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Extremal vertex-degree function index of trees with some given parameters

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Abstract. For a graph G, the vertex-degree function index of G is defined as $H_f(G) = \sum_{u \in V(G)} f(deg_G(u))$, where $deg_G(u)$ stands for the degree of vertex u in G and $f(x)$ is a function defined on positive real numbers. In this article, we determine the extremal values of the vertex-degree function index of trees with given number of pendent vertices/segments/branching vertices/maximum degree vertices and with a perfect matching when $f(x)$ is strictly convex (resp. concave). Moreover, we use the results directly to some famous topological indices which belong to the type of vertex-degree function index, such as the zeroth-order general Randić index, sum lordeg index, variable sum exdeg index, Lanzhou index, first and second multiplicative Zagreb indices.

1. Introduction

In this article, just simple connected graphs are taken into account. For such a graph G, we represent the sets of vertices and edges by $V(G)$ and $E(G)$, respectively. Let $deg_G(x)$ be the degree of $x \in V(G)$ and $\Delta(G)$ (Δ for short) be the maximum degree of G. A vertex of degree one is called a pendent vertex. Let $G - xy$ and $G + xy$ be the graphs gotten from G by deleting the edge $xy \in E(G)$ and by adding an edge $xy \notin E(G)$ ($x, y \in V(G)$), respectively. Denoted by $N_G(y)$ the set of neighborhoods of a vertex $y \in V(G)$ and n_i the number of vertices with degree i in G. As usual, we use S_n and P_n to denote the n-vertex star and n-vertex path, respectively.

It is obvious that an n-vertex tree has the degree sequence $(deg_1, deg_2, \cdots, deg_n)$ which is arranged in a non-increasing order if and only if $\sum_{i=1}^{n} deg_i = 2(n-1)$. The segment of a tree T (see [7]) is a path-subtree S whose terminal vertices are branching vertices or pendent vertices of T, that is, each internal vertex u of S has $deg_T(u) = 2$. The squeeze $S(T)$ of a tree T, as in [18], is the tree gotten from T by replacing every segment of T by an edge. A tree is called a caterpillar if the removal of all pendent vertices results in a path. In a tree T, the edge rotating capacity of vertex $x \in V(T)$ with $2 \le deg_T(x) \le \Delta - 1$ is defined as $deg_T(x) - 1$. The sum of the edge rotating capacities of all vertices with $2 \le deg_T(x) \le \Delta - 1$ in T is called the total edge rotating capacity of T. Let us denote by $\boldsymbol{PT}_{n,p}$, $\boldsymbol{ST}_{n,s}$, $\boldsymbol{BT}_{n,b}$, $\boldsymbol{DT}_{n,k}$ and $\boldsymbol{MT}_{2m}$ the set of the n-vertex trees with p

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pendent vertices, n-vertex trees with s segments, n-vertex trees with b branching vertices, n-vertex trees with k maximum degree vertices and $2m$-vertex trees with a perfect matching, respectively. For terminologies and notations, not defined here, we refer the readers to relevant standard book [4].

The zeroth-order general Randić index of a graph G (denoted by ${}^0R_\alpha(G)$) [15, 17] was defined as ${}^0R_\alpha(G) = \sum_{u\in V(G)} deg_G(u)^\alpha$ for any real number $\alpha \neq 0, 1$. If $\alpha = 2$ and $\alpha = 3$, it is the first Zagreb index $M_1(G)$ [9] and the forgotten topological index $F(G)$ [8]. Lately, De et al. [6], Khaksari et al. [13] and Vukicević et al. [25] independently introduced the following degree-based topological index, which is known as the Lanzhou index, and it is defined as $Lz(G) = \sum_{u\in V(G)} deg_{\overline{G}}(u)deg_G(u)^2 = (n-1)M_1(G) - F(G)$, where $\overline{G}$ is the complement of G and n is order of G. For the recent papers on Lanzhou index, we refer the readers to [3, 14], etc.

The sum lordeg index $SL(G)$ and variable sum exdeg index $SEI_a(G)$ are two of the Adriatic indices proposed in [24] and they are defined as $SL(G) = \sum_{u\in V(G)} deg_G(u)\sqrt{\ln deg_G(u)} = \sum_{u\in V(G): deg_G(u)\geq 2} deg_G(u)\sqrt{\ln deg_G(u)}$ and $SEI_a(G) = \sum_{u\in V(G)} deg_G(u)a^{deg_G(u)}$ ($a > 0$ and $a \neq 1$), respectively.

For a graph G, the first and second multiplicative Zagreb indices $\Pi_1(G)$ and $\Pi_2(G)$ [12] are defined as $\Pi_1(G) = \prod_{u\in V(G)} deg_G(u)^2$ and $\Pi_2(G) = \prod_{uv\in E(G)} deg_G(u)deg_G(v) = \prod_{u\in V(G)} deg_G(u)^{deg_G(u)}$, respectively. Notice that $\Pi_1(G)$ and $\Pi_2(G)$ are maximum (minimum) if and only if $\ln \Pi_1(G) = 2\sum_{u\in V(G)} \ln deg_G(u)$ and $\ln \Pi_2(G) = \sum_{u\in V(G)} deg_G(u) \ln deg_G(u)$ is maximum (minimum), respectively.

In recent years, seeking extremal values of topological indices of graphs is one of the hot topics in chemical graph theory. To find a family of extremal graphs, Linial and Rozenman [19] introduced the vertex-degree function index H_f of a graph G as:

$$H_f(G) = \sum_{u\in V(G)} f(deg_G(u)), \tag{1}$$

where the function $f(x)$ depends on positive real numbers. Tomescu [20] obtained the the minimum (resp. maximum) H_f of trees and unicyclic graphs with given order and independence number when $f(x)$ is strictly convex (resp. concave). Ali et al [2], Tomescu [22], Xu and Wu [26] study the properties of H_f on (n, m)-graphs (graphs with n vertices and m edges), furthermore, they also identify some (n, m)-graphs with extremal values of H_f. Other results on H_f can be found in [1, 10, 11, 16, 21, 27, 28].

In this paper, the extremal values of the vertex-degree function index of trees with given number of pendent vertices/segments/branching vertices/maximum degree vertices and with a perfect matching are determined when $f(x)$ is a strictly convex (resp. concave) function. Moreover, the results can be applied directly to some famous topological indices that belong to the type of vertex-degree function index, such as the zeroth-order general Randić index, sum lordeg index, variable sum exdeg index, first and second multiplicative Zagreb indices.

2. Preliminary results

Lemma 2.1. *[20] For $x_1 \geq x_2 + 2 > 2$, if $f(x)$ is a strictly convex function, then*

$$f(x_1) + f(x_2) > f(x_1 - 1) + f(x_2 + 1).$$

This inequality should be reversed when $f(x)$ is strictly concave.

Lemma 2.2. *[10, 11] Let T be an n-vertex tree. If $f(x)$ is a strictly convex function, then $H_f(T) \leq (n-1)f(1) + f(n-1)$ with equality if and only if $T \cong S_n$.*

Lemma 2.3. *[10] Let T be an n-vertex tree. If $f(x)$ is a strictly convex function. Then $H_f(T) \geq (n-2)f(2) + 2f(1)$ with equality if and only if $T \cong P_n$.*

3. Trees with given number of pendent vertices

Theorem 3.1. *Let* $T \in \boldsymbol{PT}_{n,p}$ *and the function* $f(x)$ *be strictly convex, where* $2 \le p \le n-1$. *Then*

$$H_f(T) \ge [n-(r-1)(n-p)-2]f(r+1) + [(r-1)(n-p)-p+2]f(r) + pf(1).$$

Equality occurs only if the degree sequence of T *is* $(\underbrace{r+1,\cdots,r+1}_{n-(r-1)(n-p)-2}, \underbrace{r,\cdots,r}_{(r-1)(n-p)-p+2}, \underbrace{1,\cdots,1}_{p})$, *where* $r = \lfloor \frac{n-2}{n-p} \rfloor + 1$.

