

under two graph constraints

$$\begin{aligned}&n_1+n_2+n_3+\cdots+n_{n-1}=n,\\&n_1+2n_2+3n_3+\cdots+(n-1)n_{n-1}=2m.\end{aligned}$$

By Lemma 2, we have the following corollary, implying the assertion of Theorem 9 for the case when $m=n-1$.

**Corollary 3.** *Let $f(x)$ be a strictly convex function. If $m = n - 1$, the function $H_f$ reaches its maximum among $(n,m)$-connected graphs at the star.*

Thus, it remains to show that Theorem 9 holds for $n \le m \le \binom{n}{2} - 2$.

Since $m = n + k(k-3)/2 + p$, where $2 \le k \le n-1$ and $0 \le p \le k-2$, we handle two cases in terms of $k = n-1$ and $2 \le k \le n-2$. We shall start by proving the theorem for $k = n-1$.

**Lemma 12.** *Let $G$ be a connected $(n,m)$-graph, where $m \le \binom{n}{2} - 2$, $m = n + k(k-3)/2 + p$, $k = n-1$ and $0 \le p \le n-4$. Inequality* (1) *holds for the graph $G$.*

*Proof.* Since $k = n-1$, $m = (n^2 - 3n + 4 + 2p)/2 = (n-1)(n-2)/2 + p + 1$, where $0 \le p \le n-3$. Then the minimum degree of $G$ must be greater than or equal to p + 1. In contrast, if $G$ contains a vertex whose degree is $p$ (or less), then the deletion of a vertex of degree $p$ results a graph $G'$ (without necessarily connected) with more edges than the complete graph on $n-1$ vertices.

Let the minimum degree of $G$ be $p + j + 1$, where $j$ is a nonnegative integer. Since $m \le \binom{n}{2} - 2$, $j \le n - p - 4$. Otherwise, $j = n - p - 3$, then the degree of the vertex in $G$ is either $n-2$ or $n-1$. Thus there are four distinct vertices $v_1, v_2, v_3$ and $v_4$ of degree $n-2$ such that $v_1$ and $v_2$ are nonadjacent, $v_3$ and $v_4$ are nonadjacent in $G$. Now, construct a new graph $G' = G - v_2v_3 + v_3v_4$. By Corollary 2, we have $H_f(G') - H_f(G) = f(n-1) + f(n-3) - 2f(n-2) > 0$, which contradicts the maximality of $G$.

Denote by $P^{(p,p+j+1)}$ the problem for given $p$ when the minimum degree of $G$ is $p + j + 1$, and by $H_f^{(p,p+j+1)}$ the optimal value of $H_f$ for the problem $P^{(p,p+j+1)}$. The optimal value of $H_f$ for a given $p$ is $H_f^p = \max_{0 \le j \le n-p-4} H_f^{(p,p+j+1)}$. Since the minimum degree of $G$ is $p + j + 1$, it follows from Lemma 6 that we have $n_{n-1} \le p + j + 1$. Let us solve the problem $P^{(p,p+j+1)}$, $0 \le p \le n-4$, $0 \le j \le n-p-4$.

$$\max n_{p+j+1} f(p+j+1) + n_{p+j+2} f(p+j+2) + \cdots + n_{n-1} f(n-1)$$

under the constraints:

$$n_{p+j+1} + n_{p+j+2} + n_{p+j+3} + \cdots + n_{n-1} = n,$$
$$(p+j+1)n_{p+j+1} + (p+j+2)n_{p+j+2} + \cdots + (n-1)n_{n-1} = n^2 - 3n + 4 + 2p,$$
$$n_{n-1} = p + j + 1 - \xi,$$

where $0 \le \xi \le p + j$. Let us solve the system of the latter three equalities in $n_{n-1}$, $n_{n-2}$ and $n_{p+j+1}$ :

$$\begin{aligned} n_{n-2} =& \frac{n^2 - n(2p+2j+5) + p^2 + 2pj + 5p + j^2 + 3j + 6}{n-p-j-3} \\ & - \frac{n_{p+j+2}}{n-p-j-3} - \frac{2n_{p+j+3}}{n-p-j-3} - \frac{3n_{p+j+4}}{n-p-j-3} \\ & - \cdots - \frac{(n-p-j-4)n_{n-3}}{n-p-j-3} + \frac{(n-p-j-2)\xi}{n-p-j-3}, \\ n_{p+j+1} =& \frac{n-p+j-3}{n-p-j-3} - \left(1 - \frac{1}{n-p-j-3}\right) n_{p+j+2} \\ & - \left(1 - \frac{2}{n-p-j-3}\right) n_{p+j+3} - \left(1 - \frac{3}{n-p-j-3}\right) n_{p+j+4} \\ & - \cdots - \left(1 - \frac{n-p-j-4}{n-p-j-3}\right) n_{n-3} + \left(1 - \frac{n-p-j-2}{n-p-j-3}\right) \xi. \end{aligned}$$

By replacing $n_{p+j+1}$, $n_{n-2}$, $n_{n-1}$ in $H_f$, we obtain

$$\begin{aligned} H_f =& \frac{n-p+j-3}{n-p-j-3} f(p+j+1) + (p+j+1) f(n-1) \\ & + \frac{n^2 - n(2p+2j+5) + p^2 + 2pj + 5p + j^2 + 3j + 6}{n-p-j-3} f(n-2) \\ & + \sum_{i=p+j+2}^{n-3} n_i \left( f(i) - \frac{n-i-2}{n-p-j-3} f(p+j+1) - \frac{i-p-j-1}{n-p-j-3} f(n-2) \right) \\ & + \xi \left( -f(n-1) - \frac{1}{n-p-j-3} f(p+j+1) + \frac{n-p-j-2}{n-p-j-3} f(n-2) \right). \end{aligned}$$

Following Lemma 4, it holds that

$$(n-p-j-3)f(i) \le (n-i-2)f(p+j+1) + (i-p-j-1)f(n-2) \quad (4)$$

for $p+j+1 \leq i \leq n-2$ and

$$(n-p-j-2)f(i) \leq (n-i-1)f(p+j+1)+(i-p-j-1)f(n-1) \quad (5)$$

for $p+j+1 \leq i \leq n-1$.
After taking the value of $i$ in the inequity (5) to be $n-2$, we get the following equation

$$(n-p-j-2)f(n-2) \leq f(p+j+1)+(n-p-j-3)f(n-1). \quad (6)$$

Inequalities (4) and (6) means that if we take $n_{p+j+2} = n_{p+j+3} = \cdots = n_{n-3} = \xi = 0$ then we can get an upper bound $\tilde{H}_f^{(p,p+j+1)}$ for $H_f^{(p,p+j+1)}$, where

$$\begin{aligned}\tilde{H}_f^{(p,p+j+1)} =& \frac{n-p+j-3}{n-p-j-3}f(p+j+1)+(p+j+1)f(n-1) \\ &+ \frac{n^2-n(2p+2j+5)+p^2+2pj+5p+j^2+3j+6}{n-p-j-3}f(n-2)\end{aligned}$$

for $p \in \{0,1,\ldots,n-4\}$ and $j \in \{0,1,\ldots,n-p-4\}$. Keep in mind that the upper bound $\tilde{H}_f^{(p,p+j+1)}$ may not always correspond to a graph (except for $j=0, \tilde{H}_f^{(p,p+1)} = H_f^{(p,p+1)}$).

Now we show that for a given number $p$, $H_f^{(p,p+1)}$ is the maximum value of $H_f$, that is, $H_f^{(p,p+1)} > H_f^{(p,p+j+1)}$ for $j \in \{1,2,\ldots,n-p-4\}$. Since $H_f^{(p,p+j+1)} \leq \tilde{H}_f^{(p,p+j+1)}$, it is enough to show that $H_f^{(p,p+1)} > \tilde{H}_f^{(p,p+j+1)}$ for $j \in \{1,2,\ldots,n-p-4\}$. Therefore, we are required to prove the following inequality:

$$\tilde{H}_f^{(p,p+j+1)} < f(p+1)+(n-p-2)f(n-2)+(p+1)f(n-1) \quad (7)$$

for $p \in \{0,1,\ldots,n-4\}$ and $j \in \{1,\ldots,n-p-4\}$. Since $j \leq n-p-4$, $n-p-j-3 \geq 1$. We transform inequality (7) into (8)

$$\begin{aligned}&(n-p-j-3)f(p+1)-(n-p+j-3)f(p+j+1) \\ &\quad +j(n-p-j-1)f(n-2)-j(n-p-j-3)f(n-1) > 0 \quad (8)\end{aligned}$$

for $p \in \{0,1,\ldots,n-4\}$ and $j \in \{1,2,\ldots,n-p-4\}$. Observe that under known conditions, $f(x)$ satisfies the inequality (8).

We have shown that for a given number $p$, the maximum value of $H_f$ is $H_f^{(p,p+1)}$ :

$$H_f^{(p,p+1)} = f(p+1) + (n-p-2)f(n-2) + (p+1)f(n-1)$$

for $p \in \{0, 1, \ldots, n-4\}$. This value is attained by a graph with $n_{n-1} = p+1$, $n_{n-2} = n-p-2$ and $n_{p+1} = 1$. ■

For $k = n-1$, in which case $m \geq (n-1)(n-2)/2+1$, Theorem 9 has been proved. It remains to prove the theorem for $n \leq m \leq \left(n^2 - 3n + 2\right)/2$.

**Lemma 13** (Hu, Li, Shi and Xu [12]). *Let $G^*$ be a maximum connected $(n,m)$-graph. If a function $f(x)$ is strictly convex and the maximum graph $G^*$ has $r$ $(r \leq n-3)$ vertices of degree $n-1$, then the minimum degree of $G^*$ is $r$.*

**Lemma 14.** *Assume that a function $f(x)$ satisfy conditions (i), (ii), (iii), and at least one of the conditions (iv), (v) and (vi). Let $n, m, k, p$ be integers satisfying that $m = n + k(k-3)/2 + p$ and $n \leq m \leq (n^2 - 3n + 2)/2$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-2$. If $G^*$ is a maximum connected $(n,m)$-graph, then $n_1 \neq 0$.*

*Proof.* Note that according to Proposition 8, the function $f(x)$ must satisfy condition (vi). Toward a contradiction, suppose $n_1 = 0$. Let $r$ be the minimum degree of $G^*$, in other words, $n_1 = n_2 = \cdots = n_{r-1} = 0$ and $n_r \neq 0$, where $r \geq 2$. Then $n_{n-1} = r$. Otherwise, if $n_{n-1} = k$, where $k \neq r$, then by Lemma 13 the minimum degree of $G^*$ is $k$, not $r$, a contradiction. Let $u$ be a vertex of degree $r$. Then $u$ is adjacent to all the $r$ vertices $w_1, w_2, \ldots, w_r$ of degree $n-1$.

Let $S = V(G)^* \setminus \{u, w_1, w_2, \ldots, w_r\}$, and $K(S)$ be the complete graph on $S$. Then

$$\begin{aligned}
|E(K(S))| - |E(G[S])| &= \binom{n-r-1}{2} - \left(m - r(n-r) - \binom{r}{2}\right) \\
&\geq \binom{n-r-1}{2} - \frac{n^2 - 3n + 2}{2} + r(n-r) + \binom{r}{2} \\
&= r.
\end{aligned}$$

This implies that we can add to $G[S]$ at least $r-1$ edges, and these vertices still do not form a complete graph after adding these edges. Furthermore, $|S| \geq 3$, which leads to $n \geq r+4$.

