



Article Extremal Graphs to Vertex Degree Function Index for Convex Functions

Dong He¹, Zhen Ji², Chenxu Yang² and Kinkar Chandra Das^{3,*}

- ² School of Computer, Qinghai Normal University, Xining 810008, China
- ³ Department of Mathematics, Sungkyunkwan University, Suwon 16419, Republic of Korea
- Correspondence: kinkardas2003@gmail.com or kinkar@skku.edu

Abstract: The *vertex-degree function index* $H_f(\Gamma)$ is defined as $H_f(\Gamma) = \sum_{v \in V(\Gamma)} f(d(v))$ for a function f(x) defined on non-negative real numbers. In this paper, we determine the extremal graphs with the maximum (minimum) vertex degree function index in the set of all *n*-vertex chemical trees, trees, and connected graphs. We also present the Nordhaus–Gaddum-type results for $H_f(\Gamma) + H_f(\overline{\Gamma})$ and $H_f(\Gamma) \cdot H_f(\overline{\Gamma})$.

Keywords: vertex degree function index; tree; cemical tree; connected graph; Nordhaus–Gaddum-type result

MSC: 05C07; 05C09; 05C92



Citation: He, D.; Ji, Z.; Yang, C.; Das, K.C. Extremal Graphs to Vertex Degree Function Index for Convex Functions. *Axioms* **2023**, *12*, 31. https://doi.org/10.3390/ axioms12010031

Academic Editor: Federico G. Infusino

Received: 30 October 2022 Accepted: 23 December 2022 Published: 27 December 2022

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/).

1. Introduction

In this paper, the graphs we discuss are simple graphs without multiple edges and loops. The vertex and edge set of Γ will be denoted by $V(\Gamma)$ and $E(\Gamma)$, and the order and size of Γ will usually be denoted by n and m, respectively. Let a vertex $v \in V(\Gamma)$; we denote the *degree* of v by $d_{\Gamma}(v)$ in Γ . The *neighbors* of v in $V(\Gamma)$ are denoted by $N_{\Gamma}(v)$. For a graph Γ , we denote the maximum and minimum degree of Γ by $\Delta(\Gamma)$ and $\delta(\Gamma)$, respectively. A *leaf* $v \in V(\Gamma)$ is a vertex v satisfied $d_{\Gamma}(v) = 1$. We call a connected graph without a cycle a *tree*, denoted by T. A tree whose maximum degree is no more than 4 is called a *chemical tree*. The *star graph* with order n, denoted by S_n , is a tree with one center vertex and n - 1 leaves. The *disjoint union* of two vertex-disjoint graphs Γ_1 and Γ_2 will be denoted by $\Gamma_1 \cup \Gamma_2$, whose vertex and edge sets are $V(\Gamma_1) \cup V(\Gamma_2)$ and $E(\Gamma_1) \cup E(\Gamma_2)$, respectively. We denote the *union* of k copies of a graph Γ by $k \Gamma$. The *join* of Γ_1 and Γ_2 is obtained by joining edges between each vertex of Γ_1 and all vertices of Γ_2 , denoted by $\Gamma_1 \vee \Gamma_2$. For a graph Γ , the edge $uv \in E(\Gamma)$ and the vertex $w \in V(\Gamma)$, $\Gamma - uv$ mean removing uv from Γ and $\Gamma - w$, which means removing w from Γ .

A *universal vertex* of Γ with order n is a vertex v that have d(v) = n - 1. An (n, m)-graph is the graph with n vertices and m edges. We denote by $\Gamma(n, m)$ the set of (n, m)-graphs. The *cyclomatic number* of a graph Γ is the minimum number of edges whose deletion transforms Γ into an acyclic graph, denoted by $\gamma(\Gamma)$. The set of graphs with order n and cyclomatic number γ is denoted by $\Gamma_{n,\gamma}$. We have $\gamma(\Gamma) = m - n + 1$ for a connected graph $\Gamma \in \Gamma_{n,\gamma}$.

The *vertex-degree function index* $H_f(\Gamma)$ is denoted by

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

for a function f(x) defined on non-negative real numbers in [1]. For example, the first Zagreb index [2] is defined as $M_1(\Gamma) = \sum_{v \in V(\Gamma)} d(v)^2$ when $f(x) = x^2$, and the forgotten topological index [3] is defined as $F(\Gamma) = \sum_{v \in V(\Gamma)} d(v)^3$ when $f(x) = x^3$. The general first

¹ School of Mathematics and Statistis, Qinghai Normal University, Xining 810008, China

Zagreb index, denoted by ${}^{0}R_{\alpha}(\Gamma)$, was defined in [4,5] as ${}^{0}R_{\alpha}(\Gamma) = \sum_{v \in V(\Gamma)} d(v)^{\alpha}$, where α is a real number, $\alpha \notin \{0,1\}$. For the mathematical properties of the above topological indices, see [6–11] and the references therein. Let v be a leaf of S_n , where $n \ge 3$. For $0 \le \gamma \le n-2$, the graph obtained from S_n by joining edges v with γ other pendant vertices is denoted by $H_{n,\gamma}$ in [12]. Deng [10] obtained the bounds of the Zagreb indices for trees, unicyclic graphs, and bicyclic graphs. Hu and Li determined the connected (n, m)-graphs with the minimum and maximum zeroth-order general Randić index in [13]. Li and Zheng [5] obtained a unified approach to the extremal trees for different indices. Some extremal results concerning the general zeroth-order Randić index were deduced in [14–16]; also see the survey [12].

In [17], Tomescu obtained that the function f(x) has property $(P_{\nearrow}; P_{\searrow})$ if $\varphi(i+1) > \varphi(i); \varphi(i+1) < \varphi(i)$, respectively, for every integer $i \ge 0$, where $\varphi(x) = f(x+2) + f(x) - 2f(x+1)$, and he obtained the maximum (minimum) vertex degree function index $H_f(\Gamma)$ in the set of all *n*-vertex connected graphs that have the cyclomatic number γ when $0 \le \gamma \le n - 2$ if f(x) is strictly convex (concave) and satisfies the property $P_{\nearrow}; P_{\searrow}$. Tomescu [18] obtained some structural properties of connected (n, m)-graphs which are maximum (minimum) with respect to vertex-degree function index $H_f(\Gamma)$, when f(x) is a strictly convex (concave) function. In the same paper, it is also shown that the unique graph obtained from the star S_n by adding γ edges between a fixed pendant vertex v and γ other pendant vertices has the maximum general zeroth-order Randić index ${}^0R_{\alpha}$ in the set of all *n*-vertex connected graphs that have the cyclomatic number γ when $1 \le \gamma \le n - 2$ and $\alpha \ge 2$.

Tomescu obtained the following results.

Theorem 1 ([18]). In the set of connected (n,m)-graphs Γ that have $m \ge n$, the graph that maximizes (minimizes) $H_f(\Gamma)$ where f(x) is strictly convex (concave) possesses the following properties:

- (1) Γ has a universal vertex v;
- (2) The subgraph Γv consists of some isolated vertices and a nontrivial connected component *C*, which is maximum (minimum) relatively to H_g , where g(x) = f(x+1). *C* also contains a universal vertex and no induced subgraph isomorphic to P_4 or C_p , where $p \ge 4$.