Proof. Choose $T \in \boldsymbol{PT}_{n,p}$ such that $H_f(T)$ is minimum.
Claim 1 If $x, y \in V(T)$ with $deg_T(x), deg_T(y) \ge 2$, then $|deg_T(x) - deg_T(y)| \le 1$.

To the contrary we assume that there exist two vertices, say x and y, such that $|deg_T(x) - deg_T(y)| \ge 2$. We suppose, without loss of generality, that $deg_T(x) = d_1 \ge deg_T(y) + 2 = d_2 + 2$. Let z be a neighbor of x which is not contained in the path from x to y in T. Let $T_1 = T - xz + yz$. Then $T_1 \in \boldsymbol{PT}_{n,p}$. By (1) and Lemma 2.1, one has

$$H_f(T_1) - H_f(T) = f(d_1 - 1) + f(d_2 + 1) - f(d_1) - f(d_2) < 0.$$

Hence, $H_f(T_1) < H_f(T)$, which contradicts the choice of T.

By Claim 1, it follows that the vertices in T have degree 1, r or $r+1$, where $r \ge 2$. Therefore, $p+n_r+n_{r+1} = n$, and $n_r \le n-p$. Since $p < n$, then $n_r \ge 1$. Furthermore, for a tree T, $p + rn_r + (r+1)n_{r+1} = 2(n-1)$ and we deduce that $n_r + pr = rn - (n-2)$. So $r = \frac{n-2}{n-p} + \frac{n_r}{n-p}$. Since $n_r \le n-p$, it follows that $r = \lfloor \frac{n-2}{n-p} \rfloor + 1$ and $n_{r+1} = n - (n-p)\lfloor \frac{n-2}{n-p} \rfloor - 2$, $n_r = (n-p)\lfloor \frac{n-2}{n-p} \rfloor - p + 2$. Thus the degree sequence of T is $(\underbrace{r+1,\cdots,r+1}_{n-(n-p)(r-1)-2}, \underbrace{r,\cdots,r}_{(n-p)(r-1)-p+2}, \underbrace{1,\cdots,1}_{p})$, where $r = \lfloor \frac{n-2}{n-p} \rfloor + 1$. □

Theorem 3.2. *Let* $T \in \boldsymbol{PT}_{n,p}$ *and* $f(x)$ *be strictly convex, where* $2 \le p \le n-1$. *Then*

$$H_f(T) \le pf(1) + (n-p-1)f(2) + f(p).$$

Equality occurs only if the degree sequence of T *is* $(p, \underbrace{2,\cdots,2}_{n-p-1}, \underbrace{1,\cdots,1}_{p})$.

Proof. Pick $T \in \boldsymbol{PT}_{n,p}$ such that $H_f(T)$ is maximum.
Claim 2 T contains at most one vertex $w \in V(T)$ with $deg_T(w) \ge 3$.

On the contrary, we assume that there exist two vertices, say x and y, such that $deg_T(x) = d_1 \ge deg_T(y) = d_2 \ge 3$. Let $z \in N_T(y)$ which is not contained in the path from y to x in T. Let $T_2 = T - yz + xz$. Then $T_2 \in \boldsymbol{PT}_{n,p}$. By (1) and Lemma 2.1, one has

$$H_f(T_2) - H_f(T) = f(d_1 + 1) + f(d_2 - 1) - f(d_1) - f(d_2) > 0.$$

So $H_f(T_2) > H_f(T)$, which is a contradiction with the choice of T.

By Claim 2, it follows that there exist a vertex w with $deg_T(w) = r \ge 3$, p vertices with degree 1 and $n-p-1$ vertices with degree 2 in T. Since $\sum_{v \in V(T)} deg_T(v) = p + 2(n-p-1) + r = 2(n-1)$, we deduce that $r = p$. Hence the degree sequence of T is $(p, \underbrace{2,\cdots,2}_{n-p-1}, \underbrace{1,\cdots,1}_{p})$. □

4. Trees with given number of segments

Let $T \in \boldsymbol{ST}_{n,s}$. The star S_n is the unique tree with $n-1$ segments, the path P_n is the only tree with 1 segment and there is no tree T with 2 segments. Thus, we always assume that $3 \le s \le n-2$.

Lemma 4.1. *[23] Let $T \in \boldsymbol{ST}_{n,s}$. Then there is one caterpillar $T' \in \boldsymbol{ST}_{n,s}$ such that T and T' have the same degree sequence.*

Theorem 4.1. *Let $T \in \boldsymbol{ST}_{n,s}$ and $f(x)$ be strictly convex, where $3 \le s \le n-2$. Then*

$$H_f(T) \ge \begin{cases} \frac{s-1}{2} f(3) + (n-s-1) f(2) + \frac{s+3}{2} f(1) & \text{if } s \text{ is odd,} \\ f(4) + \frac{s-4}{2} f(3) + (n-s-1) f(2) + \frac{s+4}{2} f(1) & \text{if } s \text{ is even.} \end{cases}$$

The equality occurs if and only if the degree sequence of T is $(\underbrace{3,\cdots,3}_{\frac{s-1}{2}},\underbrace{2,\cdots,2}_{n-s-1},\underbrace{1,\cdots,1}_{\frac{s+3}{2}})$ for odd s and $(4,\underbrace{3,\cdots,3}_{\frac{s-4}{2}},\underbrace{2,\cdots,2}_{n-s-1},\underbrace{1,\cdots,1}_{\frac{s+4}{2}})$ for even s.

Proof. Choose $T \in \boldsymbol{ST}_{n,s}$ such that T has the smallest H_f. In view of Lemma 4.1, there is a caterpillar $T' \in \boldsymbol{ST}_{n,s}$ such that T and T' have the same degree sequence. So $H_f(T) = H_f(T')$. Next, we prove two claims.

Claim 1. For each vertex $u \in V(T')$, $deg_{T'}(u) \le 4$.

Contrarily, we assume that there is a vertex, say x, such that $deg_{T'}(x) = d \ge 5$ in T'. Suppose $x_1, x_2, x_3 \in N_{T'}(x)$ are three pendent vertices. Let $T_1 = T' - \{xx_2, xx_3\} + \{x_1x_2, x_1x_3\}$. It is easy to see that $T_1 \in \boldsymbol{ST}_{n,s}$. By (1) and Lagrange mean value theorem, we have

$$\begin{aligned} H_f(T) - H_f(T_1) &= H_f(T') - H_f(T_1) \\ &= f(d) - f(d-2) - [f(3) - f(1)] \\ &= f'(\xi) - f'(\eta) > 0 \end{aligned}$$

since $f(x)$ is a strictly convex function, where $3 \le d-2 < \xi < d$, $1 < \eta < 3$. Thus $H_f(T) > H_f(T_1)$, which is a contradiction to the choice of T.

Claim 2. There exists at most one vertex v with $deg_{T'}(v) = 4$ in T'.