For $r \geq 2$, denote by $G'$ a connected graph obtained from $G^*$ when we delete $r-1$ edges between vertex $u$ and vertices $w_1, \dots, w_{r-1}$ and add $r-1$ new edges between $t$ vertices in $S$. Without loss of generality we can assume that these $t$ vertices are $v_1, v_2, \dots, v_t$ with degrees $j_1, j_2, \dots, j_t$ in $G^*$, and the degree of $v_i$ is $j_i + x_i$ in $G'$ for $i \in \{1, 2, \dots, t\}$. Then $j_i \geq r$ and $x_i \geq 1$ for $i \in \{1, 2, \dots, t\}$ and $\sum_{i=1}^{t} x_i = 2(r-1)$. Therefore, applying Lemma 5, we have

$$\begin{aligned} H_f(G') - H_f(G^*) &= f(1) - f(r) + (r-1)f(n-2) - (r-1)f(n-1) \\ &\quad + \sum_{i=1}^{t}(f(j_i + x_i) - f(j_i)) \\ &> f(1) - f(r) + \sum_{i=1}^{t} x_i(f(r+1) - f(r)) \\ &= f(1) - f(r) + 2(r-1)(f(r+1) - f(r)) \\ &= f(1) + (2r-2)f(r+1) - (2r-1)f(r) \\ &\geq 0 \end{aligned}$$

for $r \geq 4$, which contradicts the maximality of $G^*$.

Next, we show that the minimum degree of $G^*$ cannot be 2 or 3. Since $f(x)$ is a convex function, $f(x+1) - f(x)$ is an increasing function.

**Case 1.** $r = 2$

In this case the maximum graph $G^*$ has only two vertices of degree $n-1$, denoted by $w_1$ and $w_2$. Since $|E(K(S))| - |E(G[S])| \geq r = 2$, $n \geq 6$. We consider the number $n_2$ of vertices with degree 2.

**Subcase 1.1.** $1 \leq n_2 \leq n-3$.

Let $u$ be a vertex of degree 2. Clearly, $u$ is adjacent to $w_1$, $w_2$. We claim that there exists a vertex $v$ in $S$ with degree $j$, where $3 \leq j \leq n-3$. Since $1 \leq n_2 \leq n-3$, there exists a vertex $v_1$ in $S$ with degree $j_1$ greater than 2. If $j_1 \leq n-3$, then $v_1$ is the desired vertex. Otherwise, $j_1 = n-2$ and $v_1$ is adjacent to all vertices in $S$. So all the vertices in $S$ have degrees greater than 2, then there must exist a vertex in $S$ whose degree is less than or equal to $n-3$, this is because $|E(K(S))| - |E(G[S])| \geq r$.

Thus we can find two nonadjacent vertices $v_1$ and $v_2$ in $S$ with degree $j_1 \geq 2$ and $j_2 \geq 3$. Construct a new graph $G'' = G^* - uw_1 + v_1v_2$. We have

$$\begin{aligned} H_f(G'') - H_f(G^*) &= f(1) - f(2) + f(n-2) - f(n-1) + f(j_1+1) \\ &\quad - f(j_1) + f(j_2+1) - f(j_2) \\ &> f(1) - f(2) + f(3) - f(2) + f(4) - f(3) \\ &= f(1) - 2f(2) + f(4) \\ &\geq 0, \end{aligned}$$

a contradiction.

**Subcase 1.2.** $n_2 = n-2$.

Let $u_1, u_2, \ldots, u_{n-2}$ be the vertices of degree 2. Clearly, $u_i$ is adjacent to $w_1, w_2$ for $1 \leq i \leq n-2$.

If $n = 6$, then $G^* = K_{2,4}$. Let $G'' = FPA_1(6,4,0)$. Thus,

$$\begin{aligned} H_f(G'') - H_f(G^*) &= f(5) + 3f(3) + 2f(1) - 4f(2) - 2f(4) \\ &= f(3) - 2f(4) + f(5) + 2(f(1) - 2f(2) + f(3)) \\ &> 0, \end{aligned}$$

a contradiction. The last inequality can be derived from Lemma 2.

If $n = 7$, then $G^* = K_{2,5}$. Let $G'' = FPA_1(7,4,1)$. Hence,

$$\begin{aligned} H_f(G'') - H_f(G^*) &= 2f(1) + f(2) + 2f(3) + f(4) + f(6) - 5f(2) - 2f(5) \\ &= f(4) - 2f(5) + f(6) + 2(f(1) - 2f(2) + f(3)) \\ &> 0, \end{aligned}$$

a contradiction. The last inequality can be derived from Lemma 2.

Thus $n \geq 8$ and $n_2 = n-2 \geq 6$. Construct a new graph $G'' =$

$G^* - u_1w_1 - u_2w_1 - u_3w_1 + u_4u_5 + u_5u_6 + u_4u_6$. We have

$$\begin{aligned}H_f(G'') - H_f(G^*) &= 3(f(1) - f(2)) + f(n-4) - f(n-1) + 3(f(4) - f(2))\\ &> 3(f(1) - 2f(2) + f(4))\\ &\geq 0,\end{aligned}$$

a contradiction.

**Case 2.** $r = 3$

In this case the maximum graph $G^*$ has only three vertices with degree $n-1$, denoted by $w_1$, $w_2$ and $w_3$. Since $|E(K(S))| - |E(G[S])| \geq r = 3$, $n \geq 7$. We consider the number $n_3$ of vertices with degree 3.

**Subcase 2.1.** $1 \leq n_3 \leq n-4$.

Let $u$ be a vertex of degree 3. Clearly, $u$ is adjacent to $w_1$, $w_2$, $w_3$. With a similar approach to **Subcase 1.1**, we can find two pairs of nonadjacent vertices $v_1$ and $v_2$, $v_3$ and $v_4$ in $S$ whose degrees are $j_1, j_2, j_3$ and $j_4$, where $j_1 \geq 4$ and $j_i \geq 3$ for $i \in \{2,3,4\}$. Note that these four vertices are not necessarily distinct.

If all these four vertices are distinct, we construct a new graph $G'' = G^* - uw_1 - uw_2 + v_1v_2 + v_3v_4$. We have

$$\begin{aligned}H_f(G'') - H_f(G^*) &= f(1) - f(3) + 2(f(n-2) - f(n-1))\\ &\quad + \sum_{i=1}^{4}(f(j_i+1) - f(j_i))\\ &> f(1) - f(3) + f(5) - f(4) + 3(f(4) - f(3))\\ &= f(1) - 4f(3) + 2f(4) + f(5)\\ &\geq 0,\end{aligned}$$

a contradiction.

Next, assume that some vertices in $v_1, v_2, v_3, v_4$ are same. By symmetry, it suffices to consider two possibilities: $v_1 = v_3$ or $v_2 = v_3$.

If $v_1 = v_3$, we use $v$ to denote $v_1$. Clearly, $v$ has degree $j \geq 4$. We construct a new graph $G'' = G^* - uw_1 - uw_2 + vv_2 + vv_4$. Therefore,

$$H_f(G'') - H_f(G^*) = f(1) - f(3) + 2(f(n-2) - f(n-1)) + f(j+2)$$

$$- f(j) + (f(j_2+1) - f(j_2)) + (f(j_4+1) - f(j_4))$$
$$> f(1) - f(3) + f(6) - f(4) + 2(f(4) - f(3)).$$

By taking the values of $a$, $b$ and $y$ in Inequality (3) to be 4, 4 and 2, respectively, we have

$$f(6) - f(4) \geq 2(f(5) - f(4)).$$

Thus,

$$\begin{aligned} H_f(G'') - H_f(G^*) &> f(1) - f(3) + f(6) - f(4) + 2(f(4) - f(3)) \\ &> f(1) - f(3) + 2(f(5) - f(4)) + 2(f(4) - f(3)) \\ &> f(1) - f(3) + (f(5) - f(4)) + 3(f(4) - f(3)) \\ &= f(1) - 4f(3) + 2f(4) + f(5) \\ &\geq 0, \end{aligned}$$

a contradiction.

If $v_2 = v_3$, we use $v$ to denote $v_2$. Clearly, $v$ has degree $j \geq 3$. Construct a new graph $G'' = G^* - uw_1 - uw_2 + vv_1 + vv_4$. Hence,

$$\begin{aligned} H_f(G'') - H_f(G^*) = {} & f(1) - f(3) + 2(f(n-2) - f(n-1)) + f(j+2) \\ & - f(j) + (f(j_1+1) - f(j_1)) + (f(j_4+1) - f(j_4)) \\ > {} & f(1) - f(3) + f(5) - f(3) + f(5) - f(4) \\ & + f(4) - f(3). \end{aligned}$$

By taking the values of $a$, $b$ and $y$ in Inequality (3) to be 3, 3 and 2, respectively, we have

$$f(5) - f(3) \geq 2(f(4) - f(3)).$$

Thus,

$$\begin{aligned} & H_f(G'') - H_f(G^*) \\ & \quad > f(1) - f(3) + f(5) - f(3) + f(5) - f(4) + f(4) - f(3) \end{aligned}$$

$$
\begin{aligned}
&> f(1) - f(3) + 2(f(4) - f(3)) + f(5) - f(4) + f(4) - f(3) \\
&= f(1) - 4f(3) + 2f(4) + f(5) \\
&\geq 0,
\end{aligned}
$$

a contradiction.

**Subcase 2.2.** $n_3 = n - 3$.

Let $u_1, u_2, \ldots, u_{n-3}$ be the vertices of degree 3. Clearly, $u_i$ is adjacent to $w_1, w_2$ and $w_3$ for $1 \leq i \leq n-3$. Since $n \geq 7$, $n_3 = n-3 \geq 4$. Construct a new graph $G'' = G^* - u_1w_1 - u_1w_2 + u_2u_3 + u_3u_4$. We have

$$
\begin{aligned}
H_f(G'') - H_f(G^*) &= f(1) - f(3) + 2(f(n-2) - f(n-1)) \\
&\quad + f(5) - f(3) + 2(f(4) - f(3)) \\
&> f(1) - 4f(3) + 2f(4) + f(5) \\
&\geq 0,
\end{aligned}
$$

a contradiction. ■

Hence, we only need to consider maximum graphs which have $n_1 \neq 0$, for $2 \leq k \leq n-2$. Then $n_{n-1} = 1$ (by Lemmas 1 and 6) and all vertices of degree 1 must be adjacent to this unique vertex of degree $n-1$. Here we do not consider the case $n_1 = n-1$, since it is equivalent to the case $m = n-1$, which has been proved before. When $n_1 < n-1$, it is readily obtained that $n_1 \leq n-3$.

When $n_{n-1} = 1$ and $n_1 = l$, where $1 \leq l \leq n-3$, according to Lemma 7, problem $(P)$ can be transformed into the subsequent problem $(P^l)$ :

$$
\max l \cdot f(1) + n_2 \cdot f(2) + \cdots + n_{n-l-1} f(n-l-1) + f(n-1)
$$

under the constraints:

$$
n_2 + n_3 + n_4 + \cdots + n_{n-l-1} = n - 1 - l, \tag{9}
$$

$$
n_2 + 2n_3 + 3n_4 + \cdots + (n-l-2)n_{n-l-1} = 2(m - n + 1). \tag{10}
$$

To prove the following lemma, it is necessary to use mathematical induction. It is straightforward to verify that Theorem 9 is true for $n = 4$ and $3 \le m \le 6$. We assume that Theorem 9 is true for every connected graph $G$ in $G(i, j)$ when $4 \le i \le n-1$ and $i - 1 \le j \le \binom{i}{2}$.