Theorem 2 ([17]). *If* $n \ge 3, 1 \le \gamma \le n-2$, f(x) *is strictly convex and has property* P_{\nearrow} , and Γ *is a connected n-vertex graph with cyclomatic number* γ , *then*

$$H_f(\Gamma) \le f(n-1) + f(\gamma+1) + \gamma f(2) + (n-\gamma-2)f(1),$$

with equality if and only if $\Gamma \cong H_{n,\gamma} \cong K_1 \vee (K_{1,\gamma} \cup (n-\gamma-2)K_1)$.

In Section 2, we give upper and lower bounds for the vertex degree function index of connected graphs if f(x) is a convex and increasing function that has property P_{\nearrow} . We obtain sharp upper and lower bounds for the vertex degree function index of trees and chemical trees if f(x) is a convex and increasing function.

Let $f(\Gamma)$ be a graph invariant and n be a positive integer. The *Nordhaus–Gaddum Problem* is to determine sharp bounds for $f(\Gamma) + f(\overline{\Gamma})$ and $f(\Gamma) \cdot f(\overline{\Gamma})$ as Γ ranges over the class of all graphs of order n, and to characterize the extremal graphs, i.e., graphs that achieve the bounds. Nordhaus–Gaddum-type relations have received wide attention; see the recent survey [19] by Aouchiche and Hansen and the book chapter by Mao [20].

Denote by $\mathcal{G}(n)$ the class of connected graphs of order n whose complements are also connected. In Section 3, the upper and lower bounds for $H_f(\Gamma) + H_f(\overline{\Gamma})$ and $H_f(\Gamma) \cdot H_f(\overline{\Gamma})$ are given for $\Gamma \in \mathcal{G}(n)$.

2. Bounds on $H_f(\Gamma)$

At first, we give the following upper bound for $H_f(\Gamma)$.

Theorem 3. Let Γ be an n-vertex $(n \ge 5)$, m-edge graph with a cyclomatic number γ such that $\gamma \in [2n - t - 3, 3n - 2t - 7]$, where $t (1 \le t \le n - 4)$ is the number of pendant vertices in Γ . If f(x) is a strictly convex function that has property P_{\nearrow} , then

$$H_f(\Gamma) \le f(n-1) + tf(1) + f(n-t) + f(\gamma - n + t + 5) + (\gamma - n + t + 4)f(3) + (2n - 2t - \gamma - 5)f(2)$$

with equality if and only if $\Gamma \cong K_1 \vee \left(\left(K_1 \vee \left(K_{1,\gamma_2} \cup (n_2 - \gamma_2 - 2)K_1 \right) \right) \cup tK_1 \right)$, where $n_2 = n - t - 1$, $\gamma_2 = \gamma - n + t + 2$.

Proof. Let $\Gamma \in \Gamma_{n,\gamma}$ such that $H_f(\Gamma)$ is maximum. By (1) of Theorem 1, a universal vertex $v_1 \in V(\Gamma)$ exists, and hence

$$H_f(\Gamma) = f(n-1) + H_{g_1}(\Gamma - v_1),$$

where $g_1(x) = f(x+1)$. By (2) of Theorem 1, $\Gamma - v_1$ consists of some isolated vertices and a nontrivial connected component *C*. Let $\Gamma_1 = \Gamma - v_1$. Note that *t* is the number of isolated vertices of $\Gamma - v_1$; we have

$$H_{g_1}(\Gamma - v_1) = tg_1(0) + H_{g_1}(C).$$

Suppose that m_1, n_1, γ_1 and m_2, n_2, γ_2 are the number edges, vertices, and cyclomatic number of Γ_1, Γ_2 , respectively, where $\Gamma_1 = \Gamma - v_1$ and $\Gamma_2 = C$. Since $\gamma_2 = m_2 - n_2 + 1, m_2 = m_1 - n_1 + 1, n_2 = n_1 - t, m_1 = m - n + 1, n_1 = n - 1$, we have $m_2 = m - 2n + 3$ and $n_2 = n - t - 1$, it follows that $\gamma_2 = \gamma - 2n + t + 4$; note that $\gamma \in [2n - t - 3, 3n - 2t - 7]$, so $1 \leq \gamma_2 \leq n_2 - 2$ and $n_2 \geq 3$, which implies $m_2 \geq n_2$. Then, we know that Γ_2 is a connected n_2 -vertex graph with cyclomatic number γ_2 and $1 \leq \gamma_2 \leq n_2 - 2, n_2 \geq 3$. So, we can apply Theorem 2 for Γ_2 and we have

$$H_{g_1}(\Gamma_2) \le g_1(n_2 - 1) + g_1(\gamma_2 + 1) + \gamma_2 g_1(2) + (n_2 - \gamma_2 - 2)g_1(1)$$

with equality if only if $\Gamma_2 \cong K_1 \vee (K_{1,\gamma_2} \cup (n_2 - \gamma_2 - 2)K_1)$.

Hence, we have

$$\begin{split} H_f(\Gamma) =& f(n-1) + tg_1(0) + H_{g_1}(\Gamma_2) \\ \leq & f(n-1) + tg_1(0) + g_1(n_2-1) + g_1(\gamma_2+1) + \gamma_2 g_1(2) + (n_2-\gamma_2-2)g_1(1) \\ =& f(n-1) + tf(1) + f(n-t) + f(\gamma-n+t+5) + (\gamma-n+t+4)f(3) \\ & + (2n-2t-\gamma-5)f(2) \end{split}$$

with equality if only if $\Gamma \cong K_1 \vee \left(\left(K_1 \vee \left(K_{1,\gamma_2} \cup (n_2 - \gamma_2 - 2)K_1 \right) \right) \cup tK_1 \right)$, where $n_2 = n - t - 1$, $\gamma_2 = \gamma - n + t + 2$. \Box

A similar result holds for strictly concave functions f(x), which have property P_{\searrow} : the minimum of $H_f(\Gamma)$ is reached in $\Gamma_{n,\gamma}$ if and only if $\Gamma \cong K_1 \lor \left(\left(K_1 \lor \left(K_{1,\gamma_2} \cup (n_2 - \gamma_2 - 2)K_1 \right) \right) \cup tK_1 \right)$, where $n_2 = n - t - 1$, $\gamma_2 = \gamma - n + t + 2$.

Lemma 1. If f(x) is a convex function, then $f(x) - f(x - a) \ge f(x - b) - f(x - b - a)$ with equality if and only if b = 0, where $a, b \ge 0$.

Proof. Let h(x) = f(x) - f(x - a). Since f(x) is a convex function, it follows that f'(x) is an increasing function and $h'(x) = f'(x) - f'(x - a) \ge 0$. So, h(x) is an increasing function

and $h(x) \ge h(x-b)$ with equality if and only if b = 0, and therefore $f(x) - f(x-a) \ge f(x-b) - f(x-b-a)$. \Box

We now give a lower bound for $H_f(T)$.

Theorem 4. Let T be a tree of order $n \ (n \ge 4)$. If f(x) is a convex function, then $H_f(T) \ge (n-2)f(2) + 2f(1)$ with equality if and only if $T \cong P_n$.