On the contrary, we suppose that in T', there exist two vertices, say x, y, with $deg_{T'}(x) = deg_{T'}(y) = 4$. Let $x_1 \in N_{T'}(x)$ and $y_1 \in N_{T'}(y)$ be two pendent vertices and z be any other pendent vertex of T'. Let $T_2 = T' - \{xx_1, yy_1\} + \{zx_1, zy_1\}$. Note that $T_2 \in \boldsymbol{ST}_{n,s}$. Thus

$$\begin{aligned} H_f(T) - H_f(T_2) &= H_f(T') - H_f(T_2) \\ &= f(4) + f(4) + f(1) - 3f(3) > 0 \end{aligned}$$

by Jensen inequality ($\frac{f(4)+f(4)+f(1)}{3} > f(\frac{4+4+1}{3})$) for the function $f(x)$ which is strictly convex. We obtain $H_f(T) > H_f(T_2)$, which is a contradiction again.

We distinguish two cases to study.

Case 1. T' has no vertex of degree 4.

In this case, $n_4 = 0$. and we have

$$n_1 + 2n_2 + 3n_3 = 2(n-1) = 2n_1 + 2n_2 + 2n_3 - 2.$$

So $n_3 = n_1 - 2$. Moreover, by the definitions of the segment and the squeeze $S(T')$ of T', we have

$$s = |E(S(T'))| = |V(S(T'))| - 1 = n - n_2 - 1 = n_1 + n_3 - 1 = 2n_1 - 3,$$

which is odd. Therefore, $n_1 = \frac{s+3}{2}$, $n_2 = n - s - 1$ and $n_3 = \frac{s-1}{2}$. It is concluded that T' and T have the same degree sequence $(\underbrace{3,\cdots,3}_{\frac{s-1}{2}},\underbrace{2,\cdots,2}_{n-s-1},\underbrace{1,\cdots,1}_{\frac{s+3}{2}})$ and

$$H_f(T) = H_f(T') = \frac{s-1}{2} f(3) + (n-s-1) f(2) + \frac{s+3}{2} f(1).$$

Case 2. T' contains a vertex of degree 4.
In this case, $n_4 = 1$ and we have

$$n_1 + 2n_2 + 3n_3 + 4 = 2(n-1) = 2n_1 + 2n_2 + 2n_3.$$

So $n_3 = n_1 - 4$. Moreover,

$$s = n - n_2 - 1 = n_1 + n_3 = 2n_1 - 4,$$

which is even. Therefore, $n_1 = \frac{s+4}{2}$, $n_2 = n - s - 1$ and $n_3 = \frac{s-4}{2}$. It is concluded that T' and T have the same degree sequence $(4, \underbrace{3, \cdots, 3}_{\frac{s-4}{2}}, \underbrace{2, \cdots, 2}_{n-s-1}, \underbrace{1, \cdots, 1}_{\frac{s+4}{2}})$ and

$$H_f(T) = H_f(T') = f(4) + \frac{s-4}{2} f(3) + (n-s-1) f(2) + \frac{s+4}{2} f(1).$$

The proof is completed. □

Theorem 4.2. *Let $T \in \boldsymbol{ST}_{n,s}$ and $f(x)$ be strictly convex, where $3 \le s \le n-2$. Then*

$$H_f(T) \le f(s) + s f(1) + (n-s-1) f(2)$$

with the equality holding only if the degree sequence of T is $(s, \underbrace{2, \cdots, 2}_{n-s-1}, \underbrace{1, \cdots, 1}_{s})$.

Proof. By the definition of the squeeze $S(T)$, one gets

$$H_f(T) = n_2 f(2) + H_f(S(T)).$$

Since $n_2 = n - s - 1$, we have $H_f(T) = (n-s-1) f(2) + H_f(S(T))$. Since $S(T)$ is a tree with $s+1$ vertices and s edges, by Lemma 2.2, $H_f(S(T)) \le f(s) + s f(1)$ with the equality holding if and only if $S(T) \cong S_{s+1}$. Then

$$H_f(T) \le (n-s-1) f(2) + f(s) + s f(1)$$

with the equality holding if and only if $n_2 = n - s - 1$ and $S(T) \cong S_{s+1}$. That is, the degree sequence of $S(T)$ is $(s, \underbrace{1, \cdots, 1}_{s})$, and the degree sequence of T is $(s, \underbrace{2, \cdots, 2}_{n-s-1}, \underbrace{1, \cdots, 1}_{s})$. □

5. Trees with given number of branching vertices

Let $T \in \boldsymbol{BT}_{n,b}$. Then $b \le \frac{n}{2} - 1$ [23]. Since the path is the only tree with no branching vertex, thus, in the following we always assume that $1 \le b \le \frac{n}{2} - 1$.

Theorem 5.1. *Let $T \in \boldsymbol{BT}_{n,b}$ and $f(x)$ be strictly convex, where $1 \le b \le \frac{n}{2} - 1$. Then*

$$H_f(T) \ge b f(3) + (n-2b-2) f(2) + (b+2) f(1)$$

with the equality holding if and only if the degree sequence of T is $(\underbrace{3, \cdots, 3}_{b}, \underbrace{2, \cdots, 2}_{n-2b-2}, \underbrace{1, \cdots, 1}_{b+2})$.

Proof. Choose $T \in \boldsymbol{BT}_{n,b}$ such that T has the smallest H_f.
Claim 1. For each vertex $u \in V(T)$, $deg_T(u) \le 3$.

Contrarily, we assume that there is a vertex, say x, with $deg_T(x) = d \geq 4$ in T. Let $y \in N_T(x)$ and z $(z \neq y)$ be a pendent vertex of T. Let $T_1 = T - xy + zy$. It is easy to see that $T_1 \in \boldsymbol{BT}_{n,b}$. By (1) and Lemma 2.1, one has

$$H_f(T) - H_f(T_1) = f(d) + f(1) - f(d-1) - f(2) > 0.$$

Thus $H_f(T_1) < H_f(T)$, which contradicts the assumption of T.

By Claim 1, it follows that $n_1 + n_2 + n_3 = n$ and $n_1 + 2n_2 + 3n_3 = 2(n-1) = 2n_1 + 2n_2 + 2n_3 - 2$. So $n_3 = n_1 - 2$. We can see $b = n_3$, so $n_2 = n - 2b - 2$ and $n_1 = b + 2$. Therefore, the degree sequence of T is $(\underbrace{3,\cdots,3}_{b},\underbrace{2,\cdots,2}_{n-2b-2},\underbrace{1,\cdots,1}_{b+2})$ and

$$H_f(T) = bf(3) + (n-2b-2)f(2) + (b+2)f(1).$$

This finishes the proof. □

Theorem 5.2. *Let $T \in \boldsymbol{BT}_{n,b}$ and $f(x)$ be strictly convex, where $1 \leq b \leq \frac{n}{2} - 1$. Then*

$$H_f(T) \leq f(n-2b+1) + (b-1)f(3) + (n-b)f(1)$$

with the equality holding if and only if the degree sequence of T is $(n-2b+1,\underbrace{3,\cdots,3}_{b-1},\underbrace{1,\cdots,1}_{n-b})$.

Proof. Choose $T \in \boldsymbol{BT}_{n,b}$ such that T has the largest H_f.

Claim 2. T has no vertex of degree 2.

On the contrary, we assume that there exist the vertices of degree 2 in T. Since $T \ncong P_n$, there is a vertex, say x with $deg_T(x) = 2$, adjacent to a branching vertex, say y with $deg_T(y) = d \geq 3$. Suppose $z \in N_T(x)$ and $z \neq y$. Let $T_2 = T - xz + yz$. It is obvious that $T_2 \in \boldsymbol{BT}_{n,b}$. By (1) and Lemma 2.1, we have

$$H_f(T_2) - H_f(T) = f(d+1) + f(1) - f(d) - f(2) > 0.$$

Thus $H_f(T_2) > H_f(T)$, which is a contradiction to the assumption of T.