**Lemma 15.** *Let $G$ be a connected $(n, m)$-graph, where $m = n + k(k-3)/2 + p$, $m \ge n$, $2 \le k \le n-2$ and $0 \le p \le k-2$. If $n_{n-1} = 1$ and $1 \le n_1 \le n-3$, then Inequality (1) holds for $G$.*

*Proof.* Inequality (1) will be valid for $G$ with $n_{n-1} = 1$ and $n_1 = l$, if the following inequality holds:

$$\begin{aligned} &l \cdot f(1) + n_2 \cdot f(2) + n_3 \cdot f(3) + \cdots + n_{n-l-1} f(n-l-1) + f(n-1) \\ &\le (n-k-1)f(1) + f(p+1) + (k-p-1)f(k-1) + pf(k) + f(n-1) \end{aligned} \tag{11}$$

under constraints (9) and (10).

We first prove (11) for $l \ge 2$. Since $n_1 = l$, by Lemma 7 we have $n_{n-l} = n_{n-l+1} = \cdots = n_{n-2} = 0$. Consider the graph $G'$, which is obtained from $G$, when we delete one vertex of degree 1. The graph $G'$ has $n'_1 = l - 1$ and one vertex of degree $n-2$ (because the other vertices can have a degree at most $n-1-l$), and $n'_i = n_i$ for $i \in \{2, \ldots, n-3\}$. Then $n'_{n-l} = n'_{n-l+1} = \cdots = n'_{n-3} = 0$ and the same constraints (9) and (10) hold (because $n-1-(l-1) = n-l$). Since $G'$ has $n-1$ vertices and $n-1+k(k-3)/2+p$ edges, it satisfies the inductive hypothesis, and so,

$$\begin{aligned} &n_2 \cdot f(2) + n_3 \cdot f(3) + \cdots + n_{n-l-1} f(n-l-1) \\ &\quad = n'_2 \cdot f(2) + n'_3 \cdot f(3) + \cdots + n'_{n-l-1} f(n-l-1) \\ &\quad \le (n-1-k-1-(l-1)) \cdot f(1) + f(p+1) \\ &\qquad + (k-p-1)f(k-1) + pf(k) \end{aligned} \tag{12}$$

for every $2 \le k \le n-2$ and $0 \le p \le k-2$. Inequality (12) is equivalent to (11), which is now proved because the constraints are the same.

Now we show that (11) holds for $l = 1$, that is, the graph $G'$ has no vertex of degree one. We have $n'_i = n_i$ for $i\{2, \ldots, n-3$ and $n'_{n-2} =$

$n_{n-2}+1\}$. By the inductive hypothesis for the graph $G'$ holds

$$\begin{aligned} n_2 \cdot f(2) + n_3 \cdot f(3) + \cdots + n_{n-3} \cdot f(n-3) + (n_{n-2}+1)f(n-2) \\ = n'_2 \cdot f(2) + n'_3 \cdot f(3) + \cdots + n'_{n-3} \cdot f(n-3) + n'_{n-2} f(n-2) \\ \leq (n-1-k-1) \cdot f(1) + f(p+1) + (k-p-1)f(k-1) \\ + pf(k) + f(n-1-1) \end{aligned} \tag{13}$$

under the constraints

$$\begin{aligned} n'_2 + n'_3 + n'_4 + \cdots + n'_{n-2} = n-1, \\ 2n'_2 + 3n'_3 + 4n'_4 + \cdots + (n-2)n'_{n-2} = 2(m-1). \end{aligned}$$

Thus, we have

$$\begin{aligned} n_2 \cdot f(2) + n_3 \cdot f(3) + \cdots + n_{n-3} f(n-3) + n_{n-2} f(n-2) \\ \leq (n-k-2)f(1) + f(p+1) + (k-p-1)f(k-1) + p \cdot f(k) \end{aligned} \tag{14}$$

under the constraints

$$\begin{aligned} n_2 + n_3 + \cdots + n_{n-3} + n_{n-2} = n-2, \\ n_2 + 2n_3 + \cdots + (n-3)n_{n-3} + (n-2)n_{n-2} = 2m-n. \end{aligned} \tag{15}$$

Equalities (15) are just the constraints (9) and (10), and inequality (14) is equivalent to inequality (11) for $l=1$. Thus the lemma is proved. ■

***Proof of Theorem 9.*** We need to show that Theorem 9 holds for $n-1 \leq m \leq \binom{n}{2}$. The case $m = n-1$ has already been proved in Corollary 3, and cases $m = \binom{n}{2}$ and $\binom{n}{2} - 1$ are disregarded because they all correspond to unique graphs.

Since $m = n + k(k-3)/2 + p$, where $2 \leq k \leq n-1$ and $0 \leq p \leq k-2$, we distinguish two cases $k = n-1$ and $2 \leq k \leq n-2$. The case $k = n-1$ has already been proved in 12. The case $2 \leq k \leq n-2$ can be proved by combining Lemmas 14 and 15. Thus, Theorem 9 is proved.

■

Theorem 9 characterizes the maximum value of $H_f(G)$ among all connected $(n,m)$-graphs. Applying Theorem 9, we can also determine the maximum value of $H_f(G)$ among all $(n,m)$-graphs, as stated in Theorem 10.

***Proof of Theorem 10.*** Let $G$ be the maximum $(n,m)$-graph. By Lemma 1, $G$ consists of a set $I_1$ of isolated vertices, together with a connected graph $G_1$, which has $n'$ vertices $m$ edges. Note that $G_1$ is a maximum connected $(n',m)$-graph, otherwise, we can find a connected $(n',m)$-graph $G_2$, such that $H_f(G_2) > H_f(G_1)$, then the graph $G' := G_2 + I_1$ is an $(n,m)$-graph satisfying that $H_f(G') > H_f(G)$ holds, a contradiction.

If $m = \binom{n'}{2}$, then $G = \overline{FPA}_1(n,n',0)$, which proves the theorem.

If $m < \binom{n'}{2}$. Assume that $m = n' + k'(k'-3)/2 + p'$, where $2 \le k' \le n'-1$ and $0 \le p' \le k'-2$. By Theorem 9, $G_1$ is a fanned pineapple of type 1 with parameters $n', k', p'$, that is $G_1 = FPA_1(n',k',p')$. Let K be a copy of a clique of $k'$ vertices of $G_1$. Let $l$ be the number of vertices in $V(G_1) \setminus V(K)$ with degree 1. It is easily seen that $p'$ and $l$ cannot both be 0 simultaneously. Next, we differ the subsequent proof into the following four cases.

**Case 1.** $p' = 0$, $l = 1$.

In this case, $k' = n' - l = n' - 1$, $G_1 = FPA_1(n', n'-1, 0)$, then $G = \overline{FPA}_1(n, n'-1, 1)$, the theorem is proved.

**Case 2.** $1 \le p' \le k' - 2$, $l = 0$.

In this case, $k' = n' - l - 1 = n' - 1$, $G_1 = FPA_1(n', n'-1, p')$, then $G = \overline{FPA}_1(n, n'-1, p'+1)$, which proves the theorem.

**Case 3.** $p' = 0$, $l \ge 2$.

In this case, $k' \ge 2$, $G_1 = FPA_1(n', k', 0)$. Let $w$ be a vertex of degree $n'-1$. Let $u$ and $v$ be two vertices in $V(G_1) \setminus V(K)$ with degree 1. Let $z \in V(K) \backslash w$. Then $d(z) = k'-1$. Construct a new graph $G' = G - uw + vz$. Thus,

$$
\begin{aligned}
&H_f(G') - H_f(G) \\
&\quad = f(0) + f(2) + f(n'-2) + f(k') - 2f(1) - f(n'-1) - f(k'-1) \\
&\quad = f(0) + f(2) - 2f(1) + f(n'-2) - f(n'-1) + f(k') - f(k'-1) \\
&\quad > f(0) + f(2) - 2f(1) + f(2) - f(2-1)
\end{aligned}
$$

$$= f(0) + 2f(2) - 3f(1)$$
$$\geq 0,$$

which contradicts the maximality of $G$.

**Case 4.** $1 \leq p' \leq k' - 2$, $l \geq 1$.

In this case, $k' \geq 3$, $G_1 = FPA_1(n', k', p')$. Let $w$ be a vertex of degree $n' - 1$. Let $u$ be a vertex in $V(G_1) \setminus V(K)$ with degree 1. Let $v$ be the vertex of degree $p' + 1$ in $V(G_1) \setminus V(K)$. Let $z$ be a vertex in $V(K)$ which is not adjacent to $v$. Then $d(z) = k' - 1$. Construct a new graph $G' = G - uw + vz$. Therefore,

$$\begin{aligned}
H_f(G') - H_f(G) &= f(0) + f(p'+2) + f(n'-2) + f(k') - f(1) \\
&\quad - f(p'+1) - f(n'-1) - f(k'-1) \\
&= f(0) - f(1) + f(n'-2) + f(n'-1) + f(p'+2) \\
&\quad - f(p'+1) + f(k') - f(k'-1) \\
&> f(0) - f(1) + f(1+2) - f(1+1) + f(3) - f(3-1) \\
&= f(0) - f(1) + 2f(3) - 2f(2) \\
&\geq 0,
\end{aligned}$$

which contradicts the maximality of $G$. ■

Next, we show by Lemmas 16–23 that the function $f(x) = (x+q)^\alpha$ satisfies the assumption in Theorem 9 when $t \geq 1$, $\alpha \leq -t$ and $-1 < q \leq 2.038t - 0.038$, or $\alpha < 0$ and $-1 < q \leq 0$. Furthermore, the function $f(x) = (x+q)^\alpha$ satisfies the conditions of Theorem 10 for $t \geq 1$, $\alpha \leq -t$ and $0 < q \leq 1.413t + 0.587$.

