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On the vertex-degree-function indices of connected (n, m)-graphs of maximum degree at most four

by

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Abstract

Consider a graph G and a real-valued function f defined on the degree set of G. The sum of the outputs $f(d_v)$ over all vertices $v \in V(G)$ of G is usually known as the vertex-degree-function index and is denoted by $H_f(G)$, where d_v represents the degree of a vertex v of G. This paper gives sharp bounds on the index $H_f(G)$ in terms of order and size of G when G is connected and has the maximum degree at most 4. All the graphs achieving the derived bounds are also determined. Bounds involving several existing indices – including the general zeroth-order Randić index and coindex, the general multiplicative first/second Zagreb index, the variable sum lodeg index, the variable sum exdeg index – are deduced as the special cases of the obtained ones.

Key Words: Chemical graph theory, topological index, vertex-degree-function indices, degree of a vertex.
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1 Introduction

This study is concerned with only connected and finite graphs. The (chemical-)graph theoretical concepts used in the this paper without providing their definitions can be found in the related books like [26, 22, 6, 5].

A topological index is a function defined on the set of all graphs with the condition that it remains the same under the graph isomorphism. The degree set of a graph G is the set consisting of all distinct elements of the degree sequence of G. Consider a graph G and a real-valued function f defined on the degree set of G. The sum of the outputs $f(d_v)$ over all vertices $v \in V(G)$ of G is usually known as the vertex-degree-function index and is denoted by $H_f(G)$, where d_v represents the degree of a vertex v of G. Thus,

$$H_f(G) = \sum_{v \in V(G)} f(d_v). \tag{1}$$

Although the terminology and notation of the topological index H_f that is being used by several researchers was coined by Yao et al. [27], to the best of authors' knowledge such indices were studied first by Linial and Rozenman in [14]. These indices have been the subject of several recent papers; see for example the recent articles [20, 10, 21], recent review paper [12], and related publications cited therein.

If vertices u and v are adjacent in G, we write $u \sim v$, otherwise we write $u \nsim v$. Let $TI(G)$ be a vertex–degree–based topological index of the form:

$$TI(G) = \sum_{u \sim v} (f(d_u) + f(d_v)) = \sum_{u \in V(G)} d_u f(d_u)\,;$$

the right-handed identity is a special case of a more general identity reported in [7]. Then, the corresponding coindex, $\overline{TI}(G)$ can be defined [9, 15] as:

$$\overline{TI}(G) = \sum_{u \nsim v} (f(d_u) + f(d_v)) = \sum_{u \in V(G)} (n - 1 - d_u) f(d_u)\,.$$

The following identity is valid

$$TI(G) + \overline{TI}(G) = (n-1) \sum_{u \in V(G)} f(d_u) = (n-1) H_f(G)\,. \tag{2}$$

In what follows, some existing indices are given that are special cases of Equation (1).

- Equation (1) gives the general zeroth-order Randić index if $f(x) = x^{\alpha}$ (see for example [17, 2, 13, 16, 3]), where α is a real number.

- The general zeroth–order Randić coindex is obtained from Equation (1) corresponding to the choice $f(x) = (n - 1 - x)x^{\alpha-1}$, where n is the order of the graph under consideration and α is a real number (see e.g. [19, 18]). Particularly, if $\alpha = 3$, then the forgotten topological coindex $\overline{F}(G) = \sum_{u \in V(G)} (n - 1 - d_u) d_u^2$ is obtained (see for example [4, 8]); the forgotten topological coindex is same as the Lanzhou index [25].

- One gets the natural logarithm of the general multiplicative first Zagreb index (general multiplicative second Zagreb index, respectively) [23] by taking $f(x) = \ln x^a$ ($f(x) = \ln x^{ax}$, respectively), where $a \in \mathbb{R}$ (that is the set of real numbers).

- The substitution $f(x) = x(\ln x)^a$ in Equation (1) yields the variable sum lodeg index [24], where $a \in \mathbb{R}$

- If $f(x) = xa^x$ then Equation (1) gives the variable sum exdeg index (see for example [24, 1]), where $a > 0$ with $a \neq 1$.