Claim 3. There exists at most one vertex u in T such that $deg_T(u) \geq 4$.

Suppose, on the contrary, that there exist two vertices, say x and y, in T such that $deg_T(x) = d_1 \geq deg_T(y) = d_2 \geq 4$. Let $z \in N_T(y)$ which is not contained in the path from y to x. Let $T_3 = T - yz + xz$. It is clear that $T_3 \in \boldsymbol{BT}_{n,b}$. By (1) and Lemma 2.1, we have

$$H_f(T_3) - H_f(T) = f(d_1+1) + f(d_2-1) - f(d_1) - f(d_2) > 0.$$

Thus $H_f(T_3) > H_f(T)$, which contradicts the assumption of T again.

By Claims 2 and 3, it can be concluded that the degree sequence of T is $(r,\underbrace{3,\cdots,3}_{b-1},\underbrace{1,\cdots,1}_{n-b})$, where $r \geq 3$. Therefore,

$$r + 3(b-1) + n - b = 2(n-1).$$

So $r = n - 2b + 1$. Therefore, the degree sequence of T is $(n-2b+1,\underbrace{3,\cdots,3}_{b-1},\underbrace{1,\cdots,1}_{n-b})$. □

6. Trees with given number of maximum degree vertices

Let $T \in \boldsymbol{DT}_{n,k}$. If $k = n-2$, then $T \cong P_n$ and $\Delta = 2$. For $k \leq n-3$, $\Delta \geq 3$ and the maximum degree vertices are branching vertices, we have $k \leq b \leq \frac{n}{2} - 1$. Thus $1 \leq k \leq \frac{n}{2} - 1$.

Lemma 6.1. *[5] Let $T \in \boldsymbol{DT}_{n,k}$ with the maximum degree Δ. Then $\Delta \leq \lfloor \frac{n-2}{k} \rfloor + 1$.*

Theorem 6.1. *Let $T \in \boldsymbol{DT}_{n,k}$ and $f(x)$ be strictly convex, where $1 \leq k \leq \frac{n}{2} - 1$. Then*

$$H_f(T) \geq kf(3) + (n-2k-2)f(2) + (k+2)f(1)$$

with the equality holding only if the degree sequence of T is $(\underbrace{3, \cdots, 3}_{k}, \underbrace{2, \cdots, 2}_{n-2k-2}, \underbrace{1, \cdots, 1}_{k+2})$.

Proof. Choose $T \in \boldsymbol{DT}_{n,k}$ such that T has the smallest H_f.
Claim 1. $\Delta = 3$.

On the contrary, we assume that $\Delta \geq 4$ and $x \in V(T)$ with $deg_T(x) = \Delta$. Let $P = y_0 y_1 \cdots y_{i-1} x (= y_i) y_{i+1} \cdots y_l$ be the longest path such that x is contained in T. Denote $N_T(x) = \{y_{i-1}, y_{i+1}, x_1, x_2, \cdots, x_{\Delta-2}\}$. Suppose w_1 is the pendent vertex connecting x via x_1 (maybe $w_1 = x_1$). Let

$$T_1 = T - xx_2 + x_2 w_1. \tag{2}$$

By (1) and Lemma 2.1, we have

$$H_f(T) - H_f(T_1) = f(\Delta) + f(1) - f(\Delta - 1) - f(2) > 0.$$

Thus $H_f(T_1) < H_f(T)$.

In a similar way, we use transformations described in (2) on each vertex with maximum degree Δ. In every step from a tree T_j, one can obtain a tree T_{j+1} $(1 \leq j \leq k-1)$ such that $H_f(T_{j+1}) < H_f(T_j)$. Repeating these transformations k times, we obtain the tree T_k which contains k vertices with maximum degree $\Delta - 1$. It is clear that $T_k \in \boldsymbol{DT}_{n,k}$ and $H_f(T_k) < H_f(T)$, which contradicts the assumption of T.

By Claim 1, it can be concluded that the degree sequence of T is $(\underbrace{3, \cdots, 3}_{k}, \underbrace{2, \cdots, 2}_{n_2}, \underbrace{1, \cdots, 1}_{n_1})$. Therefore, $n_1 + 2n_2 + 3k = 2(n_1 + n_2 + k - 1)$ and we deduce that $n_1 = k+2$ and $n_2 = n - n_1 - k = n - 2k - 2$. So the degree sequence of T is $(\underbrace{3, \cdots, 3}_{k}, \underbrace{2, \cdots, 2}_{n-2k-2}, \underbrace{1, \cdots, 1}_{k+2})$ and

$$H_f(T) = kf(3) + (n-2k-2)f(2) + (k+2)f(1),$$

which completes the proof. □

Theorem 6.2. *Let $T \in \boldsymbol{DT}_{n,k}$ and $f(x)$ be strictly convex, where $1 \leq k \leq \frac{n}{2} - 1$. Then*

$$H_f(T) \leq kf(\Delta) + tf(\Delta - 1) + f(\lambda) + (n-k-t-1)f(1)$$

with the equality holding only if the degree sequence of T is $(\underbrace{\Delta, \cdots, \Delta}_{k}, \underbrace{\Delta-1, \cdots, \Delta-1}_{t}, \lambda, \underbrace{1, \cdots, 1}_{n-k-t-1})$, where $\Delta = \lfloor \frac{n-2}{k} \rfloor + 1$, $t = \lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \rfloor$ and $\lambda = n - 1 - t(\Delta - 2) - k(\Delta - 1)$.

Proof. Choose $T \in \boldsymbol{DT}_{n,k}$ such that T has the largest H_f. Let $V(T) = \{y_1, y_2, \cdots, y_n\}$ and T have the degree sequence $\pi = (deg_1, deg_2, \cdots, deg_n)$.
Claim 2. $\Delta = \lfloor \frac{n-2}{k} \rfloor + 1$.

By Lemma 6.1, $\Delta \leq \lfloor \frac{n-2}{k} \rfloor + 1$. Denote $\Delta^* = \lfloor \frac{n-2}{k} \rfloor + 1$ and $n - 2 = k \lfloor \frac{n-2}{k} \rfloor + \alpha$, where $0 \leq \alpha < k$.

Contrarily, we assume that $\Delta < \Delta^*$. So

$$\Delta = deg_1 = \cdots = deg_k = \Delta^* - \beta, \ \beta > 0.$$

Notice that

$$n_1 + n_2 + \cdots + n_\Delta = n \tag{3}$$

and

$$n_1 + 2n_2 + \cdots + \Delta n_\Delta = 2(n-1). \tag{4}$$

From (3) and (4), one gets

$$n_1 = n_3 + 2n_4 + \cdots + (\Delta-2)n_\Delta + 2 \geq (\Delta-2)n_\Delta + 2 = (\Delta-2)k + 2. \tag{5}$$

Let $n_1 = (\Delta-2)k + 2 + \gamma$, where $\gamma \geq 0$. By (3), we have

$$n = (\Delta-2)k + 2 + \gamma + n_2 + \cdots + n_{\Delta-1} + k,$$

it implies that

$$\gamma + n_2 + \cdots + n_{\Delta-1} = \alpha + k\beta. \tag{6}$$

Also, from (4), we can deduce that

$$\gamma + 2n_2 + \cdots + (\Delta-1)n_{\Delta-1} = 2(\alpha + k\beta). \tag{7}$$

By subtracting the relations (6) and (7), one has

$$n_2 + 2n_3 \cdots + (\Delta-2)n_{\Delta-1} = \alpha + k\beta \geq k\beta \geq k. \tag{8}$$

Thus the total edge rotating capacity of T is equal to or greater than k.