Proof. If n = 4, then $T \cong S_4$ or $T \cong P_4$. One can easily check that

$$H_f(S_4) = 3f(1) + f(3) > 2f(2) + 2f(1) = H_f(P_4)$$

as f(3) - f(2) > f(2) - f(1), by Lemma 1. The result holds for n = 4.

We now suppose that $n \ge 5$. We prove this result by the induction on n. Assume that the result holds for n - 1 and prove it for n. Let T' be a tree of order n - 1 such that $T - v_j = T'$, where $d_T(v_j) = 1$, $v_i = N_T(v_j)$ and $d_{T'}(v_i) = d_T(v_i) - 1 = p - 1$. Thus, we have $H_f(T') \ge (n - 3)f(2) + 2f(1)$ with equality if and only if $T' \cong P_{n-1}$. One can easily see that

$$H_f(T) = H_f(T') + f(p) - f(p-1) + f(1).$$

Since f(x) is a convex function, it follows from Lemma 1 that $f(p) - f(p-1) \ge f(2) - f(1)$ with equality if and only if p = 2. Therefore, by the induction hypothesis with the above results, we obtain

$$H_f(T) = H_f(T') + f(p) - f(p-1) + f(1)$$

$$\ge (n-3)f(2) + 3f(1) + f(p) - f(p-1)$$

$$\ge (n-2)f(1) + 2f(1)$$

and the result holds by induction. Moreover, the equality holds if and only if $T' \cong P_{n-1}$ and $d_T(v_i) = p = 2$, that is, if and only if $T \cong P_n$. \Box

Corollary 1. Let *T* be a chemical tree of order $n \ (n \ge 4)$. If f(x) is a convex function, then $H_f(T) \ge (n-2) f(2) + 2 f(1)$ with equality if and only if $T \cong P_n$.

Using Theorem 4, we obtain a lower bound for $H_f(\Gamma)$.

Theorem 5. Let Γ be a connected graph of order $n \ (n \ge 4)$. If f(x) is a convex and increasing function, then $H_f(\Gamma) \ge (n-2)f(2) + 2f(1)$ with equality if and only if $\Gamma \cong P_n$.

Proof. Since f(x) is an increasing function, it follows that $f(x + 1) + f(y + 1) \ge f(x) + f(y)$, and hence $H_f(\Gamma + e) \ge H_f(\Gamma)$, where e is an edge joining between two non-adjacent vertices in Γ . Clearly, for the graph Γ of order n, we have $H_f(\Gamma) \ge H_f(T)$, where T is a tree of order n. This result with Theorem 4, we obtain $H_f(\Gamma) \ge H_f(T) \ge (n-2)f(2) + 2f(1)$. Moreover, the equality holds if and only if $T \cong P_n$. \Box

A complete split graph $CS(n, \alpha)$ is defined as the graph join $\overline{K}_{\alpha} \vee K_{n-\alpha}$, where α is the independence number of graph $CS(n, \alpha)$.

Theorem 6. Let Γ be a connected graph of order $n \ (n \ge 4)$ with independence number α . If f(x) is a strictly increasing function, then $H_f(\Gamma) \le (n - \alpha) f(n - 1) + \alpha f(n - \alpha)$ with equality if and only if $\Gamma \cong CS(n, \alpha)$.

Proof. Since f(x) is a strictly increasing function, it follows that f(x + 1) + f(y + 1) > f(x) + f(y), and hence $H_f(\Gamma + e) > H_f(\Gamma)$, where *e* is an edge joining between two non-adjacent vertices in Γ . Since Γ is a graph of order *n* with independence number α , we must

have that Γ is a subgraph of $CS(n, \alpha)$. If $\Gamma \cong CS(n, \alpha)$, then $H_f(\Gamma) = (n - \alpha) f(n - 1) + \alpha f(n - \alpha)$; hence, the equality holds. Otherwise, $\Gamma \ncong CS(n, \alpha)$. Since Γ is a subgraph of $CS(n, \alpha)$ and $H_f(\Gamma + e) > H_f(\Gamma)$, we obtain $H_f(\Gamma) < H_f(\Gamma + e) < \cdots < H_f(CS(n, \alpha) - e_1) < H_f(CS(n, \alpha)) = (n - \alpha) f(n - 1) + \alpha f(n - \alpha)$, where e_1 is an edge in $CS(n, \alpha)$. This completes the proof of the theorem. \Box

Let *C* be the set of pendant vertices, and let *A* be the set of non-leaf vertices that have at least 2 neighbor vertices, each of which are not leaves. Let *B* be the set of non-leaf vertices that have only one neighbor vertex, which is not a leaf. Note that $V(\Gamma) = A \cup B \cup C$.

Lemma 2. Let Γ be a graph of order n, and f(x) be a convex function.

- (1) If $u \in A$, $w \in B$, and $xw \in E(\Gamma)$ such that $d_{\Gamma}(x) = 1$, $d_{\Gamma}(u) = 2$ or 3, $d_{\Gamma}(w) = 2$ or 3, then $H_f(\Gamma_1) \ge H_f(\Gamma)$, where $\Gamma_1 = \Gamma wx + ux$.
- (2) If $u \in A$, $w \in B$, and xw, $yw \in E(\Gamma)$ such that $d_{\Gamma}(x) = d_{\Gamma}(y) = 1$, $d_{\Gamma}(u) = 2$, $d_{\Gamma}(w) = 4$, then $H_f(\Gamma_2) = H_f(\Gamma)$, where $\Gamma_2 = \Gamma - wx - wy + ux + uy$.
- (3) If $u \in A$, $w \in B$, and $xw \in E(\Gamma)$ such that $d_{\Gamma}(x) = 1$, $d_{\Gamma}(u) = 3$, $d_{\Gamma}(w) = 4$, then $H_f(\Gamma_3) = H_f(\Gamma)$, where $\Gamma_3 = \Gamma wx + ux$.
- (4) If $u, v \in B$, and $xu \in E(\Gamma)$ such that $d_{\Gamma}(x) = 1$, $d_{\Gamma}(u) = 2$ or 3, $d_{\Gamma}(v) = 3$, then $H_f(\Gamma_4) \ge H_f(\Gamma)$, where $\Gamma_4 = \Gamma ux + vx$.
- (5) If $u, v, w \in B$, and $xu, yv \in E(\Gamma)$ such that $d_{\Gamma}(x) = d_{\Gamma}(y) = 1$, $d_{\Gamma}(u) = d_{\Gamma}(v) = d_{\Gamma}(w) = 2$, then $H_f(\Gamma_5) \ge H_f(\Gamma)$, where $\Gamma_5 = \Gamma xu yv + wx + wy$.
- (6) If $u, v \in B$, and $xu \in E(\Gamma)$ such that $d_{\Gamma}(x) = 1$, $d_{\Gamma}(u) = 2$ and $d_{\Gamma}(v) = 2$, then $H_f(\Gamma_6) \ge H_f(\Gamma)$, where $\Gamma_6 = \Gamma ux + vx$.