A graph with n vertices and m edges is known as an (n, m)-graph. A chemical graph is the one with the maximum degree at most four. This paper gives sharp bounds on the index $H_f(G)$ for chemical (n, m)-graphs in terms of m and n. All the graphs achieving the derived bounds are also identified. Bounds involving the above-mentioned existing indices (that is, the general zeroth-order Randić index and coindex, the general multiplicative first/second Zagreb index, the variable sum lodeg index, the variable sum exdeg index) are deduced as the special cases of the obtained bounds.

2 Main results

For a graph G, its number of vertices having the degree r is denoted by n_r. If G is a chemical (n,m)-graph, then

$$H_f(G) = \sum_{i=1}^{4} n_i\, f(i), \tag{3}$$

$$\sum_{i=1}^{4} n_i = n, \tag{4}$$

$$\sum_{i=1}^{4} i\, n_i = 2m, \tag{5}$$

We solve Equations (4) and (5) for the quantities n_1, n_4, and then substitute their values in Equation (3):

$$H_f(G) = \frac{1}{3}\Big(4f(1) - f(4)\Big)n + \frac{2}{3}\Big(f(4) - f(1)\Big)m$$
$$+ \left(f(2) - \frac{2}{3}f(1) - \frac{1}{3}f(4)\right) n_2 + \left(f(3) - \frac{1}{3}f(1) - \frac{2}{3}f(4)\right) n_3\,. \tag{6}$$

Let us take

$$\Gamma_f(G) = \left(f(2) - \frac{2}{3}f(1) - \frac{1}{3}f(4)\right) n_2 + \left(f(3) - \frac{1}{3}f(1) - \frac{2}{3}f(4)\right) n_3\,. \tag{7}$$

Now, Equation (6) yields

$$H_f(G) = \frac{1}{3}\Big(4f(1) - f(4)\Big)n + \frac{2}{3}\Big(f(4) - f(1)\Big)m + \Gamma_f(G)\,. \tag{8}$$

Let

$$\xi_1 = f(2) - \frac{2}{3}f(1) - \frac{1}{3}f(4) \quad \text{and} \quad \xi_2 = f(3) - \frac{1}{3}f(1) - \frac{2}{3}f(4) \tag{9}$$

be the coefficients of n_2 and n_3, respectively, in (7). From Equation (8), it is evident that if one wants to establish a bound on H_f for chemical (n,m)-graphs in terms of m and n, it is enough to determine the least or greatest Γ_f-value for chemical (n,m)-graphs. Thence, in the next lemma, we derive a bound on Γ_f for chemical (n,m)-graphs.

Lemma 2.1. *Let G be a chemical (n,m)-graph such that $n_2 + n_3 \geq 2$.*

(i). *If both ξ_1 and ξ_2 are negative such that $2\xi_2 < \xi_1 < \xi_2/2$, then*

$$\Gamma_f(G) < \min\{\xi_1, \xi_2\}\,.$$

(ii). *If both ξ_1 and ξ_2 are positive such that $\xi_2/2 < \xi_1 < 2\xi_2$, then*

$$\Gamma_f(G) > \max\{\xi_1, \xi_2\}\,.$$

Proof. (i) Take $\max\{\xi_1,\xi_2\}=\xi_{max}$. Note that

$$\Gamma_f(G)=\xi_1 n_2+\xi_2 n_3 \le (n_2+n_3)\xi_{max} \le 2\xi_{max} < \min\{\xi_1,\xi_2\}.$$

(ii) Let $\min\{\xi_1,\xi_2\}=\xi_{min}$. Then

$$\Gamma_f(G)=\xi_1 n_2+\xi_2 n_3 \ge (n_2+n_3)\xi_{min} \ge 2\xi_{min} > \max\{\xi_1,\xi_2\}.$$

□

Recall that the degree set of a graph G is the set of all unequal degrees of vertices of G.

Theorem 2.2. *Let G be a chemical (n,m)-graph, where $n\ge 5$. Let ξ_1 and ξ_2 be the numbers defined in* (9).