Suppose $y_i \in T$ $(k < i \leq n)$ is a vertex of degree deg_i which has positive edge rotating capacity, where $2 \leq deg_i \leq \Delta - 1$. Let T_1 be a tree with the degree sequence $\pi_1 = (deg_1^{(1)}, deg_2^{(1)}, \cdots, deg_n^{(1)})$ such that $deg_1^{(1)} = deg_1 + 1 = \Delta + 1$, $deg_i^{(1)} = deg_i - 1$ and $deg_j^{(1)} = deg_j$, where $j \neq i$ and $j \in \{2, 3, \cdots, n\}$. By (1) and Lemma 2.1, we have

$$H_f(T) - H_f(T_1) = f(deg_1) + f(deg_i) - f(deg_1 + 1) - f(deg_i - 1) < 0.$$

Thus $H_f(T_1) > H_f(T)$. Notice that the maximum degree of T_1 is $\Delta + 1$, so $T_1 \notin \boldsymbol{DT}_{n,k}$. Since T_1 contains $k-1$ vertices with degree Δ and the total edge rotating capacity of $deg_2, deg_3, \cdots, deg_\Delta$ is at least $k-1$, from (8), one can get the following conclusions.

One can repeat recursively the above-described transformation of the tree T_1 $k-1$ times on each vertex of degree Δ. In every step, we can define a tree T_r having degree sequence $\pi_r = (deg_1^{(r)}, deg_2^{(r)}, \cdots, deg_n^{(r)})$ such that $deg_r^{(r)} = \Delta + 1$, $deg_i^{(r)} = deg_i^{(r-1)} - 1$ and $deg_j^{(r)} = deg_j^{(r-1)}$ $(j \neq i, r$ and $j \in \{1, \cdots, n\})$, where $r = 2, \cdots, k$ and $deg_i^{(r-1)}$ is the degree of an arbitrary vertex $y_i \in V(T_{r-1})$ $(k < i \leq n)$ that has positive edge rotating capacity (since the total edge rotating capacity of T_{r-1} is at least $k - r + 1$, this vertex must exist). It naturally occurs that we can get a tree whose degrees $deg_{k+1}, \cdots, deg_n$ are in an increasing order after some described transformations. Moreover, every application of this transformation strictly increases the H_f. After that, one can obtain a tree $T_k \in \boldsymbol{DT}_{n,k}$ with maximum degree $\Delta + 1 = (\Delta^* - \beta) + 1$ and satisfies the condition $H_f(T_k) > H_f(T_{k-1}) > \cdots > H_f(T_1) > H_f(T)$, which is a contradiction with the choice of T. Hence $\beta = 0$ and it deduces that $\Delta = \Delta^* = \lfloor \frac{n-2}{k} \rfloor + 1$. This completes the proof of Claim 2.

By Claim 2, it follows that $deg_1 = \cdots = deg_k = \Delta = \lfloor \frac{n-2}{k} \rfloor + 1$. Just as the proof of Claim 2, let $n-2 = k\lfloor \frac{n-2}{k} \rfloor + \alpha = k(\Delta-1) + \alpha$, where $0 \leq \alpha < k$. According to (5), we deduce that $n_1 \geq (\Delta-2)k + 2 = n - k - \alpha$. Thus, $deg_n = deg_{n-1} = \cdots = deg_{k+\alpha+1} = 1$.

Notice that $n_\Delta = k$ and $n_1 = (\Delta-2)k + 2 + \gamma$, where $\gamma \geq 0$. By using (3), (4) and $\beta = 0$, in a similar way as in (6) and (8), one gets

$$\gamma + n_2 + \cdots + (\Delta-1)n_{\Delta-1} = \alpha \tag{9}$$

and

$$n_2 + 2n_3 \cdots + (\Delta - 2)n_{\Delta-1} = \alpha. \tag{10}$$

Since $n_i \geq 0$ $(i = 2, \cdots, \Delta - 1)$, by (10), we deduce that $t = n_{\Delta-1} \leq \frac{\alpha}{\Delta-2}$. So $t \leq \lfloor \frac{\alpha}{\Delta-2} \rfloor$ since $t \geq 0$ is an integer.

Now we assume that $t < \lfloor \frac{\alpha}{\Delta-2} \rfloor$ and $\lfloor \frac{\alpha}{\Delta-2} \rfloor > 0$. From (10), we have $n_2 + 2n_3 \cdots + (\Delta - 3)n_{\Delta-2} \geq \Delta - 2$. Therefore, there exist n_i and n_j $(n_i, n_j \neq 0$ and $2 \leq i < j \leq \Delta - 2)$ or there exists $n_i \geq 2$ $(2 \leq i \leq \Delta - 2)$ such that (10) holds. In addition, since $\pi = (\underbrace{\Delta, \cdots, \Delta}_{k}, deg_{k+1}, \cdots, deg_{k+\alpha}, 1, \cdots, 1)$, there exist deg_{k+i_1} and deg_{k+j_1} $(1 \leq j_1 < i_1 \leq \alpha)$ such that $deg_{k+j_1} = j > deg_{k+i_1} = i$ or $deg_{k+i_1} = deg_{k+j_1} = i$ when $n_i \geq 2$.

Let $\pi' = (deg'_1, deg'_2, \cdots, deg'_n)$ be a degree sequence satisfying $deg'_{k+i_1} = deg_{k+i_1} - 1 = i - 1$ and $deg'_{k+j_1} = deg_{k+j_1} + 1 = j + 1$, where $deg'_l = deg_l$ if $l \neq k + i_1, k + j_1$. It is clear that $\sum_{i=1}^{n} deg'_i = 2(n - 1)$ and π' is a degree sequence of a tree T'. By (1) and Lemma 2.1, we have

$$H_f(T') - H_f(T) = f(j + 1) + f(i - 1) - f(i) - f(j) > 0.$$

Thus $H_f(T') > H_f(T)$, a contradiction with the assumption of T. And we deduce that $t = n_{\Delta-1} = \lfloor \frac{\alpha}{\Delta-2} \rfloor = \lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \rfloor$ and the relation (10) now changes to

$$n_2 + 2n_3 \cdots + (\Delta - 3)n_{\Delta-2} = \alpha - t(\Delta - 2) \leq \Delta - 3.$$

In a similar way as previously, one can prove easily that $n_\lambda = 1$ $(2 \leq \lambda \leq \Delta - 2)$, where $\lambda = \alpha - t(\Delta - 2) + 1$, that is $\lambda = n - 1 - t(\Delta - 2) - k(\Delta - 1)$ and $n_i = 0$ when $i \neq \lambda$, $2 \leq i \leq \Delta - 2$, since in the opposite case one can construct a tree whose H_f is greater than $H_f(T)$ again.

Hence, T has the degree sequence $(\underbrace{\Delta, \cdots, \Delta}_{k}, \underbrace{\Delta-1, \cdots, \Delta-1}_{t}, \lambda, \underbrace{1, \cdots, 1}_{n-k-t-1})$ and

$$H_f(T) = kf(\Delta) + tf(\Delta - 1) + f(\lambda) + (n - k - t - 1)f(1).$$

The proof is completed. □

7. Trees with a perfect matching

Let $\mathscr{T}_{2m}$ be a collection of $2m$-vertex trees obtained from S_{m+1} by adding a pendent edge to its $m - 1$ pendent vertices. By Lemma 2.3, one can get the following theorem immediately.