**Lemma 16.** *Let $n, p, j$ be integers with $n \geq 5$. Let $f(x) = (x+q)^\alpha$. If $\alpha < 0$ and $q > -1$, then*

$$\begin{aligned}
g(p,j) =& (n-p-j-3)f(p+1) - (n-p+j-3)f(p+j+1) \\
&+ j(n-p-j-1)f(n-2) - j(n-p-j-3)f(n-1) > 0,
\end{aligned}$$

*for each $p \in \{0, 1, \ldots, n-4\}$ and for each $j \in \{1, \ldots, n-p-4\}$.*

*Proof.* In the following, we prove that the partial derivative of $g(p,j)$ with respect to $p$ is less than 0. Firstly,

$$\begin{aligned}\frac{\partial g(p,j)}{\partial p} =& -(p+1+q)^{\alpha}+\alpha(n-p-j-3)(p+1+q)^{\alpha-1}\\ &+(p+j+1+q)^{\alpha}-\alpha(n-p+j-3)(p+j+1+q)^{\alpha-1}\\ &-j(n-2+q)^{\alpha}+j(n-1+q)^{\alpha}.\end{aligned}$$

Since $\alpha(\alpha-1)(n-p-j-3)\left((p+1+q)^{\alpha-2}-(p+j+1+q)^{\alpha-2}\right)\geq 0$ for $\alpha<0$, we have

$$\begin{aligned}&\frac{\partial^2 g(p,j)}{\partial p^2}\\ &=-2\alpha(p+1+q)^{\alpha-1}+2\alpha(p+j+1+q)^{\alpha-1}\\ &\quad+\alpha(\alpha-1)(n-p-j-3)(p+1+q)^{\alpha-2}\\ &\quad-\alpha(\alpha-1)(n-p+j-3)(p+j+1+q)^{\alpha-2}\\ &=-2\alpha(p+1+q)^{\alpha-1}+2\alpha(p+j+1+q)^{\alpha-1}\\ &\quad+\alpha(\alpha-1)(n-p-j-3)\left((p+1+q)^{\alpha-2}-(p+j+1+q)^{\alpha-2}\right)\\ &\quad-\alpha(\alpha-1)\cdot 2j\cdot(p+j+1+q)^{\alpha-2}\\ &\geq-2\alpha\left((p+1+q)^{\alpha-1}-(p+j+1+q)^{\alpha-1}\right)\\ &\quad-2\alpha(\alpha-1)j(p+j+1+q)^{\alpha-2}\\ &=-2j\alpha(\alpha-1)\left(-\xi^{\alpha-2}+(p+j+1+q)^{\alpha-2}\right)\geq 0,\end{aligned}$$

where $\xi\in(p+1+q,p+j+1+q)$. Since $p\leq n-j-3$,

$$\begin{aligned}\frac{\partial g(p,j)}{\partial p}\leq& -(n-j-2+q)^{\alpha}+(n-2+q)^{\alpha}-2j\alpha(n-2+q)^{\alpha-1}\\ &-j\left((n-2+q)^{\alpha}-(n-1+q)^{\alpha}\right).\end{aligned}$$

Define a function $h(j)=-(n-j-2+q)^{\alpha}+(n-2+q)^{\alpha}-2j\alpha(n-2+q)^{\alpha-1}-j\left((n-2+q)^{\alpha}-(n-1+q)^{\alpha}\right)$. Since $\frac{\partial^2 h(j)}{\partial j^2}=-\alpha(\alpha-1)(n-j-2+q)^{\alpha-2}\leq 0$, $\left[(n-1+q)^{\alpha-1}+(n-3+q)^{\alpha-1}-2(n-2+q)^{\alpha-1}\right]>0$

(by Corollary 2) and $j \geq 1$, we have

$$\begin{aligned}\frac{\partial h(j)}{\partial j} &= \alpha(n-j-2+q)^{\alpha-1} - 2\alpha(n-2+q)^{\alpha-1} \\ &\quad - ((n-2+q)^{\alpha} - (n-1+q)^{\alpha}) \\ &\leq \alpha(n-3+q)^{\alpha-1} - 2\alpha(n-2+q)^{\alpha-1} \\ &\quad - ((n-2+q)^{\alpha} - (n-1+q)^{\alpha}) \\ &= \alpha\left[(n-1+q)^{\alpha-1} + (n-3+q)^{\alpha-1} - 2(n-2+q)^{\alpha-1}\right] \\ &\quad - ((n-2+q)^{\alpha} - (n-1+q)^{\alpha}) - \alpha(n-1+q)^{\alpha-1} \\ &\leq \alpha\eta^{\alpha-1} - \alpha(n-1+q)^{\alpha-1} \leq 0,\end{aligned}$$

where $\eta \in (n-2+q, n-1+q)$. Thus, $\frac{\partial g(p,j)}{\partial p} \leq h(j) \leq h(1)$.

Since for any $x, x_0 \in [a,b]$, where $a$ and $b$ are real numbers, there exists $\xi \in (a,b)$ such that $f(x) = f(x_0) + \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{x=x_0}(x-x_0) + \frac{1}{2!}\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\Big|_{x=\xi}(x-x_0)^2$, so we have

$$\begin{aligned}(n-1+q)^{\alpha} &= (n-2+q)^{\alpha} + \alpha(n-2+q)^{\alpha-1} + \frac{\alpha(\alpha-1)}{2!}(n-2+\xi_1+q)^{\alpha-2}, \\ (n-3+q)^{\alpha} &= (n-2+q)^{\alpha} - \alpha(n-2+q)^{\alpha-1} + \frac{\alpha(\alpha-1)}{2!}(n-2-\xi_2+q)^{\alpha-2},\end{aligned}$$

where $0 < \xi_1 < 1$ and $0 < \xi_2 < 1$. Then

$$\begin{aligned}h(1) =&(n-1+q)^{\alpha} - (n-3+q)^{\alpha} - 2\alpha(n-2+q)^{\alpha-1} \\ =&(n-2+q)^{\alpha} + \alpha(n-2+q)^{\alpha-1} + \frac{\alpha(\alpha-1)}{2}(n-2+\xi_1+q)^{\alpha-2} \\ &- (n-2+q)^{\alpha} + \alpha(n-2+q)^{\alpha-1} - \frac{\alpha(\alpha-1)}{2}(n-2-\xi_2+q)^{\alpha-2} \\ &- 2\alpha(n-2+q)^{\alpha-1} \\ =&\frac{\alpha(\alpha-1)}{2}\left((n-2+\xi_1+q)^{\alpha-2} - (n-2-\xi_2+q)^{\alpha-2}\right) < 0.\end{aligned}$$

Consequently, $\frac{\partial g(p,j)}{\partial p} \leq h(j) \leq h(1) < 0$. Thus, $g(p,j) \geq g(n-j-4,j) > g(n-j-3,j) = 0$. ■

**Lemma 17.** *Let* $f(x) = (x+q)^{\alpha}$. *If* $\alpha \leq -t$, $-1 < q \leq 2.038t - 0.038$,

$t \geq 1$ *and* $r \geq 3$, *then*

$$f(1) + (2r-2)f(r+1) - (2r-1)f(r) \geq 0.$$

*Proof.* Let $f_1(\alpha, q, r) = f(1) + (2r-2)f(r+1) - (2r-1)f(r) = (1+q)^\alpha + (2r-2)(r+1+q)^\alpha - (2r-1)(r+q)^\alpha$ and $g(\alpha, q, r) = \frac{f_1(\alpha,q,r)}{(r+q)^\alpha} = \left(\frac{1+q}{r+q}\right)^\alpha + (2r-2)\left(\frac{r+1+q}{r+q}\right)^\alpha - (2r-1)$. Firstly,

$$\frac{\partial g}{\partial q} = \frac{\alpha}{(r+q)^2}\left[(r-1)\left(\frac{1+q}{r+q}\right)^{\alpha-1} - (2r-2)\left(\frac{r+1+q}{r+q}\right)^{\alpha-1}\right].$$

Let $g_1(t) = (t+1)\ln\left(\frac{2.038t+3.962}{2.038t+0.962}\right) - \ln 2$. According to Lemma 10, Since $2 \times 2.038^2 - 2.038 \times 3.962 - 2.038 \times 0.962 < 0$, $2.038 \times 3.962 + 2.038 \times 0.962 - 2 \times 3.962 \times 0.962 > 0$ and $\frac{\mathrm{d}g_1}{\mathrm{d}t}$ has no root on the interval $(1, \infty)$, it follows that $g_1(t) \geq g_1(1) \approx 0.69 > 0$. Thus,

$$\begin{aligned}
\frac{(r-1)\left(\frac{1+q}{r+q}\right)^{\alpha-1}}{(2r-2)\left(\frac{r+1+q}{r+q}\right)^{\alpha-1}} &= \frac{1}{2}\left(\frac{1+q}{r+1+q}\right)^{\alpha-1} \geq \frac{1}{2}\left(\frac{r+1+q}{1+q}\right)^{t+1} \\
&\geq \frac{1}{2}\left(1+\frac{r}{1+q}\right)^{t+1} \\
&\geq \frac{1}{2}\left(1+\frac{3}{1+2.038t-0.038}\right)^{t+1} \\
&= \frac{1}{2}\left(\frac{2.038t+3.962}{2.038t+0.962}\right)^{t+1} \\
&> 1
\end{aligned}$$

and $\frac{\partial g}{\partial q} < 0$.

We now prove that the partial derivative of the function $g(\alpha, q, r)$ with respect to $\alpha$ is less than or equal to 0. By Lemmas 8 and 11, $\frac{\ln\left(\frac{2.038t+r+0.962}{2.038t+r-0.038}\right)}{\ln\left(\frac{2.038t+r-0.038}{2.038t+0.962}\right)}\left(\frac{2.038t+0.962}{2.038t+r+0.962}\right)^t \leq \frac{3}{(r-1)(r+3)}$ and $\frac{\ln\left(\frac{q+r+1}{q+r}\right)}{\ln\left(\frac{q+r}{q+1}\right)}$ is monotonically increasing with respect to $q$. We have $\frac{(2r-2)\ln\left(\frac{q+r+1}{q+r}\right)\left(\frac{q+r+1}{q+r}\right)^a}{\ln\left(\frac{q+r}{q+1}\right)\left(\frac{q+1}{q+r}\right)^a} = (2r-2)\frac{\ln\left(\frac{q+r+1}{q+r}\right)}{\ln\left(\frac{q+r}{q+1}\right)}\left(\frac{q+r+1}{q+1}\right)^a \leq (2r-2)\frac{\ln\left(\frac{q+r+1}{q+r}\right)}{\ln\left(\frac{q+r}{q+1}\right)}\left(\frac{q+1}{q+r+1}\right)^t$

$\leq (2r-2)\,\frac{\ln\left(\frac{2.038t+r+0.962}{2.038t+r-0.038}\right)}{\ln\left(\frac{2.038t+r-0.038}{2.038t+0.962}\right)}\left(\frac{2.038t+0.962}{2.038t+r+0.962}\right)^t \leq (2r-2)\,\frac{3}{(r-1)(r+3)} \leq 1$. Since $\frac{\partial g}{\partial \alpha} = (2r-2)\ln\left(\frac{q+r+1}{q+r}\right)\left(\frac{q+r+1}{q+r}\right)^a - \ln\left(\frac{q+r}{q+1}\right)\left(\frac{q+1}{q+r}\right)^a$, $\frac{\partial g}{\partial \alpha} \leq 0$.