(i). *If both ξ_1 and ξ_2 are negative such that $2\xi_2<\xi_1<\xi_2/2$, then*

$$H_f(G) \le \frac{1}{3}\Big(4f(1)-f(4)\Big)n+\frac{2}{3}\Big(f(4)-f(1)\Big)m + \begin{cases} f(2)-\frac{2}{3}f(1)-\frac{1}{3}f(4) & \text{if } 2m-n\equiv 1 \pmod 3 \\ f(3)-\frac{1}{3}f(1)-\frac{2}{3}f(4) & \text{if } 2m-n\equiv 2 \pmod 3 \\ 0 & \text{if } 2m-n\equiv 0 \pmod 3 \end{cases}$$

with equality if and only if
- *G contains no vertex of degree 3 and it contains only one vertex of degree 2 whenever $2m-n\equiv 1 \pmod 3$;*
- *G contains no vertex of degree 2 and it contains only one vertex of degree 3 whenever $2m-n\equiv 2 \pmod 3$;*
- *G contains neither any vertex of degree 2 nor any vertex of degree 3 whenever $2m-n\equiv 0 \pmod 3$.*

(ii) *If both ξ_1 and ξ_2 are positive such that $\xi_2/2<\xi_1<2\xi_2$, then*

$$H_f(G) \ge \frac{1}{3}\Big(4f(1)-f(4)\Big)n+\frac{2}{3}\Big(f(4)-f(1)\Big)m + \begin{cases} f(2)-\frac{2}{3}f(1)-\frac{1}{3}f(4) & \text{if } 2m-n\equiv 1 \pmod 3 \\ f(3)-\frac{1}{3}f(1)-\frac{2}{3}f(4) & \text{if } 2m-n\equiv 2 \pmod 3 \\ 0 & \text{if } 2m-n\equiv 0 \pmod 3 \end{cases}$$

with equality if and only if
• *G contains no vertex of degree 3 and it contains only one vertex of degree 2 whenever* $2m - n \equiv 1 \pmod 3$*;*
• *G contains no vertex of degree 2 and it contains only one vertex of degree 3 whenever* $2m - n \equiv 2 \pmod 3$*;*
• *G contains neither any vertex of degree 2 nor any vertex of degree 3 whenever* $2m - n \equiv 0 \pmod 3$.

Proof. Because the proofs of the both parts are similar to each other, we prove only Part (i). If the inequality $n_2 + n_3 \geq 2$ holds, then by using Lemma 2.1 and Equation (8), one has

$$\begin{aligned} H_f(G) &< \frac{1}{3}\Big(4f(1) - f(4)\Big)n + \frac{2}{3}\Big(f(4) - f(1)\Big)m \\ &\quad + \min\left\{f(2) - \frac{2}{3}f(1) - \frac{1}{3}f(4), f(3) - \frac{1}{3}f(1) - \frac{2}{3}f(4)\right\} \\ &< \frac{1}{3}\Big(4f(1) - f(4)\Big)n + \frac{2}{3}\Big(f(4) - f(1)\Big)m \end{aligned}$$

as desired.
In the remaining proof, assume that $n_2 + n_3 \leq 1$. Then, $(n_2, n_3) \in \{(0,0), (1,0), (0,1)\}$. From Equations (4) and (5), it follows that $n_2 + 2n_3 \equiv 2m - n \pmod 3$ (see for example [11]), which gives

$$(n_2, n_3) = \begin{cases} (1,0) & \text{if } \; 2m - n \equiv 1 \pmod 3, \\ (0,1) & \text{if } \; 2m - n \equiv 2 \pmod 3, \\ (0,0) & \text{if } \; 2m - n \equiv 0 \pmod 3. \end{cases}$$

The required result follows now from Equation (6). □

In what follows, we consider some well-known topological indices that satisfy the assumptions of Theorem 2.2 and hence yield different corollaries of Theorem 2.2.