Theorem 7.1. *Let $T \in \boldsymbol{MT}_{2m}$ and $f(x)$ be strictly convex, where $m \geq 2$. Then*

$$H_f(T) \geq 2(m - 1)f(2) + 2f(1)$$

with equality only if $T \cong P_{2m}$.

Theorem 7.2. *Let $T \in \boldsymbol{MT}_{2m}$ and $f(x)$ be strictly convex, where $m \geq 2$. Then*

$$H_f(T) \leq f(m) + (m - 1)f(2) + mf(1)$$

with equality only if $T \cong \mathscr{T}_{2m}$.

Proof. For $m = 2$, $T \cong \mathscr{T}_4 \cong P_4$, the result is true.

For $m \geq 3$, pick $T \in \boldsymbol{MT}_{2m}$ such that T has the largest H_f. Suppose M is a perfect matching of T. Let $y \in V(T)$ is a maximum degree vertex in T.

Claim 1. For any other vertex $u \in V(T)$ $(u \neq y)$, $deg_T(u) \leq 2$.

Contrarily, we assume that T contains $y' \in V(T) \backslash \{y\}$ with $deg_T(y') \geq 3$. Let $N_T(y) = \{u_1, u_2, \cdots, u_r\}$ and $N_T(y') = \{v_1, v_2, \cdots, v_s\}$, where $r \geq s \geq 3$. Let P be the path connecting y and y' in T. Suppose without loss of generality that $u_1, v_1 \in V(P)$ (maybe $u_1 = y'$ or $v_1 = y$). Notice that $|\{v_2y', v_3y', \cdots, v_sy'\} \cap M| \leq 1$. One can assume that $v_3y', \cdots, v_sy' \notin M$. Let $T_1 = T - \{v_3y', \cdots, v_sy'\} + \{yv_3, \cdots, yv_s\}$. Clearly, $T_1 \in \boldsymbol{MT}_{2m}$. By (1) and Lagrange mean value theorem, it follows that

$$\begin{aligned} H_f(T_1) - H_f(T) =& f(r+s-2) - f(r) - [f(s) - f(2)] \\ =& f'(\xi) - f'(\eta) > 0, \end{aligned}$$

where $r < \xi < r+s-2$, $2 < \eta < s$. Thus $H_f(T_1) > H_f(T)$, which contradicts the choice of T.

From Claim 1, T must be a starlike tree and y is the central vertex.

Claim 2. $deg_T(y) \geq 3$.

On the contrary assume that $deg_T(y) \leq 2$. Furthermore, $deg_T(y) \geq 2$ since y has the maximum degree in T. Hence $deg_T(y) = 2$ and $T \cong P_{2m}$. Furthermore, $\mathscr{T}_{2m} \ncong P_{2m}$ since $m \geq 3$. By Lemma 2.3, $H_f(\mathscr{T}_{2m}) > H_f(P_{2m})$, which contradicts the assumption of T.

Let us use $P_1, P_2, \cdots, P_t$ to denote the paths attached to y in T, where $t \geq 3$.

Claim 3. $|E(P_i)| \leq 2$, $i = 1, 2, \cdots, t$.

Contrarily, if T contains P_i ($i \in \{1, 2, \cdots, t\}$) with $|E(P_i)| \geq 3$, without loss of generality, suppose that $|E(P_t)| \geq 3$. Denote $P_t = y_1y_2\cdots y_k$, where $y_1 = y$ and $k \geq 4$. Then there exists at least one edge y_jy_{j+1} with $y_jy_{j+1} \notin M$ in P_t, $j \in \{2, 3, \cdots, k-1\}$. Let $T_2 = T - y_jy_{j+1} + yy_{j+1}$. Obviously, $T_2 \in \boldsymbol{MT}_{2m}$. By (1) and Lemma 2.1, for $t \geq 3$, one has

$$H_f(T_2) - H_f(T) = f(t+1) + f(1) - f(t) - f(2) > 0.$$

Thus $H_f(T_2) > H_f(T)$, a contradiction again.

Denote $PV_1 = \{v \in V(T) | deg_T(v) = 1, vy \in E(T)\}$. By Claim 3 and $T \in \boldsymbol{MT}_{2m}$, we have $|PV_1| = 1$. It implies that $T \cong \mathscr{T}_{2m}$. □

8. Concluding remark and applications

Remark 8.1. *If $f(x)$ is a strictly concave function, the inequalities in Theorems 3.1, 3.2, 4.1, 4.2, 5.1, 5.2, 6.1, 6.2, 7.1 and 7.2 should be reversed, and the corresponding results for the concave function can also be obtained.*

The topological indices mentioned in Section 1 belong to the vertex-degree function indices $H_f(G)$: zeroth-order general Randić index ${}^0R_\alpha(G)$ corresponds to $f(x) = x^\alpha$ ($x \geq 1$) which is strictly concave for $0 < \alpha < 1$ and strictly convex for $\alpha > 1$ or $\alpha < 0$; variable sum exdeg index $SEI_a(G)$ corresponds to $f(x) = xa^x$ ($x \geq 1$) which is strictly convex for $a > 1$; sum lordeg index $SL(G)$ corresponds to $f(x) = x\sqrt{\ln x}$ which is strictly convex for $x \geq 2$; natural logarithm of the first multiplicative Zagreb index $\ln \Pi_1(G)$ corresponds to $f(x) = 2\ln x$ which is strictly concave for $x \geq 1$; natural logarithm of the second multiplicative Zagreb index $\ln \Pi_2(G)$ corresponds to $f(x) = x \ln x$ which is strictly convex for $x \geq 1$. By Theorems 3.1, 3.2, 4.1, 4.2, 5.1, 5.2, 6.1, 6.2, 7.1, 7.2 and Remark 8.1, we can get the following corollaries.

Corollary 8.1. *Let $T \in \boldsymbol{PT}_{n,p}$, where $2 \leq p \leq n-1$. Then*

$${}^0R_\alpha(G) \geq [n - (r-1)(n-p) - 2](r+1)^\alpha + [(r-1)(n-p) - p + 2]r^\alpha + p$$

for $\alpha > 1$ or $\alpha < 0$;

$${}^0R_\alpha(G) \leq [n - (r-1)(n-p) - 2](r+1)^\alpha + [(r-1)(n-p) - p + 2]r^\alpha + p$$

for $0 < \alpha < 1$;

$$SEI_a(G) \geq [n - (r-1)(n-p) - 2](r+1)a^{(r+1)} + [(r-1)(n-p) - p + 2]ra^r + pa$$

for $a > 1$*;*

$$SL(G) \geq [n-(r-1)(n-p)-2](r+1)\sqrt{\ln(r+1)} + [(r-1)(n-p)-p+2]r\sqrt{\ln r};$$
$$\Pi_1(G) \leq (r+1)^{2[n-(r-1)(n-p)-2]} r^{2[(r-1)(n-p)-p+2]};$$
$$\Pi_2(G) \geq (r+1)^{[n-(r-1)(n-p)-2](r+1)} r^{[(r-1)(n-p)-p+2]r}.$$

The equalities occur only if the degree sequence of T *is* $(\underbrace{r+1,\cdots,r+1}_{n-(r-1)(n-p)-2},\ \underbrace{r,\cdots,r}_{(r-1)(n-p)-p+2},\ \underbrace{1,\cdots,1}_{p})$*, where* $r = \lfloor \frac{n-2}{n-p} \rfloor + 1$*.*