Proof. Suppose that Γ is the graph of order n and f(x) is convex. For (1), from Lemma 1, $f(d_{\Gamma}(u) + 1) - f(d_{\Gamma}(u)) + f(d_{\Gamma}(w) - 1) - f(d_{\Gamma}(w)) \ge 0$ holds for $d_{\Gamma}(u) = 2,3$ and $d_{\Gamma}(w) = 2,3$, and hence

$$H_f(\Gamma_1) = H_f(\Gamma) + f(d_{\Gamma}(u) + 1) - f(d_{\Gamma}(u)) + f(d_{\Gamma}(w) - 1) - f(d_{\Gamma}(w)) \ge H_f(\Gamma).$$

For (2), we can easily obtain

$$H_f(\Gamma_2) = H_f(\Gamma) + f(d_{\Gamma}(u) + 2) - f(d_{\Gamma}(u)) + f(d_{\Gamma}(w) - 2) - f(d_{\Gamma}(w))$$

= $H_f(\Gamma) + f(4) - f(2) + f(2) - f(4) = H_f(\Gamma).$

For (3), we have

$$H_f(\Gamma_3) = H_f(\Gamma) + f(d_{\Gamma}(u) + 1) - f(d_{\Gamma}(u)) + f(d_{\Gamma}(w) - 1) - f(d_{\Gamma}(w))$$

= $H_f(\Gamma) + f(4) - f(3) + f(3) - f(4) = H_f(\Gamma).$

For (4), from Lemma 1, we know that $f(d_{\Gamma}(v) + 1) - f(d_{\Gamma}(v)) + f(d_{\Gamma}(u) - 1) - f(d_{\Gamma}(u)) \ge 0$ holds for $d_{\Gamma}(u) = 2, 3$ and $d_{\Gamma}(v) = 3$, and hence

$$H_{f}(\Gamma_{4}) = H_{f}(\Gamma) + f(d_{\Gamma}(v) + 1) - f(d_{\Gamma}(v)) + f(d_{\Gamma}(u) - 1) - f(d_{\Gamma}(u)) \ge H_{f}(\Gamma).$$

For (5), since f(x) is a convex function, it follows that $f(1) + f(3) \ge 2f(2)$. From Lemma 1, we have $f(1) + f(4) \ge f(2) + f(3)$, and hence $2f(1) + f(4) \ge 3f(2)$. Then,

$$\begin{split} H_f(\Gamma_5) = & H_f(\Gamma) + f(d_{\Gamma}(v) - 1) - f(d_{\Gamma}(v)) + f(d_{\Gamma}(u) - 1) - f(d_{\Gamma}(u)) \\ & + f(d_{\Gamma}(w) + 2) - f(d_{\Gamma}(w)) \\ = & H_f(\Gamma) + 2f(1) - 2f(2) + f(4) - f(2) \\ = & H_f(\Gamma) + 2f(1) + f(4) - 3f(2) \ge H_f(\Gamma). \end{split}$$

For (6), from Lemma 1, we know that $f(d_{\Gamma}(v) + 1) - f(d_{\Gamma}(v)) + f(d_{\Gamma}(u) - 1) - f(d_{\Gamma}(u)) \ge 0$ holds for $d_{\Gamma}(u) = 2$ and $d_{\Gamma}(v) = 2$, and hence

$$H_{f}(\Gamma_{6}) = H_{f}(\Gamma) + f(d_{\Gamma}(v) + 1) - f(d_{\Gamma}(v)) + f(d_{\Gamma}(u) - 1) - f(d_{\Gamma}(u)) \ge H_{f}(\Gamma).$$

For chemical trees, we have the following upper bound.

Theorem 7. Let *T* be a chemical tree of order $n \ (n \ge 5)$. If f(x) is a convex function, then three integers (m_1, m_2, m_3) exist such that

$$H_{f}(T) \leq \begin{cases} m_{1}f(4) + (n - m_{1} - 1)f(1) + f(2) & \text{if } i = 0, \\ m_{2}f(4) + (n - m_{2} - 1)f(1) + f(3) & \text{if } i = 1, \\ m_{3}f(4) + (n - m_{3})f(1) & \text{if } i = 2 \end{cases}$$

with equality if and only if T contains only one 2-degree vertex but contains no 3-degree vertices for i = 0; T contains only one 3-degree vertex but contains no 2-degree vertices for i = 1; and T only contains 1-degree vertices and 4-degree vertices for i = 2, where $n \equiv i \pmod{3}$.

Proof. Suppose that *T* is a chemical tree of order *n* and f(x) is a convex function. By operations (1), (2), and (3) of Lemma 2, we can obtain a new tree *T'* with V(T') = V(T) containing no 2-degree vertices or 3-degree vertices in *A*. That is to say, all of the 2-degree vertices and 3-degree vertices are in *B*. Suppose that $n \equiv i \pmod{3}$ and n_1, n_2, n_3, n_4 are the number of vertices with degree 1, 2, 3, 4, respectively, in *T'*.

Note that $H_f(T') \ge H_f(T)$. We distinguish the following cases to show this theorem.

Case 1. *i* = 0.

We claim that $n_2 \neq 0$ or $n_3 \neq 0$; otherwise, T' contains only 1-degree and 4-degree vertices. Since $n_1 + n_4 = n$ and $n_1 + 4n_4 = 2(n - 1)$, we have $n = 3n_4 + 2$, contradicting the fact that $n \equiv 0 \pmod{3}$.

Since $n_1 + n_2 + n_3 + n_4 = n$ and $n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1)$, we have $n_2 + 2n_3 \equiv 1 \pmod{3}$, and so $n_2 - n_3 \equiv 1 \pmod{3}$ and $n_3 - n_2 \equiv 2 \pmod{3}$.

If $n_2 \ge n_3$, then it follows from (4) of Lemma 2 that

$$H_f(T') = n_1 f(1) + n_2 f(2) + n_3 f(3) + n_4 f(4)$$

$$\leq (n_1 + n_3) f(1) + (n_2 - n_3) f(2) + (n_4 + n_3) f(4).$$

Suppose that $n_2 - n_3 = 3k_1 + 1$. From (5) of Lemma 2, we have

$$H_f(T') \le (n_1 + n_3 + 2k_1)f(1) + f(2) + (n_4 + n_3 + k_1)f(4).$$

Let $m_1 = n_4 + n_3 + k_1$, and thus we are done.

If $n_2 < n_3$, then it follows from (4) of Lemma 2 that $H_f(T') = n_1f(1) + n_2f(2) + n_3f(3) + n_4f(4) \le (n_1 + n_2)f(1) + (n_3 - n_2)f(3) + (n_4 + n_2)f(4)$. Suppose that $n_3 - n_2 = 3\ell_1 + 2$. From (4) of Lemma 2, we have

$$H_f(T') \le (n_1 + n_2)f(1) + (\ell_1 + 1)f(2) + \ell_1 f(3) + (n_4 + n_2 + \ell_1 + 1)f(4) \le (n_1 + n_2 + \ell_1)f(1) + f(2) + (n_4 + n_2 + 2\ell_1 + 1)f(4).$$

Let $m_1 = n_4 + n_2 + 2\ell_1 + 1$, and thus we are done.

Case 2. *i* = 1.

We claim that $n_2 \neq 0$ or $n_3 \neq 0$; otherwise, T' contains only 1-degree and 4-degree vertices. Since $n_1 + n_4 = n$ and $n_1 + 4n_4 = 2(n - 1)$, we have $n = 3n_4 + 2$, contradicting the fact that $n \equiv 1 \pmod{3}$.