First, we take $f(x) = x^\alpha$. Then H_f is the general zeroth-order Randić index ${}^0R_\alpha$. Here, we have

$$\xi_1 = f(2) - \frac{2}{3}f(1) - \frac{1}{3}f(4) = \begin{cases} -\dfrac{(2^\alpha - 2)(2^\alpha - 1)}{3} < 0 & \text{if either } \alpha > 1 \text{ or } \alpha < 0, \\ -\dfrac{(2^\alpha - 2)(2^\alpha - 1)}{3} > 0 & \text{if } 0 < \alpha < 1, \end{cases}$$

and

$$\xi_2 = f(3) - \frac{1}{3}f(1) - \frac{2}{3}f(4) = \begin{cases} \dfrac{3^{\alpha+1} - 2^{2\alpha+1} - 1}{3} < 0 & \text{if either } \alpha > 1 \text{ or } \alpha < 0, \\ \dfrac{3^{\alpha+1} - 2^{2\alpha+1} - 1}{3} > 0 & \text{if } 0 < \alpha < 1. \end{cases}$$

Also,

$$2\xi_2 = \frac{2(3^{\alpha+1} - 2^{2\alpha+1} - 1)}{3} < \xi_1 = -\frac{(2^\alpha - 2)(2^\alpha - 1)}{3} < \frac{\xi_2}{2} = \frac{3^{\alpha+1} - 2^{2\alpha+1} - 1}{6} \tag{10}$$

holds if either $\alpha > 1$ or $\alpha < 0$. If each inequality sign "$<$" of (10) is replaced with "$>$" then the resulting inequality holds for $0 < \alpha < 1$. Thus, we have the following known [11] result as a direct consequence of Theorem 2.2.

Corollary 2.3. *Let G be a chemical (n,m)-graph, where $n \geq 5$. If either $\alpha > 1$ or $\alpha < 0$, then*

$$^0R_\alpha(G) \leq \frac{4-4^\alpha}{3}n + \frac{2(4^\alpha - 1)}{3}m + \begin{cases} -\dfrac{(2^\alpha - 2)(2^\alpha - 1)}{3} & \text{if } 2m - n \equiv 1 \pmod 3 \\ \dfrac{3^{\alpha+1} - 2^{2\alpha+1} - 1}{3} & \text{if } 2m - n \equiv 2 \pmod 3 \\ 0 & \text{if } 2m - n \equiv 0 \pmod 3 \end{cases}$$

where the equality characterization is the same as specified in Theorem 2.2. If $0 < \alpha < 1$ then the above inequality for $^0R_\alpha(G)$ is reversed.

Now, we take $f(x) = xa^x$ with $a > 0$ but $a \neq 1$. Then H_f is the variable sum exdeg index SEI_a. Here, we have

$$\xi_1 = f(2) - \frac{2}{3}f(1) - \frac{1}{3}f(4) = \begin{cases} -\dfrac{2a(a-1)(2a^2+2a-1)}{3} < 0 & \text{if either } 0 < a < \dfrac{1}{3} \text{ or } a > 1 \\ -\dfrac{2a(a-1)(2a^2+2a-1)}{3} > 0 & \text{if } \dfrac{1}{2} < a < 1, \end{cases}$$

and

$$\xi_2 = f(3) - \frac{1}{3}f(1) - \frac{2}{3}f(4) = \begin{cases} -\dfrac{a(a-1)(8a^2-a-1)}{3} < 0 & \text{if either } 0 < a < \dfrac{1}{3} \text{ or } a > 1 \\ -\dfrac{a(a-1)(8a^2-a-1)}{3} > 0 & \text{if } \dfrac{1}{2} < a < 1, \end{cases}$$

Also,

$$\begin{aligned} 2\xi_2 = -\frac{2a(a-1)(8a^2-a-1)}{3} &< \xi_1 = -\frac{2a(a-1)(2a^2+2a-1)}{3} \\ &< \frac{\xi_2}{2} = -\frac{a(a-1)(8a^2-a-1)}{6} \end{aligned} \tag{11}$$

holds if either $a > 1$ or $0 < a < \frac{1}{3}$. If each inequality sign "$<$" in (11) is replaced with "$>$" then the resulting inequality holds for $\frac{1}{2} < a < 1$. Thus, we have the next result that follows directly from Theorem 2.2.