Since $\frac{\partial g}{\partial q} < 0$ and $\frac{\partial g}{\partial \alpha} \leq 0$, $g(\alpha,q,r) \geq g(-t, 2.038t-0.038, r) = g_2(t,r)$, where $g_2(t,r) = \left(\frac{2.038t+r-0.038}{2.038t+0.962}\right)^t + (2r-2)\left(\frac{2.038t+r-0.038}{2.038t+r+0.962}\right)^t - (2r-1)$. The partial derivative of $g_2(t,r)$ with respect to $r$ is given by: $\frac{\partial g_2}{\partial r} = 2\left(\frac{2.038t+r-0.038}{2.038t+r+0.962}\right)^t + \frac{t\left(\frac{2.038t+r-0.038}{2.038t+0.962}\right)^{t-1}}{2.038t+0.962} + \frac{t(2r-2)\left(\frac{2.038t+r-0.038}{2.038t+r+0.962}\right)^{t-1}}{(2.038t+r+0.962)^2} - 2 \geq 2h_1(t) + h_2(t)h_3(t) + \frac{t(2r-2)\left(\frac{2.038t+r-0.038}{2.038t+r+0.962}\right)^{t-1}}{(2.038t+r+0.962)^2} - 2$, where $h_1(t) = \left(\frac{2.038t+2.962}{2.038t+3.962}\right)^t$, $h_2(t) = \frac{t}{2.038t+2.962}$ and $h_3(t) = \left(\frac{2.038t+2.962}{2.038t+0.962}\right)^t$. Let $h_4(t) = t\ln\left(\frac{2.038t+2.962}{2.038t+0.962}\right)$ and $h(t) = 2h_1(t) + h_2(t)h_3(t) - 2$. By Lemma 9, we have $h_1(t)$, $\frac{\mathrm{d}h_2}{\mathrm{d}t}$ and $\frac{\mathrm{d}h_4}{\mathrm{d}t}$ are positive and monotonically decreasing on the interval $[1,\infty)$. On the interval $[1,\infty)$, $h_2(t)$, $h_3(t)$ and $h_4(t)$ are positive monotonically increasing functions, while $\frac{\mathrm{d}h_1}{\mathrm{d}t}$ is a negative monotonically increasing function. For two constants $a$ and $b$, let $h_5(a,b) = 2\,\frac{\mathrm{d}h_1}{\mathrm{d}t}\Big|_{t=a} + \frac{\mathrm{d}h_2}{\mathrm{d}t}\Big|_{t=b} h_3(a) + h_2(a)e^{h_4(a)}\,\frac{\mathrm{d}h_4}{\mathrm{d}t}\Big|_{t=b}$, where $1 \leq a \leq b$. When $t \in [a,b]$, $\frac{\mathrm{d}h}{\mathrm{d}t} = 2\frac{\mathrm{d}h_1}{\mathrm{d}t} + \frac{\mathrm{d}h_2}{\mathrm{d}t}h_3(t) + h_2(t)e^{h_4(t)}\frac{\mathrm{d}h_4}{\mathrm{d}t} \geq h_5(a,b)$. If $h_5(a,b) \geq 0$, then $\frac{\mathrm{d}h}{\mathrm{d}t} \geq 0$ on the interval $[a,b]$. One can verify that $h_5(a,b) > 0$ when $a = 1+0.4i$ and $b = a+0.4$ for $i \in \{0,1,\ldots,7\}$. Thus, $\frac{\mathrm{d}h}{\mathrm{d}t} \geq 0$ and $h(t) \geq h(1) = 0$ on the interval $[1,4]$. When $t \geq 4$, $h(t) = 2h_1(t) + h_2(t)h_3(t) - 2 \geq 2h_1(\infty) + h_2(4)h_3(4) - 2 > 0$. Thus, $\frac{\partial g_2}{\partial r} > h(t) \geq 0$ and $g_2(t,r) \geq g_2(t,3) = h_6(t) + 4h_7(t) - 5$, where $h_6(t) = \left(\frac{2.038t+2.962}{2.038t+0.962}\right)^t$ and $h_7(t) = \left(\frac{2.038t+2.962}{2.038t+3.962}\right)^t$.

Let $h_8(t) = t\ln\left(\frac{2.038t+2.962}{2.038t+0.962}\right)$ and $h_9(t) = h_6(t) + 4h_7(t) - 5$. By Lemma 9, we have $h_7(t)$ and $\frac{\mathrm{d}h_8}{\mathrm{d}t}$ are positive and monotonically decreasing on the interval $[1,\infty)$. On the interval $[1,\infty)$, $h_6(t)$ and $h_8(t)$ are positive monotonically increasing functions, while $\frac{\mathrm{d}h_7}{\mathrm{d}t}$ is a negative monotonically increasing function. For two constants $a$ and $b$, let $h_{10}(a,b) = e^{h_8(a)}\,\frac{\mathrm{d}h_8}{\mathrm{d}t}\Big|_{t=b} + 4\,\frac{\mathrm{d}h_7}{\mathrm{d}t}\Big|_{t=a}$, where $1 \leq a \leq b$. When $t \in [a,b]$, $\frac{\mathrm{d}h_9}{\mathrm{d}t} = e^{h_8(t)}\frac{\mathrm{d}h_8}{\mathrm{d}t} + 4\frac{\mathrm{d}h_7}{\mathrm{d}t} \geq h_{10}(a,b)$. If $h_{10}(a,b) \geq 0$, then $\frac{\mathrm{d}h_9}{\mathrm{d}t} \geq 0$ on the interval $[a,b]$. It can be verified that $h_{10}(a,b) > 0$ when $a = 1+0.04i$ and $b = a+0.04$ for $i \in \{0,1,\ldots,500\}$. Thus, $\frac{\mathrm{d}h_9}{\mathrm{d}t} \geq 0$ and $h_9(t) \geq h_9(1) = 0$ on the interval $[1,21]$. When $t \geq 21$, $h_9(t) \geq h_6(21) + 4h_7(\infty) - 5 > 0$.

Hence, $g(\alpha, q, r) \geq g_2(t, r) \geq g_2(t, 3) = h_9(t) \geq 0$ and $f(\alpha, q, r) = g(\alpha, q, r)(r + q)^\alpha \geq 0$. ■

**Lemma 18.** *Let $f(x) = (x + q)^\alpha$. If $\alpha \leq -t$, $-1 < q \leq 2.038t - 0.038$ and $t \geq 1$, then*

$$f(1) - 2f(2) + f(4) \geq 0.$$

*Proof.* Let $f(\alpha, q) = f(1) - 2f(2) + f(4) = (1 + q)^\alpha - 2(2 + q)^\alpha + (4 + q)^\alpha$ and $g(\alpha, q) = \frac{f(\alpha,q)}{(2+q)^\alpha} = \left(\frac{1+q}{2+q}\right)^\alpha + \left(\frac{4+q}{2+q}\right)^\alpha - 2$. Firstly,

$$\frac{\partial g}{\partial q} = \frac{\alpha}{(2 + q)^2} \left[\left(\frac{1 + q}{2 + q}\right)^{\alpha-1} - 2\left(\frac{4 + q}{2 + q}\right)^{\alpha-1}\right].$$

Let $g_1(t) = (t + 1)\ln\left(\frac{2.038t+3.962}{2.038t+0.962}\right) - \ln 2$. According to Lemma 10, since $2\times 2.038^2 - 2.038\times 3.962 - 2.038\times 0.962 < 0$, $2.038\times 3.962 + 2.038\times 0.962 - 2\times 3.962\times 0.962 > 0$ and $\frac{\mathrm{d}g_1}{\mathrm{d}t} > 0$ has no root on the interval $(1, \infty)$, it follows that $g_1(t) \geq g_1(1) \approx 0.693 > 0$. Thus, $\frac{\left(\frac{1+q}{2+q}\right)^{\alpha-1}}{2\left(\frac{4+q}{2+q}\right)^{\alpha-1}} = \frac{1}{2}\left(\frac{1+q}{4+q}\right)^{\alpha-1} \geq \frac{1}{2}\left(\frac{4+q}{1+q}\right)^{t+1} \geq \frac{1}{2}\left(\frac{2.038t+3.962}{2.038t+0.962}\right)^{t+1} > 1$ and $\frac{\partial g}{\partial q} < 0$.

We now prove that the partial derivative of the function $g(\alpha, q)$ with respect to $\alpha$ is less than or equal to 0. By Lemmas 8 and 11, $\frac{\ln\left(\frac{2.038t+3.962}{2.038t+1.962}\right)}{\ln\left(\frac{2.038t+1.962}{2.038t+0.962}\right)}\left(\frac{2.038t+0.962}{2.038t+3.962}\right)^t \leq 1$ and $\frac{\ln\left(\frac{q+4}{q+2}\right)}{\ln\left(\frac{q+2}{q+1}\right)}$ is monotonically increasing with respect to $q$, we have

$$\begin{aligned}
\frac{\ln\left(\frac{q+4}{q+2}\right)\left(\frac{q+4}{q+2}\right)^a}{\ln\left(\frac{q+2}{q+1}\right)\left(\frac{q+1}{q+2}\right)^a} &= \frac{\ln\left(\frac{q+4}{q+2}\right)}{\ln\left(\frac{q+2}{q+1}\right)}\left(\frac{q + 4}{q + 1}\right)^a \\
&\leq \frac{\ln\left(\frac{q+4}{q+2}\right)}{\ln\left(\frac{q+2}{q+1}\right)}\left(\frac{q + 1}{q + 4}\right)^t \\
&\leq \frac{\ln\left(\frac{2.038t+3.962}{2.038t+1.962}\right)}{\ln\left(\frac{2.038t+1.962}{2.038t+0.962}\right)}\left(\frac{2.038t + 0.962}{2.038t + 3.962}\right)^t \\
&\leq 1.
\end{aligned}$$

Since $\frac{\partial g}{\partial \alpha} = \ln\left(\frac{q+4}{q+2}\right)\left(\frac{q+4}{q+2}\right)^a - \ln\left(\frac{q+2}{q+1}\right)\left(\frac{q+1}{q+2}\right)^a$, $\frac{\partial g}{\partial \alpha} < 0$.

Since $\frac{\partial g}{\partial q} < 0$ and $\frac{\partial g}{\partial \alpha} < 0$, $g(\alpha, q) \geq g(-t, 2.038t - 0.038) = h_1(t) + h_2(t) - 2$, where $h_1(t) = \left(\frac{2.038t+1.962}{2.038t+0.962}\right)^t$ and $h_2(t) = \left(\frac{2.038t+1.962}{2.038t+3.962}\right)^t$. Let $h_3(t) = t \ln\left(\frac{2.038t+1.962}{2.038t+0.962}\right)$ and $h(t) = h_1(t) + h_2(t) - 2$. By Lemma 9, we have $h_2(t)$ and $\frac{\mathrm{d}h_3}{\mathrm{d}t}$ are positive and monotonically decreasing on the interval $[1, \infty)$. On the interval $[1, \infty)$, $h_1(t)$ and $h_3(t)$ are positive monotonically increasing functions, while $\frac{\mathrm{d}h_2}{\mathrm{d}t}$ is a negative monotonically increasing function. For two constants $a$ and $b$, let $h_4(a, b) = e^{h_3(a)} \left.\frac{\mathrm{d}h_3}{\mathrm{d}t}\right|_{t=b} + \left.\frac{\mathrm{d}h_2}{\mathrm{d}t}\right|_{t=a}$, where $1 \leq a \leq b$. When $t \in [a, b]$, $\frac{\mathrm{d}h}{\mathrm{d}t} = e^{h_3(t)} \frac{\mathrm{d}h_3}{\mathrm{d}t} + \frac{\mathrm{d}h_2}{\mathrm{d}t} \geq h_4(a, b)$. If $h_4(a, b) \geq 0$, then $\frac{\mathrm{d}h}{\mathrm{d}t} \geq 0$ on the interval $[a, b]$. It can be verified that $h_4(a, b) > 0$ when $a = 1 + 0.0002i$ and $b = a + 0.0002$ for $i \in \{0, 1, \ldots, 3000\}$, as well as when $a = 1.6 + 0.01i$ and $b = a + 0.01$ for $i \in \{0, 1, \ldots, 6740\}$. Thus, $\frac{\mathrm{d}h}{\mathrm{d}t} \geq 0$ and $h(t) \geq h(1) = 0$ on the interval $[1, 69]$. When $t \geq 69$, $h(t) \geq h_1(69) + h_2(\infty) - 2 > 0$.