Since $n_1 + n_2 + n_3 + n_4 = n$ and $n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1)$, we have $n_2 + 2n_3 \equiv 2 \pmod{3}$, and so $n_2 - n_3 \equiv 2 \pmod{3}$, $n_3 - n_2 \equiv 1 \pmod{3}$.

If $n_2 \ge n_3$, then it follows from (4) of Lemma 2 that

$$H_f(T') = n_1 f(1) + n_2 f(2) + n_3 f(3) + n_4 f(4)$$

$$\leq (n_1 + n_3) f(1) + (n_2 - n_3) f(2) + (n_4 + n_3) f(4).$$

If $n_2 - n_3 = 3k_2 + 2$, it follows from (5) and (6) of Lemma 2 that

$$H_f(T') \le (n_1 + n_3 + 2k_2)f(1) + 2f(2) + (n_4 + n_3 + k_2)f(4)$$

$$\le (n_1 + n_3 + 2k_2 + 1)f(1) + f(3) + (n_4 + n_3 + k_2)f(4).$$

Let $m_2 = n_4 + n_3 + k_2$, and thus we are done.

If $n_2 < n_3$, then it follows from (4) of Lemma 2 that

$$H_f(T') = n_1 f(1) + n_2 f(2) + n_3 f(3) + n_4 f(4)$$

$$\leq (n_1 + n_2) f(1) + (n_3 - n_2) f(3) + (n_4 + n_2) f(4).$$

If $n_3 - n_2 = 3\ell_2 + 1$, then it follows from (4) of Lemma 2 that

$$H_{f}(T') \leq (n_{1}+n_{2})f(1) + (3\ell_{2}+1)f(3) + (n_{4}+n_{2})f(4)$$

$$\leq (n_{1}+n_{2})f(1) + \ell_{2}f(2) + (\ell_{2}+1)f(3) + (n_{4}+n_{2}+\ell_{2})f(4)$$

$$\leq (n_{1}+n_{2}+\ell_{2})f(1) + f(3) + (n_{4}+n_{2}+2\ell_{2})f(4).$$

Let $m_2 = n_4 + n_2 + 2\ell_2$, and thus we are done.

Case 3. *i* = 2.

Since $n_1 + n_2 + n_3 + n_4 = n$ and $n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1)$, we have $n_2 + 2n_3 \equiv 0 \pmod{3}$, and so $n_2 - n_3 \equiv 0 \pmod{3}$, $n_3 - n_2 \equiv 0 \pmod{3}$.

If $n_2 \ge n_3$, then it follows from (4) of Lemma 2 that $H_f(T') = n_1f(1) + n_2f(2) + n_3f(3) + n_4f(4) \le (n_1 + n_3)f(1) + (n_2 - n_3)f(2) + (n_4 + n_3)f(4)$. Suppose that $n_2 - n_3 = 3k_3$. By (5) of Lemma 2, we have

$$H_f(T') \le (n_1 + n_3 + 2k_3)f(1) + (n_4 + n_3 + k_3)f(4).$$

Let $m_3 = n_4 + n_3 + k_3$, and thus we are done.

If $n_2 < n_3$, then it follows from (4) of Lemma 2 that

$$H_f(T') = n_1 f(1) + n_2 f(2) + n_3 f(3) + n_4 f(4)$$

$$\leq (n_1 + n_2) f(1) + (n_3 - n_2) f(3) + (n_4 + n_2) f(4).$$

Suppose that $n_3 - n_2 = 3\ell_3$. By (4) of Lemma 2, we have

$$\begin{aligned} H_f(T') &\leq (n_1 + n_2)f(1) + 3\ell_3f(3) + (n_4 + n_2)f(4) \\ &\leq (n_1 + n_2)f(1) + \ell_3f(2) + \ell_3f(3) + (n_4 + n_2 + \ell_3)f(4) \\ &\leq (n_1 + n_2 + \ell_3)f(1) + (n_4 + n_2 + 2\ell_3)f(4). \end{aligned}$$

Let $m_3 = (n_4 + n_2 + 2\ell_3)$, and thus we are done. \Box

For trees, we have the following upper bound.

Theorem 8. Let T be a tree of order $n \ (n \ge 4)$. If f(x) is a convex function, then $H_f(T) \le (n-1)f(1) + f(n-1)$ with equality if and only if $T \cong S_n$.

Proof. If n = 4, then by the proof of Theorem 4, we obtain $H_f(S_4) > H_f(P_4)$. The result holds for n = 4.

We now suppose that $n \ge 5$. We prove this result by induction on n. Assume that the result holds for n - 1 and prove it for n. Let T' be a tree of order n - 1 such that $T - v_j = T'$, where $d_T(v_j) = 1$, $v_i = N_T(v_j)$ and $d_{T'}(v_i) = d_T(v_i) - 1 = p - 1$, (say). Thus, we have $H_f(T') \le (n-2)f(1) + f(n-2)$ with equality if and only if $T' \cong S_{n-1}$. One can easily see that

$$H_f(T) = H_f(T') + f(p) - f(p-1) + f(1).$$

Since f(x) is a convex function, it follows from Lemma 1 that $f(n-1) - f(n-2) \ge f(p) - f(p-1)$ with equality if and only if p = n - 1. Therefore, by the induction hypothesis with the above results, we obtain

$$H_f(T) = H_f(T') + f(p) - f(p-1) + f(1)$$

$$\leq (n-1)f(1) + f(n-2) + f(p) - f(p-1)$$

$$\leq (n-1)f(1) + f(n-1)$$

and the result holds by induction. Moreover, the equality holds if and only if $T' \cong S_{n-1}$ and $d_T(v_i) = p = n - 1$, that is, if and only if $T \cong S_n$. \Box

Remark 1. If f(x) is a convex function, then by Theorems 4 and 8, we conclude that the path P_n gives the minimum $H_f(T)$ and the star gives the maximum $H_f(T)$ among all trees of order n.

3. Nordhaus–Gaddum-Type Results

In this section, we give the Nordhaus–Gaddum-type results for the vertex degree function index.

Theorem 9. Let Γ be a graph of order n. If f(x) is a convex function, then

$$H_f(\Gamma) + H_f(\overline{\Gamma}) \ge \begin{cases} 2n f(\frac{n-1}{2}) & \text{if } n \text{ is odd,} \\ n \left[f(\frac{n}{2}) + f(\frac{n}{2} - 1) \right] & \text{if } n \text{ is even.} \end{cases}$$

Moreover, the equality holds if and only if Γ *is a* $\lfloor \frac{n}{2} \rfloor$ *-regular graph.*

Proof. We have

$$H_{f}(\Gamma) + H_{f}(\overline{\Gamma}) = \sum_{i=1}^{n} f(d_{\Gamma}(v_{i})) + \sum_{i=1}^{n} f(n-1-d_{\Gamma}(v_{i}))$$

$$= \sum_{i=1}^{n} \left[f(d_{\Gamma}(v_{i})) + f(n-1-d_{\Gamma}(v_{i})) \right].$$
 (1)

We consider two cases.

Case 1. *n* is odd.