Corollary 8.2. *Let* $T \in \boldsymbol{PT}_{n,p}$*, where* $2 \leq p \leq n-1$*. Then*

$${}^0R_\alpha(G) \leq p^\alpha + (n-p-1)2^\alpha + p$$

for $\alpha > 1$ *or* $\alpha < 0$*;*

$${}^0R_\alpha(G) \geq p^\alpha + (n-p-1)2^\alpha + p$$

for $0 < \alpha < 1$*;*

$$SEI_a(G) \leq pa^p + 2(n-p-1)a^2 + pa$$

for $a > 1$*;*

$$SL(G) \leq p\sqrt{\ln p} + 2(n-p-1)\sqrt{\ln 2};$$
$$\Pi_1(G) \geq p^2 2^{2(n-p-1)};$$
$$\Pi_2(G) \leq p^p 2^{2(n-p-1)}.$$

The equalities occur only if the degree sequence of T *is* $(p, \underbrace{2,\cdots,2}_{n-p-1}, \underbrace{1,\cdots,1}_{p})$*.*

Corollary 8.3. *Let* $T \in \boldsymbol{ST}_{n,s}$*, where* $3 \leq s \leq n-2$*. Then*

$${}^0R_\alpha(G) \geq \begin{cases} \frac{s-1}{2}3^\alpha + (n-s-1)2^\alpha + \frac{s+3}{2} & \text{if } s \text{ is odd,} \\ 4^\alpha + \frac{s-4}{2}3^\alpha + (n-s-1)2^\alpha + \frac{s+4}{2} & \text{if } s \text{ is even} \end{cases}$$

for $\alpha > 1$ *or* $\alpha < 0$*;*

$${}^0R_\alpha(G) \leq \begin{cases} \frac{s-1}{2}3^\alpha + (n-s-1)2^\alpha + \frac{s+3}{2} & \text{if } s \text{ is odd,} \\ 4^\alpha + \frac{s-4}{2}3^\alpha + (n-s-1)2^\alpha + \frac{s+4}{2} & \text{if } s \text{ is even} \end{cases}$$

for $0 < \alpha < 1$*;*

$$SEI_a(G) \geq \begin{cases} \frac{3(s-1)}{2}a^3 + 2(n-s-1)a^2 + \frac{s+3}{2}a & \text{if } s \text{ is odd,} \\ 4a^4 + \frac{3(s-4)}{2}a^3 + 2(n-s-1)a^2 + \frac{s+4}{2}a & \text{if } s \text{ is even} \end{cases}$$

for $a > 1$*;*

$$SL(G) \geq \begin{cases} \frac{3(s-1)}{2}\sqrt{\ln 3} + 2(n-s-1)\sqrt{\ln 2} & \text{if } s \text{ is odd,} \\ 4\sqrt{\ln 4} + \frac{3(s-4)}{2}\sqrt{\ln 3} + 2(n-s-1)\sqrt{\ln 2} & \text{if } s \text{ is even;} \end{cases}$$
$$\Pi_1(G) \leq \begin{cases} 3^{s-1}2^{2(n-s-1)} & \text{if } s \text{ is odd,} \\ 16 \cdot 3^{s-4}2^{2(n-s-1)} & \text{if } s \text{ is even;} \end{cases}$$
$$\Pi_2(G) \geq \begin{cases} 3^{\frac{3(s-1)}{2}}2^{2(n-s-1)} & \text{if } s \text{ is odd,} \\ 4^4 3^{\frac{3(s-4)}{2}}2^{2(n-s-1)} & \text{if } s \text{ is even.} \end{cases}$$

The equalities occur only if the degree sequence of T is $(\underbrace{3,\cdots,3}_{\frac{s-1}{2}},\underbrace{2,\cdots,2}_{n-s-1},\underbrace{1,\cdots,1}_{\frac{s+3}{2}})$ *for odd s and* $(4,\underbrace{3,\cdots,3}_{\frac{s-4}{2}},\underbrace{2,\cdots,2}_{n-s-1},\underbrace{1,\cdots,1}_{\frac{s+4}{2}})$ *for even s.*

Corollary 8.4. *Let* $T \in \boldsymbol{ST}_{n,s}$*, where* $3 \le s \le n-2$*. Then*

$$^{0}R_{\alpha}(G) \le s^{\alpha} + (n-s-1)2^{\alpha} + s$$

for $\alpha > 1$ *or* $\alpha < 0$*;*

$$^{0}R_{\alpha}(G) \ge s^{\alpha} + (n-s-1)2^{\alpha} + s$$

for $0 < \alpha < 1$*;*

$$SEI_{a}(G) \le sa^{s} + 2(n-s-1)a^{2} + sa$$

for $a > 1$*;*

$$SL(G) \le s\sqrt{\ln s} + 2(n-s-1)\sqrt{\ln 2};$$
$$\Pi_1(G) \ge s^{2}2^{2(n-s-1)};$$
$$\Pi_2(G) \le s^{s}2^{2(n-s-1)}.$$

The equalities occur only if the degree sequence of T is $(s,\underbrace{2,\cdots,2}_{n-s-1},\underbrace{1,\cdots,1}_{s})$.

Corollary 8.5. *Let* $T \in \boldsymbol{BT}_{n,b}$*, where* $1 \le b \le \frac{n}{2} - 1$*. Then*

$$^{0}R_{\alpha}(G) \ge 3^{\alpha}b + (n-2b-2)2^{\alpha} + b + 2$$

for $\alpha > 1$ *or* $\alpha < 0$*;*

$$^{0}R_{\alpha}(G) \le 3^{\alpha}b + (n-2b-2)2^{\alpha} + b + 2$$

for $0 < \alpha < 1$*;*

$$SEI_{a}(G) \ge 3ba^{3} + 2(n-2b-2)a^{2} + (b+2)a$$

for $a > 1$*;*

$$SL(G) \ge 3b\sqrt{\ln 3} + 2(n-2b-2)\sqrt{\ln 2};$$
$$\Pi_1(G) \le 3^{2b}2^{2(n-2b-2)};$$
$$\Pi_2(G) \ge 3^{3b}2^{2(n-2b-2)}.$$

The equalities occur only if the degree sequence of T is $(\underbrace{3,\cdots,3}_{b},\underbrace{2,\cdots,2}_{n-2b-2},\underbrace{1,\cdots,1}_{b+2})$.

Corollary 8.6. *Let* $T \in \boldsymbol{BT}_{n,b}$*, where* $1 \le b \le \frac{n}{2} - 1$*. Then*

$$^{0}R_{\alpha}(G) \le (n-2b+1)^{\alpha} + (b-1)3^{\alpha} + n - b$$

for $\alpha > 1$ *or* $\alpha < 0$*;*

$$^{0}R_{\alpha}(G) \ge (n-2b+1)^{\alpha} + (b-1)3^{\alpha} + n - b$$

for $0 < \alpha < 1$*;*

$$SEI_a(G) \leq (n-2b+1)a^{(n-2b+1)} + 3(b-1)a^3 + a(n-b)$$

for $a > 1$*;*

$$SL(G) \leq (n-2b+1)\sqrt{\ln(n-2b+1)} + 3(b-1)\sqrt{\ln 3};$$
$$\Pi_1(G) \geq (n-2b+1)^2 3^{2(b-1)};$$
$$\Pi_2(G) \leq (n-2b+1)^{(n-2b+1)} 3^{3(b-1)}.$$

The equalities occur only if the degree sequence of T *is* $(n-2b+1, \underbrace{3, \cdots, 3}_{b-1}, \underbrace{1, \cdots, 1}_{n-b})$.