Hence, $g(\alpha, q) \geq h(t) \geq 0$ and $f(\alpha, q) = g(\alpha, q)(2 + q)^\alpha \geq 0$. ■

**Lemma 19.** *Let $f(x) = (x + q)^\alpha$. If $\alpha < 0$, $-1 < q \leq 0$ and $r \geq 4$, then*

$$f(1) + (2r - 2)f(r + 1) - (2r - 1)f(r) > 0.$$

*Proof.* Let $f(\alpha, q) = f(1) + (2r - 2)f(r + 1) - (2r - 1)f(r) = (1 + q)^\alpha + (2r - 2)(r + 1 + q)^\alpha - (2r - 1)(r + q)^\alpha$ and $g(\alpha, q) = \frac{f(\alpha, q)}{(r+q)^\alpha} = \left(\frac{1+q}{r+q}\right)^\alpha + (2r - 2)\left(\frac{r+1+q}{r+q}\right)^\alpha - (2r - 1)$. Firstly,

$$\frac{\partial g}{\partial q} = \frac{\alpha}{(r + q)^2} \left[(r - 1)\left(\frac{1 + q}{r + q}\right)^{\alpha-1} - (2r - 2)\left(\frac{r + 1 + q}{r + q}\right)^{\alpha-1}\right].$$

Since $\frac{(r-1)\left(\frac{1+q}{r+q}\right)^{\alpha-1}}{(2r-2)\left(\frac{r+1+q}{r+q}\right)^{\alpha-1}} = \frac{1}{2}\left(\frac{1+q}{r+1+q}\right)^{\alpha-1} \geq \frac{1}{2}\left(\frac{r+1+q}{1+q}\right) \geq \frac{1}{2}\left(1 + \frac{r}{1+q}\right) \geq \frac{1}{2}\left(1 + \frac{4}{1+0}\right) = \frac{5}{2} > 1$, $\frac{\partial g}{\partial q} < 0$. Thus, $g(\alpha, q) \geq g(\alpha, 0) = \left(\frac{1}{r}\right)^\alpha + (2r - 2)\left(\frac{r+1}{r}\right)^\alpha - (2r - 1)$.

We now prove that the partial derivative of $g(\alpha, 0)$ with respect to $\alpha$ is less than 0. Set $g_1(r) = (2r - 2)\ln(r + 1) - (2r - 1)\ln r$. Consider the derivative of $g_1(r)$ with respect to $r$, we have $\frac{\mathrm{d}g_1}{\mathrm{d}r} = 2\ln\frac{r+1}{r} + \frac{1-3r}{r(r+1)}$. Set $g_2(r) = \frac{3r-1}{2r(r+1)\ln\frac{r+1}{r}}$. Then $\frac{\mathrm{d}g_2}{\mathrm{d}r} = \frac{3r-1-\ln(1+\frac{1}{r})(3r^2-2r-1)}{2r^2\ln^2(1+\frac{1}{r})(r+1)^2}$. Since

$\frac{\ln(1+\frac{1}{r})(3r^2-2r-1)}{3r-1} = \ln(1+\frac{1}{r})^{\frac{(3r^2-2r-1)}{3r-1}} = \frac{(3r-1)(r-\frac{1}{3})-\frac{4}{3}}{3r-1}\ln(1+\frac{1}{r}) < r\cdot\ln(1+\frac{1}{r}) = \ln(1+\frac{1}{r})^r$, $(1+\frac{1}{r})^r$ is monotonically increasing in $(0,+\infty)$ and $\lim_{r\to+\infty}(1+\frac{1}{r})^r = \mathrm{e}$, $\frac{\ln(1+\frac{1}{r})(3r^2-2r-1)}{3r-1} < \ln(1+\frac{1}{r})^r < \ln\mathrm{e} = 1$. Thus, $\frac{\mathrm{d}g_2}{\mathrm{d}r} > 0$ and $g_2(r) \geq g_2(4) = \frac{11}{40\ln\frac{5}{4}} > 1$, it implies that $\frac{3r-1}{r(r+1)} > 2\ln\frac{r+1}{r}$ and $\frac{\mathrm{d}g_1}{\mathrm{d}r} = 2\ln\frac{r+1}{r} + \frac{1-3r}{r(r+1)} < 0$. Thus, $g_1(r) \leq g_1(4) = 6\ln(5) - 7\ln 4 < 0$ and $\frac{(2r-2)\ln\frac{r+1}{r}\cdot\left(\frac{r+1}{r}\right)^\alpha}{\ln r\cdot(\frac{1}{r})^\alpha} = \frac{(2r-2)\ln\frac{r+1}{r}}{\ln r}\cdot(r+1)^\alpha \leq \frac{(2r-2)(\ln(r+1)-\ln r)}{\ln r} = \frac{g_1(r)+\ln r}{\ln r} < 1$. Since $\frac{\partial g(\alpha,0)}{\partial\alpha} = (2r-2)\ln\frac{r+1}{r}\cdot\left(\frac{r+1}{r}\right)^\alpha - \ln r\cdot(\frac{1}{r})^\alpha$, $\frac{\partial g(\alpha,0)}{\partial\alpha} < 0$. Consequently, $g(\alpha,q) \geq g(\alpha,0) > g(0,0) = 1+(2r-2)-(2r-1) = 0$. Thus $f(\alpha,q) = g(\alpha,q)(r+q)^\alpha > 0$. ∎

**Lemma 20.** *Let $f(x) = (x+q)^\alpha$. If $\alpha < 0$ and $-1 < q \leq 0$, then*

$$f(1) - 2f(2) + f(4) > 0.$$

*Proof.* Let $f(\alpha,q) = f(1)-2f(2)+f(4) = (1+q)^\alpha - 2(2+q)^\alpha + (4+q)^\alpha$ and $g(\alpha,q) = \frac{f(\alpha,q)}{(2+q)^\alpha} = \left(\frac{1+q}{2+q}\right)^\alpha + \left(\frac{4+q}{2+q}\right)^\alpha - 2$. Firstly,

$$\frac{\partial g}{\partial q} = \frac{\alpha}{(2+q)^2}\left[\left(\frac{1+q}{2+q}\right)^{\alpha-1} - 2\left(\frac{4+q}{2+q}\right)^{\alpha-1}\right].$$

Since $\frac{\left(\frac{1+q}{2+q}\right)^{\alpha-1}}{2\left(\frac{4+q}{2+q}\right)^{\alpha-1}} = \frac{1}{2}\left(\frac{1+q}{4+q}\right)^{\alpha-1} \geq \frac{1}{2}\left(1-\frac{3}{4+q}\right)^{-1} \geq \frac{1}{2}\left(1-\frac{3}{4}\right)^{-1} = 2 > 1$, $\frac{\partial g}{\partial q} < 0$. Thus, $g(\alpha,q) \geq g(\alpha,0) = \left(\frac{1}{2}\right)^\alpha + 2^\alpha - 2$. Since $\frac{\mathrm{d}g(\alpha,0)}{\mathrm{d}\alpha} = \ln 2\cdot 2^\alpha - \ln 2\cdot(\frac{1}{2})^\alpha < 0$, $g(\alpha,q) \geq g(\alpha,0) > g(0,0) = 0$. Thus $f(\alpha,q) = g(\alpha,q)(2+q)^\alpha > 0$. ∎

**Lemma 21.** *Let $f(x) = (x+q)^\alpha$. If $\alpha < 0$ and $-1 < q \leq 0$, then*

$$f(1) + 2f(4) + f(5) - 4f(3) > 0.$$

*Proof.* Let $f(\alpha,q) = f(1)+2f(4)+f(5)-4f(3) = (1+q)^\alpha + 2(4+q)^\alpha + (5+q)^\alpha - 4(3+q)^\alpha$ and $f_1(\alpha,q) = \frac{f(\alpha,q)}{(3+q)^\alpha} = \left(\frac{1+q}{3+q}\right)^\alpha + 2\left(\frac{4+q}{3+q}\right)^\alpha + \left(\frac{5+q}{3+q}\right)^\alpha - 4$. Firstly, $\frac{\partial f_1}{\partial q} = \frac{\alpha}{(3+q)^2}\left[2\left(\frac{1+q}{3+q}\right)^{\alpha-1} - 2\left(\frac{4+q}{3+q}\right)^{\alpha-1} - 2\left(\frac{5+q}{3+q}\right)^{\alpha-1}\right]$. Set $f_2(\alpha,q) = 2\left(\frac{1+q}{3+q}\right)^{\alpha-1} - 2\left(\frac{4+q}{3+q}\right)^{\alpha-1} - 2\left(\frac{5+q}{3+q}\right)^{\alpha-1}$ and $f_3(\alpha,q) = \frac{f_2(\alpha,q)}{2\left(\frac{5+q}{3+q}\right)^{\alpha-1}}$

$= \left(\frac{1+q}{5+q}\right)^{\alpha-1} - \left(\frac{4+q}{5+q}\right)^{\alpha-1} - 1.$

Since $\frac{\partial f_3}{\partial q} = \frac{\alpha-1}{(5+q)^2}\left[4\left(\frac{1+q}{5+q}\right)^{\alpha-2} - \left(\frac{4+q}{5+q}\right)^{\alpha-2}\right]$ and $4\frac{\left(\frac{1+q}{5+q}\right)^{\alpha-2}}{\left(\frac{4+q}{5+q}\right)^{\alpha-2}} = 4\left(\frac{1+q}{4+q}\right)^{\alpha-2}$ $\geq 4\left(1-\frac{3}{4+q}\right)^{-2} \geq 4\left(1-\frac{3}{4}\right)^{-2} = 64 > 1$ , $\frac{\partial f_3}{\partial q} < 0$. Thus, $f_3(\alpha,q) \geq f_3(\alpha,0) = (\frac{1}{5})^{\alpha-1} - (\frac{4}{5})^{\alpha-1} - 1$. Since $\frac{\mathrm{d}f_3(\alpha,0)}{\mathrm{d}\alpha} = \ln\frac{5}{4}\cdot(\frac{4}{5})^{\alpha-1} - \ln 5\cdot(\frac{1}{5})^{\alpha-1}$ and $\frac{\ln\frac{5}{4}\cdot(\frac{4}{5})^{\alpha-1}}{\ln 5\cdot(\frac{1}{5})^{\alpha-1}} = \frac{\ln\frac{5}{4}}{\ln 5}\cdot 4^{\alpha-1} \leq \frac{\ln\frac{5}{4}}{\ln 5}\cdot 4^{-1} < 1$, $\frac{\mathrm{d}f_3(\alpha,0)}{\mathrm{d}\alpha} < 0$. Thus, $f_3(\alpha,q) \geq f_3(\alpha,0) > f_3(0,0) = 5 - \frac{5}{4} - 1 > 0$, $\frac{\partial f_1}{\partial q} = \frac{\alpha}{(3+q)^2}f_2(\alpha,q) = \frac{\alpha}{(3+q)^2}f_3(\alpha,q)\cdot 2\left(\frac{5+q}{3+q}\right)^{\alpha-1} < 0$ and $f_1(\alpha,q) \geq f_1(\alpha,0) = (\frac{1}{3})^\alpha + 2(\frac{4}{3})^\alpha + (\frac{5}{3})^\alpha - 4$.