First, we assume that $\frac{n-1}{2} \le d_{\Gamma}(v_i) \le n-1$. Setting $x = d_{\Gamma}(v_i)$, $a = b = d_{\Gamma}(v_i) - \frac{n-1}{2}$ in Lemma 1, we obtain

$$f(d_{\Gamma}(v_i)) - f\left(\frac{n-1}{2}\right) \ge f\left(\frac{n-1}{2}\right) - f(n-d_{\Gamma}(v_i)-1),$$

that is,

$$f(d_{\Gamma}(v_i)) + f(n - d_{\Gamma}(v_i) - 1) \ge 2f\left(\frac{n-1}{2}\right)$$

with equality if and only if $d_{\Gamma}(v_i) = \frac{n-1}{2}$. From (1), we obtain

$$H_f(\Gamma) + H_f(\overline{\Gamma}) \ge 2 \sum_{i=1}^n f\left(\frac{n-1}{2}\right) = 2nf\left(\frac{n-1}{2}\right)$$

with equality if and only if Γ is an $\frac{(n-1)}{2}$ -regular graph, that is, if and only if Γ is a $\lfloor \frac{n}{2} \rfloor$ -regular graph.

Next, we assume that $0 \le d_{\Gamma}(v_i) \le \frac{n-1}{2} - 1$, that is, $\frac{n-1}{2} < d_{\overline{\Gamma}}(v_i) \le n - 1$. Setting $x = d_{\overline{\Gamma}}(v_i)$, $a = b = d_{\overline{\Gamma}}(v_i) - \frac{n-1}{2}$ in Lemma 1, we obtain

$$f\left(d_{\overline{\Gamma}}(v_i)\right) - f\left(\frac{n-1}{2}\right) \ge f\left(\frac{n-1}{2}\right) - f\left(n - d_{\overline{\Gamma}}(v_i) - 1\right),$$

that is,

$$f\left(d_{\overline{\Gamma}}(v_i)\right) + f\left(n - d_{\overline{\Gamma}}(v_i) - 1\right) \ge 2f\left(\frac{n-1}{2}\right)$$

with equality if and only if $d_{\overline{\Gamma}}(v_i) = \frac{n-1}{2}$. Hence, $H_f(\Gamma) + H_f(\overline{\Gamma}) = \sum_{i=1}^n \left[f\left(d_{\Gamma}(v_i)\right) + f\left(d_{\overline{\Gamma}}(v_i)\right) \right] = \sum_{i=1}^n \left[f\left(n-1-d_{\overline{\Gamma}}(v_i)\right) + f\left(d_{\overline{\Gamma}}(v_i)\right) \right] \ge 2n f\left(\frac{n-1}{2}\right)$ with equality if and only if Γ is an $\frac{(n-1)}{2}$ -regular graph, that is, if and only if Γ is a $\lfloor \frac{n}{2} \rfloor$ -regular graph.

Case 2. *n* is even.

In this case, first we assume that $\frac{n}{2} \leq d_{\Gamma}(v_i) \leq n-1$. Setting $x = d_{\Gamma}(v_i)$, $a = d_{\Gamma}(v_i) - \frac{n}{2} + 1$, $b = d_{\Gamma}(v_i) - \frac{n}{2}$ in Lemma 1, we obtain

$$f(d_{\Gamma}(v_i)) - f\left(\frac{n}{2} - 1\right) \ge f\left(\frac{n}{2}\right) - f(n - d_{\Gamma}(v_i) - 1)$$

with equality if and only if $d_{\Gamma}(v_i) = \frac{n}{2}$, and hence

$$H_f(\Gamma) + H_f(\overline{\Gamma}) \ge \sum_{i=1}^n \left(f\left(\frac{n}{2}\right) + f\left(\frac{n}{2} - 1\right) \right) \ge n \left[f\left(\frac{n}{2}\right) + f\left(\frac{n}{2} - 1\right) \right]$$

with equality if and only if Γ is an $\frac{n}{2}$ -regular graph, that is, if and only if Γ is a $\lfloor \frac{n}{2} \rfloor$ -regular graph.

Next, we assume that $0 \le d_{\Gamma}(v_i) \le \frac{n}{2} - 1$, that is, $\frac{n}{2} \le d_{\overline{\Gamma}}(v_j) \le n - 1$. Setting $x = d_{\overline{\Gamma}}(v_j), a = d_{\overline{\Gamma}}(v_j) - \frac{n}{2} + 1, b = d_{\overline{\Gamma}}(v_j) - \frac{n}{2}$ in Lemma 1, we obtain

$$f\left(d_{\overline{\Gamma}}(v_j)\right) - f\left(\frac{n}{2} - 1\right) \ge f\left(\frac{n}{2}\right) - f\left(n - d_{\overline{\Gamma}}(v_j) - 1\right),$$

that is,

$$f\left(d_{\overline{\Gamma}}(v_j)\right) + f\left(n - d_{\overline{\Gamma}}(v_j) - 1\right) \ge f\left(\frac{n}{2}\right) + f\left(\frac{n}{2} - 1\right)$$

with equality if and only if $d_{\overline{\Gamma}}(v_j) = \frac{n}{2}$. Hence,

$$\begin{split} H_f(\Gamma) + H_f(\overline{\Gamma}) &= \sum_{i=1}^n \left[f\left(d_{\Gamma}(v_i) \right) + f\left(d_{\overline{\Gamma}}(v_i) \right) \right] = \sum_{i=1}^n \left[f\left(n - 1 - d_{\overline{\Gamma}}(v_i) \right) + f\left(d_{\overline{\Gamma}}(v_i) \right) \right] \\ &\geq n \left[f\left(\frac{n}{2} \right) + f\left(\frac{n}{2} - 1 \right) \right]. \end{split}$$

with equality if and only if Γ is an $\frac{n}{2}$ -regular graph, that is, if and only if Γ is a $\lfloor \frac{n}{2} \rfloor$ -regular graph. \Box

Theorem 10. Let Γ be a graph of order n with maximum degree Δ . If f(x) is a convex function, then

$$H_f(\Gamma) + H_f(\overline{\Gamma}) \le n \left[f(\Delta) + f(n-1-\Delta) \right]$$

with equality if and only if Γ is a regular graph or graph Γ has only two type of degrees Δ and $n - 1 - \Delta$ ($\Delta > (n - 1)/2$).

Proof. Setting $x = \Delta$, $a = \Delta - d_{\Gamma}(v_i)$ and $b = \Delta + d_{\Gamma}(v_i) - (n-1)$, by Lemma 1 we obtain

$$f(d_{\Gamma}(v_i)) + f(n-1 - d_{\Gamma}(v_i)) \le f(\Delta) + f(n-1 - \Delta)$$

with equality if and only if $d_{\Gamma}(v_i) = n - 1 - \Delta$ or i = 1. Hence,

$$H_f(\Gamma) + H_f(\overline{\Gamma}) = \sum_{i=1}^n f(d_{\Gamma}(v_i)) + \sum_{i=1}^n f(n-1-d_{\Gamma}(v_i))$$
$$\leq \sum_{i=1}^n \left[f(\Delta) + f(n-1-\Delta) \right] = n \left[f(\Delta) + f(n-1-\Delta) \right].$$

Moreover, the equality holds if and only if $d_{\Gamma}(v_i) = \Delta$ or $d_{\Gamma}(v_i) = n - 1 - \Delta$ for any vertex $v_i \in V(\Gamma)$, that is, if and only if Γ is a regular graph or graph Γ has only two type of degrees Δ and $n - 1 - \Delta$ ($\Delta > (n - 1)/2$). \Box

Corollary 2. Let Γ be a graph of order *n*. If f(x) is a convex function, then

$$H_f(\Gamma) + H_f(\overline{\Gamma}) \le n \left[f(n-1) + f(0) \right]$$

with equality if and only if Γ is a complete graph or Γ is an empty graph.