Corollary 2.4. *Let G be a chemical (n,m)-graph, where $n \geq 5$. If either $a > 1$ or $0 < a < \frac{1}{3}$, then*

$$SEI_a(G) \leq \frac{4a(1-a^3)n}{3} + \frac{2a(4a^3-1)m}{3} + \begin{cases} \dfrac{2a(1-a)(2a^2+2a-1)}{3} & \text{if } 2m-n \equiv 1 (\text{mod } 3) \\ \dfrac{a(1-a)(8a^2-a-1)}{3} & \text{if } 2m-n \equiv 2 (\text{mod } 3) \\ 0 & \text{if } 2m-n \equiv 0 (\text{mod } 3) \end{cases}$$

where the equality characterization is the same as specified in Theorem 2.2. If $\frac{1}{2} < a < 1$ then the above inequality for $SEI_a(G)$ is reversed.

Next, we take $f(x) = x(\ln x)^a$ with $a > 0$. Then H_f is the variable sum lodeg index SLI_a. Here, for $a > \frac{\ln 3 - \ln 4}{\ln(\ln 2) - \ln(\ln 3)}$ (≈ 0.6246), we have

$$\xi_1 = f(2) - \frac{2}{3}f(1) - \frac{1}{3}f(4) = \frac{2\big(3(\ln 2)^a - 2(\ln 4)^a\big)}{3} < 0,$$

$$\xi_2 = f(3) - \frac{1}{3}f(1) - \frac{2}{3}f(4) = \frac{9(\ln 3)^a - 8(\ln 4)^a}{3} < 0$$

and

$$2\xi_2 = \frac{2\big(9(\ln 3)^a - 8(\ln 4)^a\big)}{3} < \xi_1 = \frac{2\big(3(\ln 2)^a - 2(\ln 4)^a\big)}{3} < \frac{\xi_2}{2} = \frac{9(\ln 3)^a - 8(\ln 4)^a}{6}.$$

Hence, the following corollary is another direct consequence of Theorem 2.2.

Corollary 2.5. *Let G be a chemical (n,m)-graph, where $n \geq 5$. If*

$$a > \frac{\ln 3 - \ln 4}{\ln(\ln 2) - \ln(\ln 3)} \quad (\approx 0.6246),$$

then

$$SLI_a(G) \leq \frac{8(\ln 4)^a}{3} m - \frac{4(\ln 4)^a}{3} n + \begin{cases} \dfrac{2\big(3(\ln 2)^a - 2(\ln 4)^a\big)}{3} & \text{if } 2m-n \equiv 1 \,(\text{mod } 3) \\ \dfrac{9(\ln 3)^a - 8(\ln 4)^a}{3} & \text{if } 2m-n \equiv 2 \,(\text{mod } 3) \\ 0 & \text{if } 2m-n \equiv 0 \,(\text{mod } 3) \end{cases}$$

where the equality characterization is the same as specified in Theorem 2.2.

Finally, if we take $f(x) = (n-1-x)x^2$, or $f(x) = \ln x^{ax}$, or $f(x) = \ln x^a$, then H_f is the forgotten topological coindex $\overline{F}(G)$ (see [4, 8]), or the natural logarithm of the general multiplicative first Zagreb index $\ln \Pi_{1,a}$, or the natural logarithm of the general multiplicative second Zagreb index $\ln \Pi_{2,a}$, respectively.

- If we take $f(x) = (n-1-x)x^2$ with $n \geq 11$, or $f(x) = \ln x^{ax}$ with $a > 0$, or $f(x) = \ln x^a$ with $a < 0$, then f satisfies the conditions of Theorem 2.2(i).

- If we take $f(x) = \ln x^a$ with $a > 0$, or $f(x) = \ln x^{ax}$ with $a < 0$, then f satisfies the conditions of Theorem 2.2(ii).

Hence, the next result follows immediately from Theorem 2.2.

Corollary 2.6. *Let G be a chemical (n,m)-graph, where $n \geq 5$. If $a < 0$ then*

$$\Pi_{1,a}(G) \leq \begin{cases} 2^{\frac{a(4m-2n+1)}{3}} & \text{if} \quad 2m-n \equiv 1 \pmod 3 \\ 2^{\frac{2a(2m-n-2)}{3}} 3^a & \text{if} \quad 2m-n \equiv 2 \pmod 3 \\ 2^{\frac{2a(2m-n)}{3}} & \text{if} \quad 2m-n \equiv 0 \pmod 3, \end{cases}$$