Set $f_4(\alpha) = \frac{\mathrm{d}f_1(\alpha,0)}{\mathrm{d}\alpha}/(\frac{5}{3})^\alpha = \ln\frac{5}{3} + 2\ln\frac{4}{3}\cdot(\frac{4}{5})^\alpha - \ln 3\cdot(\frac{1}{5})^\alpha$. Since $\frac{\mathrm{d}f_4}{\mathrm{d}\alpha} = \ln 3\cdot\ln 5\cdot(\frac{1}{5})^\alpha - 2\ln\frac{4}{3}\cdot\ln\frac{5}{4}\cdot(\frac{4}{5})^\alpha$ and $\frac{\ln 3\cdot\ln 5\cdot(\frac{1}{5})^\alpha}{2\ln\frac{4}{3}\cdot\ln\frac{5}{4}\cdot(\frac{4}{5})^\alpha} = \frac{\ln 3\cdot\ln 5}{2\ln\frac{4}{3}\cdot\ln\frac{5}{4}}\cdot(\frac{1}{4})^\alpha \geq \frac{\ln 3\cdot\ln 5}{2\ln\frac{4}{3}\cdot\ln\frac{5}{4}}\cdot(\frac{1}{4})^0 > 1$, $\frac{\mathrm{d}f_4}{\mathrm{d}\alpha} > 0$. Consequently, $f_4(\alpha) < f_4(0) = \ln\frac{5}{3} + 2\ln\frac{4}{3} - \ln 3 < 0$ and $\frac{\mathrm{d}f_1(\alpha,0)}{\mathrm{d}\alpha} = f_4(\alpha)(\frac{5}{3})^\alpha < 0$. Thus, $f_1(\alpha,q) \geq f_1(\alpha,0) > f_1(0,0) = 0$ and $f(\alpha,q) = f_1(\alpha,q)(3+q)^\alpha > 0$. ∎

**Lemma 22.** *Let $f(x) = (x+q)^\alpha$. If $\alpha \leq -t$, $0 < q \leq 1.413t + 0.587$ and $t \geq 1$, then*

$$f(0) + 2f(2) - 3f(1) \geq 0.$$

*Proof.* Let $f(\alpha,q) = f(0) + 2f(2) - 3f(1) = q^\alpha + 2(2+q)^\alpha - 3(1+q)^\alpha$ and $g(\alpha,q) = \frac{f(\alpha,q)}{(1+q)^\alpha} = \left(\frac{q}{1+q}\right)^\alpha + 2\left(\frac{2+q}{1+q}\right)^\alpha - 3$. Firstly,

$$\frac{\partial g}{\partial q} = \frac{\alpha}{(1+q)^2}\left[\left(\frac{q}{1+q}\right)^{\alpha-1} - 2\left(\frac{2+q}{1+q}\right)^{\alpha-1}\right].$$

Let $g_1(t) = (t+1)\ln\left(\frac{1.413t+2.587}{1.413t+0.587}\right) - \ln 2$. According to Lemma 10, since $2\times 1.413^2 - 1.413\times 2.587 - 1.413\times 0.587 < 0$, $1.413\times 2.587 + 1.413\times 0.587 - 2\times 2.587\times 0.587 > 0$ and $\frac{\mathrm{d}g_1}{\mathrm{d}t} > 0$ has a unique root $t_1$ on the interval $(1,\infty)$, where $t_1 \approx 1.625$, it follows that $g_1(t) \geq g_1(t_1) \approx 0.69 > 0$. Thus, $\frac{\left(\frac{q}{1+q}\right)^{\alpha-1}}{2\left(\frac{2+q}{1+q}\right)^{\alpha-1}} = \frac{1}{2}\left(\frac{q}{2+q}\right)^{\alpha-1} \geq \frac{1}{2}\left(\frac{2+q}{q}\right)^{t+1} \geq \frac{1}{2}\left(\frac{1.413t+2.587}{1.413t+0.587}\right)^{t+1} > 1$ and $\frac{\partial g}{\partial q} < 0$.

We now prove that the partial derivative of the function $g(\alpha,q)$ with respect to $\alpha$ is less than or equal to 0. By Lemmas 8 and 11, $\frac{2\ln\left(\frac{1.413t+2.587}{1.413t+1.587}\right)}{\ln\left(\frac{1.413t+1.587}{1.413t+0.587}\right)}\left(\frac{1.413t+0.587}{1.413t+2.587}\right)^t \leq 1$ and $\frac{\ln\left(\frac{q+2}{q+1}\right)}{\ln\left(\frac{q+1}{q}\right)}$ is monotonically increasing with respect to $q$, we have

$$\frac{2\ln\left(\frac{q+2}{q+1}\right)\left(\frac{q+2}{q+1}\right)^a}{\ln\left(\frac{q+1}{q}\right)\left(\frac{q}{q+1}\right)^a} \leq \frac{2\ln\left(\frac{q+2}{q+1}\right)}{\ln\left(\frac{q+1}{q}\right)}\left(\frac{q}{q+2}\right)^t \leq \frac{2\ln\left(\frac{1.413t+2.587}{1.413t+1.587}\right)}{\ln\left(\frac{1.413t+1.587}{1.413t+0.587}\right)}\left(\frac{1.413t+0.587}{1.413t+2.587}\right)^t \leq 1.$$

Since $\frac{\partial g}{\partial \alpha} = 2\ln\left(\frac{q+2}{q+1}\right)\left(\frac{q+2}{q+1}\right)^a - \ln\left(\frac{q+1}{q}\right)\left(\frac{q}{q+1}\right)^a \leq 0$, $\frac{\partial g}{\partial \alpha} \leq 0$.

Since $\frac{\partial g}{\partial q} \leq 0$ and $\frac{\partial g}{\partial \alpha} \leq 0$, $g(\alpha, q) \geq g(-t, 1.413t + 0.587) = h_1(t) + 2h_2(t) - 3$, where $h_1(t) = \left(\frac{1.413t+1.587}{1.413t+0.587}\right)^t$ and $h_2(t) = \left(\frac{1.413t+1.587}{1.413t+2.587}\right)^t$. Let $h_3(t) = t\ln\left(\frac{1.413t+1.587}{1.413t+0.587}\right)$ and $h(t) = h_1(t) + 2h_2(t) - 3$. By Lemma 9, we have $h_2(t)$ and $\frac{dh_3}{dt}$ are positive and monotonically decreasing on the interval $[1, \infty)$. On the interval $[1, \infty)$, $h_1(t)$ and $h_3(t)$ are positive monotonically increasing functions, while $\frac{dh_2}{dt}$ is a negative monotonically increasing function. For two constants $a$ and $b$, let $h_4(a, b) = e^{h_3(a)} \left.\frac{dh_3}{dt}\right|_{t=b} + 2\left.\frac{dh_2}{dt}\right|_{t=a}$, where $1 \leq a \leq b$. When $t \in [a, b]$, $\frac{dh}{dt} = e^{h_3(t)}\frac{dh_3}{dt} + 2\frac{dh_2}{dt} \geq h_4(a, b)$. If $h_4(a, b) \geq 0$, then $\frac{dh}{dt} \geq 0$ on the interval $[a, b]$. It can be verified that $h_4(a, b) > 0$ when $a = 1 + 0.0001i$ and $b = a + 0.0001$ for $i \in \{0, 1, \ldots, 6000\}$, as well as when $a = 1.6 + 0.01i$ and $b = a + 0.01$ for $i \in \{0, 1, \ldots, 7240\}$. Thus, $\frac{dh}{dt} \geq 0$ and $h(t) \geq h(1) = 0$ on the interval $[1, 74]$. When $t \geq 74$, $h(t) = h_1(t) + 2h_2(t) - 3 \geq h_1(74) + 2h_2(\infty) - 3 > 0$.

Hence, $g(\alpha, q) \geq h(t) \geq 0$ and $f(\alpha, q) = g(\alpha, q)(1 + q)^\alpha \geq 0$. ■

**Lemma 23.** *Let $f(x) = (x + q)^\alpha$. If $\alpha \leq -t$, $0 < q \leq 1.413t + 0.587$ and $t \geq 1$, then*

$$f(0) - f(1) - 2f(2) + 2f(3) > 0.$$

*Proof.* Let $f(\alpha, q) = f(0) - f(1) - 2f(2) + 2f(3) = q^\alpha - (1 + q)^\alpha - 2(2 + q)^\alpha + 2(3 + q)^\alpha$ and $f_1(\alpha, q) = \frac{f(\alpha,q)}{q^\alpha} = 1 - \left(\frac{1+q}{q}\right)^\alpha - 2\left(\frac{2+q}{q}\right)^\alpha + 2\left(\frac{3+q}{q}\right)^\alpha$. Firstly,

$$\frac{\partial f_1}{\partial q} = \frac{\alpha}{q^2}\left[-6\left(\frac{3+q}{q}\right)^{\alpha-1} + \left(\frac{1+q}{q}\right)^{\alpha-1} + 4\left(\frac{2+q}{q}\right)^{\alpha-1}\right].$$

Let $f_2(\alpha, q) = -6\left(\frac{3+q}{q}\right)^{\alpha-1} + \left(\frac{1+q}{q}\right)^{\alpha-1} + 4\left(\frac{2+q}{q}\right)^{\alpha-1}$ and $f_3(\alpha, q) = \frac{f_2(\alpha,q)}{\left(\frac{3+q}{q}\right)^{\alpha-1}} = \left(\frac{1+q}{3+q}\right)^{\alpha-1} + 4\left(\frac{2+q}{3+q}\right)^{\alpha-1} - 6.$

Since $\frac{\partial f_3}{\partial q} = \frac{\alpha-1}{(3+q)^2}\left[4\left(\frac{2+q}{3+q}\right)^{\alpha-2} + 2\left(\frac{1+q}{3+q}\right)^{\alpha-2}\right] < 0$ and $\frac{\partial f_3}{\partial \alpha} = \ln\left(\frac{1+q}{3+q}\right)\left(\frac{1+q}{3+q}\right)^{\alpha-1} + 4\ln\left(\frac{2+q}{3+q}\right)\left(\frac{2+q}{3+q}\right)^{\alpha-1} < 0$, $f_3(\alpha,q) \geq f_3(-t, 1.413t+0.587) = e^{h_1(t)} + 4e^{h_2(t)} - 6$, where $h_1(t) = (t+1)\ln\left(\frac{1.413t+3.587}{1.413t+1.587}\right)$ and $h_2(t) = (t+1)\ln\left(\frac{1.413t+3.587}{1.413t+2.587}\right)$. According to Lemma 10, since $2\times 1.413^2 - 1.413\times 3.587 - 1.413\times 1.587 < 0$, $1.413\times 3.587 + 1.413\times 1.587 - 2\times 3.587\times 1.587 < 0$, $2\times 1.413^2 - 1.413\times 3.587 - 1.413\times 2.587 < 0$ and $1.413\times 3.587 + 1.413\times 2.587 - 2\times 3.587\times 2.587 < 0$, it follows that $h_1(t) \geq h_1(1)$ and $h_2(t) \geq h_2(1)$. Thus, $f_3(\alpha,q) \geq e^{h_1(t)} + 4e^{h_2(t)} - 6 \geq e^{h_1(1)} + 4e^{h_2(1)} - 6 = \frac{109}{36} > 0$. Since $\frac{\partial f_1}{\partial q} = \frac{\alpha}{q^2} f_2(\alpha,q) = \frac{\alpha}{q^2} f_3(\alpha,q)\cdot\left(\frac{3+q}{q}\right)^{\alpha-1}$, $\frac{\partial f_1}{\partial q} < 0$.