Proof. Setting x = n - 1, $a = n - 1 - \Delta$ and $b = \Delta$, by Lemma 1 we obtain

$$f(\Delta) + f(n-1-\Delta) \le f(n-1) + f(0)$$

with equality if and only if $\Delta = 0$ or $\Delta = n - 1$. Using this result with Theorem 10, we obtain the result. Moreover, the equality holds if and only if Γ is a complete graph or Γ is an empty graph. \Box

The following is the well-known Jensen inequality.

Lemma 3 (Jensen Inequality [21]). If f(x) is convex function, for all $x_1, x_2, \ldots, x_n \in [a, b]$, then

$$\sum_{i=0}^{n} f(x_i) \ge n f\left(\frac{\sum\limits_{i=0}^{n} x_i}{n}\right),$$

with equality if and only if $x_1 = x_2 = \cdots = x_n$.

Theorem 11. Let Γ be a graph of order n and size m. If f(x) is a convex function, then

$$H_f(\Gamma) + H_f(\overline{\Gamma}) \ge n f\left(\frac{2m}{n}\right) + n f\left(\frac{n(n-1) - 2m}{n}\right)$$

11 of 13

and

$$H_f(\Gamma) \cdot H_f(\overline{\Gamma}) \ge n^2 f\left(\frac{2m}{n}\right) \cdot f\left(\frac{n(n-1)-2m}{n}\right).$$

with equality if and only if Γ is a regular graph.

Proof. Since f(x) is a convex function and $\sum_{i=1}^{n} d_{\Gamma}(v_i) = 2m$, it follows from Lemma 3 that

$$\sum_{i=1}^{n} f(d_{\Gamma}(v_i)) \ge n f\left(\frac{\sum_{i=1}^{n} d_{\Gamma}(v_i)}{n}\right) = n f\left(\frac{2m}{n}\right)$$

and

$$\sum_{i=1}^{n} f(d_{\overline{\Gamma}}(v_i)) \ge n f\left(\frac{\sum_{i=1}^{n} d_{\overline{\Gamma}}(v_i)}{n}\right) = n f\left(\frac{n(n-1)-2m}{n}\right).$$

Hence,

$$H_f(\Gamma) + H_f(\overline{\Gamma}) = \sum_{i=1}^n f(d_{\Gamma}(v_i)) + \sum_{i=1}^n f(d_{\overline{\Gamma}}(v_i)) \ge n f\left(\frac{2m}{n}\right) + n f\left(\frac{n(n-1)-2m}{n}\right)$$

and

$$H_f(\Gamma) \cdot H_f(\overline{\Gamma}) = \sum_{i=1}^n f(d_{\Gamma}(v_i)) \cdot \sum_{i=1}^n f(d_{\overline{\Gamma}}(v_i)) \ge n^2 f\left(\frac{2m}{n}\right) \cdot f\left(\frac{n(n-1)-2m}{n}\right).$$

Moreover, the equality holds if and only if $d_{\Gamma}(v_i) = d_{\Gamma}(v_j)$ for $1 \le i, j \le n$, which means that Γ is a regular graph. \Box

Theorem 12. Let Γ be a graph of order n with maximum degree Δ and minimum degree δ . If f(x) is an increasing function, then

$$\begin{split} H_f(\Gamma) \cdot H_f(\overline{\Gamma}) \leq & (n-1)^2 f(\Delta) f(n-1-\delta) + (n-1) f(\delta) f(n-1-\delta) \\ & + (n-1) f(\Delta) f(n-1-\Delta) + f(\delta) f(n-1-\Delta) \end{split}$$

with equality if and only if Γ is a regular graph.

Proof. Since Δ is the maximum degree and δ is the minimum degree, we can assume that $\Delta = d_{\Gamma}(v_1) \ge d_{\Gamma}(v_2) \ge \cdots \ge d_{\Gamma}(v_n) = \delta$. Moreover, we obtain

$$n-1-\delta \ge n-1-d_{\Gamma}(v_i) \ge n-1-\Delta$$
 for $v_i \in V(\Gamma)$.

Since f(x) is an increasing function with the above results, we obtain

$$\begin{split} H_f(\Gamma) \cdot H_f(\overline{\Gamma}) &= \sum_{i=1}^n f(d_{\Gamma}(v_i)) \cdot \sum_{i=1}^n f(n-1-d_{\Gamma}(v_i)) = \left[f(\Delta) + \sum_{i=2}^{n-2} f(d_{\Gamma}(v_i)) + f(\delta) \right] \\ & \left[f(n-1-\delta) + \sum_{i=2}^{n-2} f(n-1-d_{\Gamma}(v_i)) + f(n-1-\Delta) \right] \\ & \leq \left[f(\delta) + (n-1) f(\Delta) \right] \left[f(n-1-\Delta) + (n-1) f(n-1-\delta) \right] \\ &= (n-1)^2 f(\Delta) f(n-1-\delta) + (n-1) f(\delta) f(n-1-\delta) \\ & + (n-1) f(\Delta) f(n-1-\Delta) + f(\delta) f(n-1-\Delta). \end{split}$$

Moreover, the above equality holds if and only if $d_{\Gamma}(v_i) = \Delta$ for all $v_i \in V(\Gamma)$ (i = 1, 2, ..., n-1), and $d_{\Gamma}(v_i) = \delta$ for all $v_i \in V(\Gamma)$ (i = 2, 3, ..., n), and hence $\Delta = \delta$, that is, if and only if Γ is a regular graph. \Box

Corollary 3. *Let* Γ *be a graph of order n with maximum degree* Δ *and minimum degree* δ *. If* f(x) *is an increasing function, then*

$$H_f(\Gamma) \cdot H_f(\overline{\Gamma}) \le n^2 f(\Delta) f(n-1-\delta)$$

with equality if and only if Γ is a regular graph.

Proof. Since f(x) is an increasing function, we have $f(\delta) \leq f(\Delta)$ and $f(n - 1 - \Delta) \leq f(n - 1 - \delta)$. Using these results in Theorem 12, we obtain the required result. Moreover, the equality holds if and only if Γ is a regular graph. \Box

Theorem 13. Let Γ be a graph of order n with maximum degree Δ and minimum degree δ . If f(x) is an increasing function, then

$$H_{f}(\Gamma) \cdot H_{f}(\overline{\Gamma}) \ge (n-1)^{2} f(\delta) f(n-1-\Delta) + (n-1) f(\delta) f(n-1-\delta) + (n-1) f(\Delta) f(n-1-\Delta) + f(\Delta) f(n-1-\delta)$$

with equality if and only if Γ is a regular graph.