Corollary 8.7. *Let* $T \in \boldsymbol{DT}_{n,k}$*, where* $1 \leq k \leq \frac{n}{2} - 1$*. Then*

$$^0R_\alpha(G) \geq 3^\alpha k + (n-2k-2)2^\alpha + k + 2$$

for $\alpha > 1$ *or* $\alpha < 0$*;*

$$^0R_\alpha(G) \leq 3^\alpha k + (n-2k-2)2^\alpha + k + 2$$

for $0 < \alpha < 1$*;*

$$SEI_a(G) \geq 3ka^3 + 2(n-2k-2)a^2 + (k+2)a$$

for $a > 1$*;*

$$SL(G) \geq 3k\sqrt{\ln 3} + 2(n-2k-2)\sqrt{\ln 2};$$
$$\Pi_1(G) \leq 3^{2k} 2^{2(n-2k-2)};$$
$$\Pi_2(G) \geq 3^{3k} 2^{2(n-2k-2)}.$$

The equalities occur only if the degree sequence of T *is* $(\underbrace{3, \cdots, 3}_{k}, \underbrace{2, \cdots, 2}_{n-2k-2}, \underbrace{1, \cdots, 1}_{k+2})$.

Corollary 8.8. *Let* $T \in \boldsymbol{DT}_{n,k}$*, where* $1 \leq k \leq \frac{n}{2} - 1$*. Then*

$$^0R_\alpha(G) \leq k\Delta^\alpha + t(\Delta-1)^\alpha + \lambda^\alpha + n - k - t - 1$$

for $\alpha > 1$ *or* $\alpha < 0$*;*

$$^0R_\alpha(G) \geq k\Delta^\alpha + t(\Delta-1)^\alpha + \lambda^\alpha + n - k - t - 1$$

for $0 < \alpha < 1$*;*

$$SEI_a(G) \leq k\Delta a^\Delta + t(\Delta-1)a^{\Delta-1} + \lambda a^\lambda + a(n-k-t-1)$$

for $a > 1$*;*

$$SL(G) \leq k\Delta\sqrt{\ln \Delta} + t(\Delta-1)\sqrt{\ln(\Delta-1)} + \lambda\sqrt{\ln \lambda};$$
$$\Pi_1(G) \geq \Delta^{2k}(\Delta-1)^{2t}\lambda^2;$$
$$\Pi_2(G) \leq \Delta^{k\Delta}(\Delta-1)^{t(\Delta-1)}\lambda^\lambda.$$

The equalities occur only if the degree sequence of T *is* $(\underbrace{\Delta, \cdots, \Delta}_{k}, \underbrace{\Delta-1, \cdots, \Delta-1}_{t}, \lambda, \underbrace{1, \cdots, 1}_{n-k-t-1})$*, where* $\Delta = \lfloor \frac{n-2}{k} \rfloor + 1$*,* $t = \lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \rfloor$ *and* $\lambda = n - 1 - t(\Delta-2) - k(\Delta-1)$.

Corollary 8.9. *Let $T \in \boldsymbol{MT}_{2m}$, where $m \geq 2$. Then*

$$^0R_\alpha(G) \geq 2(m-1)2^\alpha + 2$$

for $\alpha > 1$ or $\alpha < 0$;

$$^0R_\alpha(G) \leq 2(m-1)2^\alpha + 2$$

for $0 < \alpha < 1$;

$$SEI_a(G) \geq 4(m-1)a^2 + 2a$$

for $a > 1$;

$$SL(G) \geq 4(m-1)\sqrt{\ln 2};$$
$$\Pi_1(G) \leq 2^{4(m-1)};$$
$$\Pi_2(G) \geq 2^{4(m-1)}.$$

The equalities occur only if $T \cong P_{2m}$.

Corollary 8.10. *Let $T \in \boldsymbol{MT}_{2m}$, where $m \geq 2$. Then*

$$^0R_\alpha(G) \leq m^\alpha + (m-1)2^\alpha + m$$

for $\alpha > 1$ or $\alpha < 0$;

$$^0R_\alpha(G) \geq m^\alpha + (m-1)2^\alpha + m$$

for $0 < \alpha < 1$;

$$SEI_a(G) \leq ma^m + 2(m-1)a^2 + ma$$

for $a > 1$;

$$SL(G) \leq m\sqrt{\ln m} + 2(m-1)\sqrt{\ln 2};$$
$$\Pi_1(G) \leq m^2 2^{2(m-1)};$$
$$\Pi_2(G) \leq m^m 2^{2(m-1)}.$$

The equalities occur only if $T \cong \mathscr{T}_{2m}$.

Remark 8.2. *Since the extremal trees specified in Theorems 4.1, 5.1, 6.1, 7.1 and Corollaries 8.3, 8.5, 8.7, 8.9 are chemical trees which are the trees with maximum degree at most 4, these results determine also the respective extremal chemical trees.*

Note that the Lanzhou index $Lz(G)$ corresponds to the function $f(x) = (n-1-x)x^2$ $(x \geq 1)$ which is strictly convex for $x < \frac{n-1}{3}$. Thus, by Theorems 4.1, 5.1, 6.1 and 7.1, we have the following corollaries on the Lanzhou index of chemical trees with $n \geq 14$ (since $4 < \frac{n-1}{3}$) vertices.

Corollary 8.11. *Let $T \in \boldsymbol{ST}_{n,s}$ be a chemical tree, where $n \geq 14$ and $3 \leq s \leq n-2$. Then*

$$Lz(T) \geq \begin{cases} \frac{9(s-1)}{2}(n-4) + 4(n-s-1)(n-3) + \frac{s+3}{2}(n-2) & \text{if } s \text{ is odd,} \\ 16(n-5) + \frac{9(s-4)}{2}(n-4) + 4(n-s-1)(n-3) + \frac{s+4}{2}(n-2) & \text{if } s \text{ is even.} \end{cases}$$

The equality occurs if and only if the degree sequence of T is $(\underbrace{3,\cdots,3}_{\frac{s-1}{2}},\underbrace{2,\cdots,2}_{n-s-1},\underbrace{1,\cdots,1}_{\frac{s+3}{2}})$ for odd s and $(4,\underbrace{3,\cdots,3}_{\frac{s-4}{2}},\underbrace{2,\cdots,2}_{n-s-1},\underbrace{1,\cdots,1}_{\frac{s+4}{2}})$ for even s.

Corollary 8.12. *Let $T \in \boldsymbol{BT}_{n,b}$ be a chemical tree, where $n \geq 14$ and $1 \leq b \leq \frac{n}{2} - 1$. Then*

$$Lz(T) \geq 9b(n-4) + 4(n-2b-2)(n-3) + (b+2)(n-2)$$

with the equality holding if and only if the degree sequence of T is $(\underbrace{3,\cdots,3}_{b},\underbrace{2,\cdots,2}_{n-2b-2},\underbrace{1,\cdots,1}_{b+2})$.

Corollary 8.13. *Let $T \in \boldsymbol{DT}_{n,k}$ be a chemical tree, where $n \geq 14$ and $1 \leq k \leq \frac{n}{2} - 1$. Then*

$$Lz(T) \geq 9k(n-4) + 4(n-2k-2)(n-3) + (k+2)(n-2)$$

with the equality holding only if the degree sequence of T is $(\underbrace{3,\cdots,3}_{k},\underbrace{2,\cdots,2}_{n-2k-2},\underbrace{1,\cdots,1}_{k+2})$.

Corollary 8.14. *Let $T \in \boldsymbol{MT}_{2m}$ be a chemical tree, where $m \geq 7$. Then*

$$Lz(T) \geq 8(m-1)(2m-3) + 4(m-1)$$

with equality only if $T \cong P_{2m}$.

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