The partial derivative of $f_1(\alpha,q)$ with respect to $\alpha$ is given by: $\frac{\partial f_1}{\partial \alpha} = 2\ln\left(\frac{3+q}{q}\right)\left(\frac{3+q}{q}\right)^{\alpha} - 2\ln\left(\frac{2+q}{q}\right)\left(\frac{2+q}{q}\right)^{\alpha} - \ln\left(\frac{1+q}{q}\right)\left(\frac{1+q}{q}\right)^{\alpha}$. Set $f_4(\alpha,q) = \frac{\frac{\partial f_1}{\partial \alpha}}{\left(\frac{3+q}{q}\right)^{\alpha}} = 2\ln\left(\frac{3+q}{q}\right) - 2\ln\left(\frac{2+q}{q}\right)\left(\frac{2+q}{3+q}\right)^{\alpha} - \ln\left(\frac{1+q}{q}\right)\left(\frac{1+q}{3+q}\right)^{\alpha}$. Then $\frac{\partial f_4}{\partial \alpha} = 2\ln\left(\frac{2+q}{q}\right)\ln\left(\frac{3+q}{2+q}\right)\left(\frac{2+q}{3+q}\right)^{\alpha} + \ln\left(\frac{1+q}{q}\right)\ln\left(\frac{3+q}{1+q}\right)\left(\frac{1+q}{3+q}\right)^{\alpha} > 0$ and $\frac{\partial f_4}{\partial q} = \frac{\left(\frac{q+1}{q+3}\right)^a}{q(q+1)} - \frac{6}{q(q+3)} + \frac{4\left(\frac{q+2}{q+3}\right)^a}{q(q+2)} - \frac{2a\ln\left(\frac{q+1}{q}\right)\left(\frac{q+1}{q+3}\right)^a}{q^2+4q+3} - \frac{2a\ln\left(\frac{q+2}{q}\right)\left(\frac{q+2}{q+3}\right)^a}{q^2+5q+6} \geq \frac{1}{q(q+3)}\left(\left(\frac{q+1}{q+3}\right)^a + 4\left(\frac{q+2}{q+3}\right)^a - 6\right) \geq \frac{1}{q(q+3)}\left(\left(\frac{q+3}{q+1}\right)^t + 4\left(\frac{q+3}{q+2}\right)^t - 6\right)$ $\geq \frac{1}{q(q+3)}\left(g_1(t) + 4g_2(t) - 6\right)$, where $g_1(t) = \left(\frac{1.413t+3.587}{1.413t+1.587}\right)^t$ and $g_2(t) = \left(\frac{1.413t+3.587}{1.413t+2.587}\right)^t$. By Lemma 9, $g_1(t)$ and $g_2(t)$ are both monotonically increasing. Thus, $g_1(t) + 4g_2(t) - 6 \geq g_1(1) + 4g_2(1) - 6 = \frac{2}{3} > 0$ and $\frac{\partial f_4}{\partial q} \geq \frac{1}{q(q+3)}\left(g_1(t) + 4g_2(t) - 6\right) > 0$.

Let $g_3(t) = 2\ln\left(\frac{1.413t+3.587}{1.413t+0.587}\right) - 2\ln\left(\frac{1.413t+2.587}{1.413t+0.587}\right)\left(\frac{1.413t+3.587}{1.413t+2.587}\right)^t$, $g_4(t) = \ln\left(\frac{1.413t+1.587}{1.413t+0.587}\right)\left(\frac{1.413t+3.587}{1.413t+1.587}\right)^t$, $g_5(t) = \ln\left(\frac{1.413t+3.587}{1.413t+0.587}\right)$, $g_6(t) = \ln\left(\frac{1.413t+2.587}{1.413t+0.587}\right)$, $g_7(t) = \left(\frac{1.413t+3.587}{1.413t+2.587}\right)^t$, $g_8(t) = \ln\left(\frac{1.413t+1.587}{1.413t+0.587}\right)$, $g_9(t) = \left(\frac{1.413t+3.587}{1.413t+1.587}\right)^t$ and $g_{10}(t) = \frac{g_6(t)}{g_5(t)} = \frac{\ln\left(\frac{1.413t+2.587}{1.413t+0.587}\right)}{\ln\left(\frac{1.413t+3.587}{1.413t+0.587}\right)}$. By Lemmas 8 and 9, $\lim_{t\to+\infty} g_{10}(t) = \frac{2}{3}$, $g_5(t)$, $g_6(t)$, $g_7(t)$, $g_8(t)$, $g_9(t)$ and $g_{10}(t)$ are all positive functions, where $g_7(t)$ and $g_9(t)$ are monotonically increasing while the others are monotonically decreasing. For two constants $a$ and $b$, let $g_{11}(a,b) = 2g_5(a) - 2g_6(b)g_7(a) - g_8(b)g_9(a)$, where $1 \leq a \leq b$. When

$t \in [a,b]$, $g_3(t) - g_4(t) = 2g_5(t) - 2g_6(t)g_7(t) - g_8(t)g_9(t) \leq g_{11}(a,b)$. If $g_{11}(a,b) \leq 0$, then $g_3(t) - g_4(t) \leq 0$ on the interval $[a,b]$. It can be verified that $g_{11}(a,b) < 0$ when $a = 1 + 0.5i$ and $b = a + 0.5$ for $i \in \{0,1,2,3\}$. Thus, $g_3(t) - g_4(t) < 0$ on the interval $[1,3]$. When $t \geq 3$, $\frac{g_6(t)g_7(t)}{g_5(t)} = g_7(t)g_{10}(t) \geq g_7(3)g_{10}(\infty) = \frac{2}{3}g_7(3) > 1$, $g_3(t) < 0$ and $g_3(t) - g_4(t) < 0$.
Since $\frac{\partial f_4}{\partial q} > 0$ and $\frac{\partial f_4}{\partial \alpha} > 0$, $f_4(\alpha,q) \leq f_4(-t, 1.413t + 0.587) = g_3(t) - g_4(t) < 0$ and $\frac{\partial f_1}{\partial \alpha} = f_4(\alpha,q)(\frac{3+q}{q})^{\alpha} < 0$.

Since $\frac{\partial f_1}{\partial q} < 0$ and $\frac{\partial f_1}{\partial \alpha} < 0$, $f_1(\alpha,q) \geq f_1(-t, 1.413t + 0.587) = 1 - g_{12}(t) - 2g_{13}(t) + 2g_{14}(t)$, where $g_{12}(t) = \left(\frac{1.413t+0.587}{1.413t+1.587}\right)^t$, $g_{13}(t) = \left(\frac{1.413t+0.587}{1.413t+2.587}\right)^t$ and $g_{14}(t) = \left(\frac{1.413t+0.587}{1.413t+3.587}\right)^t$. By Lemma 9, $\lim\limits_{t\to+\infty} g_{14}(t) = e^{\frac{-3}{1.413}}$, the functions $g_{12}(t)$, $g_{13}(t)$ and $g_{14}(t)$ are all monotonically decreasing. For two constants $a$ and $b$, let $g_{15}(a,b) = 1 - g_{12}(a) - 2g_{13}(a) + 2g_{14}(b)$, where $1 \leq a \leq b$. When $t \in [a,b]$, $1 - g_{12}(t) - 2g_{13}(t) + 2g_{14}(t) \geq g_{15}(a,b)$. If $g_{15}(a,b) \geq 0$, then $1 - g_{12}(t) - 2g_{13}(t) + 2g_{14}(t) \geq 0$ on the interval $[a,b]$. It can be verified that $g_{15}(a,b) > 0$ when $a = 1 + 0.4i$ and $b = a + 0.4$ for $i \in \{0,1,\ldots,7\}$. Thus, $1 - g_{12}(t) - 2g_{13}(t) + 2g_{14}(t) > 0$ on the interval $[1,4]$. When $t \geq 4$, $1 - g_{12}(t) - 2g_{13}(t) + 2g_{14}(t) \geq 1 - g_{12}(4) - 2g_{13}(4) + 2g_{14}(\infty) > 0$, so the function $1 - g_{12}(t) - 2g_{13}(t) + 2g_{14}(t) > 0$ on the interval $[1,+\infty)$.

Thus, $f_1(\alpha,q) \geq 1 - g_{12}(t) - 2g_{13}(t) + 2g_{14}(t) > 0$ and $f(\alpha,q) = f_1(\alpha,q)q^{\alpha} > 0$. ■

***Acknowledgment*:** The research was supported by NSFC (No. 12061073).

# References

[1] A. Ali, D. Dimitrov, Z. Du, F. Ishfaq, On the extremal graphs for general sum-connectivity index ($\chi_\alpha$) with given cyclomatic number when $\alpha > 1$, *Discr. Appl. Math.* **257** (2019) 19–30.

[2] A. Ali, I. Gutman, E. Milovanović, I. Milovanović, Sum of powers of the degrees of graphs: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **80** (2018) 5–84.

[3] A. Ali, I. Gutman, H. Saber, A. M. Alanazi, On bond incident degree indices of $(n, m)$-graphs, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 89–96.

[4] M. Aouchiche, F. K. Bell, D. Cvetković, P. Hansen, P. Rowlinson, S. K. Simić, D. Stevanović, Variable neighborhood search for extremal graphs. 16. Some conjectures related to the largest eigenvalue of a graph, *Eur. J. Oper. Res.* **191** (2008) 661–676.

[5] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, London, 2008.

[6] Y. Caro, New results on the independence number, *Tech. Report*, Tel-Aviv Univ., 1979.

[7] X. Cheng, X. Li, Some bounds for the vertex degree function index of connected graphs with given minimum and maximum degrees, *MATCH Commun. Math. Comput. Chem.* **90** (2023) 175–186.

[8] S. Fajtlowicz, On conjectures of graffiti II, *Congr. Num.* **60** (1987) 189–197.

[9] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total $\pi$-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[10] L. H. Hall, L. B. Kier, The nature of structure-activity relationships and their relation to molecular connectivity, *Eur. J. Med. Chem.* **12** (1977) 307–312.

[11] Z. Hu, X. Li, D. Peng, Graphs with minimum vertex-degree function-index for convex functions, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 521–533.

[12] Y. Hu, X. Li, Y. Shi, T. Xu, Connected $(n, m)$-graphs with minimum and maximum zeroth-order general Randić index, *Discr. Appl. Math.* **155** (2007) 1044–1054.

[13] Y. Hu, X. Li, Y. Shi, T. Xu, I. Gutman, On molecular graphs with smallest and greatest zeroth-order general Randić index, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 425–434.

[14] X. Li, Y. Shi, $(n, m)$-graphs with maximum zeroth-order general Randić index for $\alpha \in (-1, 0)$, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 163–170.

[15] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 195–208.

[16] L. Pavlović, Maximal value of the zeroth-order Randić index, *Discr. Appl. Math.* **127** (2003) 615–626.

[17] L. Pavlović, M. Lazić, T. Aleksić, More on "Connected $(n, m)$-graphs with minimum and maximum zeroth-order general Randić index", *Discr. Appl. Math.* **157** (2009) 2938–2944.

[18] I. Tomescu, Graphs with given cyclomatic number extremal relatively to vertex degree function index for convex functions, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 109–114.

[19] I. Tomescu, Properties of connected $(n, m)$-graphs extremal relatively to vertex degree function index for convex functions, *MATCH Commun. Math. Comput. Chem.* **85** (2021) 285–294.

[20] V. K. Wei, A lower bound on the stability number of a simple graph, *Bell Laboratories Technical Memorandum*, 81-11217-9, Murray Hill, 1981.

[21] Y. Yao, M. Liu, F. Belardo, C. Yang, Unified extremal results of topological indices and spectral invariants of graphs, *Discr. Appl. Math.* **271** (2019) 218–232.

[22] Y. Yao, M. Liu, X. Gu, Unified extremal results for vertex-degree-based graph invariants with given diameter, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 699–714.