Proof. The proof is similar to the proof of Theorem 12. Since f(x) is an increasing function, we obtain

$$\begin{split} H_f(\Gamma) \cdot H_f(\overline{\Gamma}) &= \left[f(\Delta) + \sum_{i=2}^{n-2} f(d_{\Gamma}(v_i)) + f(\delta) \right] \left[f(n-1-\delta) + \sum_{i=2}^{n-2} f(n-1-d_{\Gamma}(v_i)) \right. \\ &+ f(n-1-\Delta) \right] \\ &\geq \left[f(\Delta) + (n-1) f(\delta) \right] \left[f(n-1-\delta) + (n-1) f(n-1-\Delta) \right] \\ &= (n-1)^2 f(\delta) f(n-1-\Delta) + (n-1) f(\delta) f(n-1-\delta) \\ &+ (n-1) f(\Delta) f(n-1-\Delta) + f(\Delta) f(n-1-\delta). \end{split}$$

Moreover, the equality holds if and only if Γ is a regular graph. \Box

Corollary 4. *Let* Γ *be a graph of order n with maximum degree* Δ *and minimum degree* δ *. If* f(x) *is an increasing function, then*

$$H_f(\Gamma) \cdot H_f(\overline{\Gamma}) \ge n^2 f(\delta) f(n-1-\Delta)$$

with equality if and only if Γ is a regular graph.

4. Concluding Remarks

In this report, the *vertex-degree function index* $H_f(\Gamma)$ has been investigated for a different class of graphs. Tight bounds of the *vertex-degree function index* $H_f(\Gamma)$ have been set up for any *n* vertex-connected graphs, trees, and chemical trees. The extremal graphs where the bounds attain have also been identified. Moreover, we present the Nordhaus–Gaddum-type results for $H_f(\Gamma) + H_f(\overline{\Gamma})$ and $H_f(\Gamma) \cdot H_f(\overline{\Gamma})$, and the characterization of the extremal graphs. We now pose the following problem related to the work presented in this paper, as a potential topic for further research.

Problem 1. To find the lower and upper bounds on the vertex-degree function index $H_f(\Gamma)$ and characterize corresponding extremal graphs for other significant classes of graphs such as bicyclic, tricyclic graphs, etc.

Author Contributions: Conceptualization, D.H., Z.J., C.Y. and K.C.D.; methodology, D.H., Z.J., C.Y. and K.C.D.; investigation, D.H., Z.J., C.Y. and K.C.D.; writing—original draft preparation, D.H., Z.J., C.Y. and K.C.D.; writing—review and editing, D.H., Z.J., C.Y. and K.C.D. All authors have read and agreed to the published version of the manuscript.

Funding: D.H. is supported by the Qinghai Key Laboratory of Internet of Things Project (2017-ZJ-Y21). K.C.D. is supported by National Research Foundation funded by the Korean government (Grant No. 2021R1F1A1050646).

Data Availability Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

References

- 1. Yao, Y.; Liu, M.; Belardo, F.; Yang, C. Unified extremal results of topological indices and spectral invariants of graphs. *Discrete Appl. Math.* **2019**, *271*, 218–232. [CrossRef]
- 2. Gutman, I.; Trinajstić, N. Graph theory and molecular orbitals, Total *φ*-electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **1972**, *17*, 535–538. [CrossRef]
- 3. Furtula, B.; Gutman, I. A forgotten topological index. J. Math. Chem. 2015, 53, 1184–1190. [CrossRef]
- 4. Hu, Y.; Li, X.; Shi, Y.; Xu, T.; Gutman, I. On molecular graphs with smallest and greatest zeroth-order general Randić index. *MATCH Commun. Math. Comput. Chem.* **2005**, *54*, 425–434.
- 5. Li, X.; Zheng, J. A unified approach to the extremal trees for different indices. *MATCH Commun. Math. Comput. Chem.* **2005**, *54*, 195–208.
- 6. Ali, A.; Das, K.C.; Akhter, S. On the extremal graphs for second Zagreb index with fixed number of vertices and cyclomatic number. *Miskolc Math. Notes* **2022**, *23*, 41–50. [CrossRef]
- An, M.; Das, K.C. First Zagreb index, *k*-connectivity, β-deficiency and *k*-hamiltonicity of graphs. *MATCH Commun. Math. Comput. Chem.* 2018, *80*, 141–151.
- Das, K.C.; Dehmer, M. Comparison between the zeroth-order Randić index and the sum-connectivity index. *Appl. Math. Comput.* 2016, 274, 585–589. [CrossRef]
- 9. Das, K.C.; Xu, K.; Nam, J. On Zagreb indices of graphs. Front. Math. China 2015, 10, 567–582. [CrossRef]
- 10. Deng, H. A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs. *MATCH Commun. Math. Comput. Chem* **2007**, *57*, 597–616.
- 11. Horoldagva, B.; Das, K.C. On Zagreb indices of graphs. MATCH Commun. Math. Comput. Chem. 2021, 85, 295–301.
- 12. Ali, A.; Dimitrov, D.; Du, Z.; Ishfaq, F. On the extremal graphs for general sum-connectivity index χ_{α} with given cyclomatic number when $\alpha > 1$. *Discrete Appl. Math.* **2019**, 257, 19–30. [CrossRef]
- 13. Hu, Y.; Li, X.; Shi, Y.; Xu, T. Connected (*n*, *m*)-graphs with minimum and maximum zeroth-order general Randić index. *Discrete Appl. Math.* **2007**, *155*, 1044–1054. [CrossRef]
- 14. Das, K.C. Maximizing the sum of the squares of the degrees of a graph. Discrete Math. 2004, 285, 57–66. [CrossRef]
- 15. Li, X.; Shi, Y. (n, m)-graphs with maximum zeroth-order general Randić index for alpha is an element of $\alpha \in (-1, 0)$. *MATCH Commun. Math. Comput. Chem.* **2009**, *62*, 163–170.
- 16. Pavlović, L.; Lazić, M.; Aleksić, T. More on connected (*n*, *m*)-graphs with minimum and maximum zeroth-order general Randić index. *Discrete Appl. Math.* **2009**, 157, 2938–2944. [CrossRef]
- 17. Tomescu, I. Graphs with given cyclomatic number extremal relatively to vertex degree function index for convex functions. *MATCH Commun. Math. Comput. Chem.* **2022**, *87*, 109–114. [CrossRef]
- 18. Tomescu, I. Properties of connected (*n*,*m*)-graphs extremal relatively to vertex degree function index for convex functions. *MATCH Commun. Math. Comput. Chem.* **2021**, *85*, 285–294.
- 19. Aouchiche, M.; Hansen, P. A survey of Nordhaus–Gaddum type relations. *Discrete Appl. Math.* 2013, 161, 466–546. [CrossRef]
- 20. Mao, Y. Nordhaus–Gaddum Type Results in Chemical Graph Theory; Bounds in Chemical Graph Theory–Advances; Gutman, I., Furtula, B., Das, K.C., Milovanović, E., Milovanovixcx, I., Eds.; University Kragujevac: Kragujevac, Serbia, 2017; pp. 3–127.
- 21. Jensen, J.L.W.V. Sur les fonctions convexes et les inégalités entre les valeurs moyennes. Acta Math. 1906, 30, 175–193. [CrossRef]

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.