$$\Pi_{2,a}(G) \geq \begin{cases} 2^{\frac{2a(8m-4n-1)}{3}} & \text{if} \quad 2m-n \equiv 1 \pmod 3 \\ 2^{\frac{8a(2m-n-2)}{3}} 3^{3a} & \text{if} \quad 2m-n \equiv 2 \pmod 3 \\ 2^{\frac{8a(2m-n)}{3}} & \text{if} \quad 2m-n \equiv 0 \pmod 3, \end{cases}$$

and if $n \geq 11$ then

$$\overline{F}(G) \leq \begin{cases} 2\Big(m(5n-26) - n(2n-11) + 8\Big) & \text{if} \quad 2m-n \equiv 1 \pmod 3 \\ 2\Big(m(5n-26) - n(2n-11) + 9\Big) & \text{if} \quad 2m-n \equiv 2 \pmod 3 \\ 2\Big(m(5n-26) - 2n(n-6)\Big) & \text{if} \quad 2m-n \equiv 0 \pmod 3, \end{cases}$$

where the equality characterization in any of the above inequalities involving $\Pi_{1,a}(G)$, $\Pi_{2,a}(G)$, $\overline{F}(G)$, is the same as specified in Theorem 2.2. If $a > 0$ then the above inequalities involving $\Pi_{1,a}(G)$ and $\Pi_{2,a}(G)$ are reversed.

From Theorem 2.2 and the identity (2), the next result follows.

Theorem 2.7. *Let G be a chemical (n,m)-graph, where $n \geq 5$. Let ξ_1 and ξ_2 be the numbers defined in (9).*

(i) *If both ξ_1 and ξ_2 are negative such that $2\xi_2 < \xi_1 < \xi_2/2$, then*

$$TI(G) + \overline{TI}(G) \leq (n-1)\left(\frac{1}{3}\Big(4f(1) - f(4)\Big)n + \frac{2}{3}\Big(f(4) - f(1)\Big)m\right)$$

$$+ \begin{cases} (n-1)\Big(f(2) - \frac{2}{3}f(1) - \frac{1}{3}f(4)\Big) & \text{if} \quad 2m-n \equiv 1 \pmod 3 \\ (n-1)\Big(f(3) - \frac{1}{3}f(1) - \frac{2}{3}f(4)\Big) & \text{if} \quad 2m-n \equiv 2 \pmod 3 \\ 0 & \text{if} \quad 2m-n \equiv 0 \pmod 3, \end{cases}$$

with equality if and only if
• *G contains no vertex of degree* 3 *and it contains only one vertex of degree* 2 *whenever* $2m - n \equiv 1 \pmod 3$*;*
• *G contains no vertex of degree* 2 *and it contains only one vertex of degree* 3 *whenever* $2m - n \equiv 2 \pmod 3$*;*
• *G contains neither any vertex of degree* 2 *nor any vertex of degree* 3 *whenever* $2m - n \equiv 0 \pmod 3$.

(ii) *If both* ξ_1 *and* ξ_2 *are positive such that* $\xi_2/2 < \xi_1 < 2\xi_2$*, then*

$$TI(G) + \overline{TI}(G) \geq (n-1)\left(\frac{1}{3}\Big(4f(1) - f(4)\Big)n + \frac{2}{3}\Big(f(4) - f(1)\Big)m\right)$$

$$+ \begin{cases} (n-1)\Big(f(2) - \frac{2}{3}f(1) - \frac{1}{3}f(4)\Big) & \text{if } \; 2m - n \equiv 1 \pmod 3 \\ (n-1)\Big(f(3) - \frac{1}{3}f(1) - \frac{2}{3}f(4)\Big) & \text{if } \; 2m - n \equiv 2 \pmod 3 \\ 0 & \text{if } \; 2m - n \equiv 0 \pmod 3 \end{cases}$$

with equality if and only if
• *G contains no vertex of degree* 3 *and it contains only one vertex of degree* 2 *whenever* $2m - n \equiv 1 \pmod 3$*;*
• *G contains no vertex of degree* 2 *and it contains only one vertex of degree* 3 *whenever* $2m - n \equiv 2 \pmod 3$*;*
• *G contains neither any vertex of degree* 2 *nor any vertex of degree* 3 *whenever* $2m - n \equiv 0 \pmod 3$.

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