

Graphs with Minimum Vertex-Degree Function-Index for Convex Functions¹

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Abstract

An (n, m) -graph is a graph with n vertices and m edges. The vertex-degree function-index $H_f(G)$ of a graph G is defined as $H_f(G) = \sum_{v \in V(G)} f(d(v))$, where f is a real function. Recently, Tomescu considered the upper bound of $H_f(G)$ and got the connected (n, m) -graph G with $m \geq n$ which maximizes $H_f(G)$ if $f(x)$ is strictly convex with two special properties. He also characterized all (n, m) -graphs G with $1 \leq m \leq n$ satisfying that $H_f(G) \leq f(m) + mf(1) + (n - m - 1)f(0)$ if $f(x)$ is strictly convex and differentiable and its derivative is strictly convex. In this paper, we will consider the lower bound of $H_f(G)$ and show that every (n, m) -graph with $1 \leq m \leq n(n - 1)/2$ satisfies that $H_f(G) \geq rf(k + 1) + (n - r)f(k)$ if $f(x)$ is strictly convex, where $k = \lfloor 2m/n \rfloor$ and $r = 2m - nk$. Moreover, the equality holds if and only if $G \in \mathcal{G}(n, m)$, where $\mathcal{G}(n, m)$ is the family of all (n, m) -graphs G satisfying that the vertex-degree $d(v) \in \{\lfloor \frac{2m}{n} \rfloor, \lceil \frac{2m}{n} \rceil\}$ for all $v \in V(G)$. Under the same condition on f we also obtain a result for the minimum of $H_f(G)$ among all connected (n, m) -graphs. It is easy to see that if $f(x)$ is strictly concave, we can get the maximum case for $H_f(G)$.

1 Introduction

We only consider simple and finite graphs in this paper. For terminology and notation not defined here, we refer the reader to [2, 20]. We use $V(G)$ and $E(G)$ to denote

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the vertex-set and edge-set of a graph G , respectively. An (n, m) -graph is a graph $G = (V(G), E(G))$, where $m = |E(G)|$ and $n = |V(G)|$. Let $G(n, m)$ represent the collection of all (n, m) -graphs. For any two vertices u and v , if u is adjacent to v , we denote it by $u \sim v$. A graph G is called k -regular if the degree $d(v) = k$ for every $v \in V(G)$. We denote a complete graph with n vertices by K_n . Moreover, we use C_n and P_n to denote a cycle and a path on n vertices, respectively.

For two disjoint graphs G and H , the union $G \cup H$ of G and H is a new graph with $V(G \cup H) = V(G) \cup V(H)$ and $E(G \cup H) = E(G) \cup E(H)$. For two disjoint graphs G and H , we use $G \vee H$ to denote a new graph obtained by adding edges joining every vertex of G to every vertex of H . For a subset F of $E(G)$, we use $G - F$ to denote the subgraph of G obtained by deleting all edges of F from G , whereas for a subset S of $V(G)$, we use $G - S$ to denote the subgraph of G induced by $V \setminus S$ in G . If M is a matching of G , we use $|M|$ to denote the number of edges in M .

Denote the degree of a vertex v in G also by d_v , and denote the sequence of degrees of a graph G with n vertices by $\mathbf{d} = (d_1, d_2, \dots, d_n)$. In this paper, we will study a kind of general chemical index, called the vertex-degree function-index $H_f(G)$ of a graph G with function $f(x)$, which was first introduced by Linial and Rozenman in [14], and is defined as follows:

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

Another topological function-index TI was introduced by Gutman in [5]. For a symmetric real function $f(x, y)$ and a graph G , the topological index is defined as

$$TI(G) = \sum_{uv \in E(G)} f(d_u, d_v).$$

This was also called the *bond-incident-degree index* $BID(G)$ by Vukićević and Durdević in [21]. Notice that by taking the symmetric real function equals to $f(x)/x + f(y)/y$ for some function $f(x)$, one could deduce that $H_f(G)$ is a special case of $TI(G)$. For more knowledge on TI we refer to [4, 5, 10, 16, 21], and we denoted $TI(G)$ by $IT_f(G)$ in [10].

In the past years, many researchers have done a lot of work on chemical indices,

including Zagreb indices; see [3, 6, 8, 9, 11–13, 17] and the references therein. Recently, Tomescu [18, 19] studied $H_f(G)$ for convex function f . He gave some upper bounds for the function-index $H_f(G)$ and the function f is required to satisfy some other properties except for the convexity. Their results are stated as follows.

Theorem 1.1. [Lemma 2.2 [18]] *If $G \in G(n, m)$ maximizes (minimizes) $H_f(G)$ where $f(x)$ is strictly convex (concave), then G has at most one nontrivial connected component C and C has a vertex of degree $|V(C)| - 1$.*

Theorem 1.2. [Theorem 2.3 [19]] *Let $n \geq 2$ and $G \in G(n, m)$ such that $1 \leq m \leq n-1$. If $f(x)$ is a strictly convex function having property that $f(x)$ is differentiable and its derivative is strictly convex, then it holds that*

$$H_f(G) \leq f(m) + mf(1) + (n - m - 1)f(0),$$

with equality if and only if $G = S_{m+1} \cup (n - m - 1)K_1$.

Theorem 1.3. [Theorem 2.4 [19]] *If $n \geq 3$, $n \leq m \leq 2n - 3$, $f(x)$ is a strictly convex function having property that $f(x)$ is differentiable and its derivative is strictly convex, and $G \in G(n, m)$ is connected, then it holds that*

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

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

As one can see, Tomescu's results are all about the upper bound of $H_f(G)$. Ali et al. in [1] gave the following lower bound for connected (n, m) -graphs under some constraints on n and m .

Theorem 1.4. [Theorem 1 [1]] *If $n \geq 4$, $3n/2 \geq m \geq n+1$ and $f(x)$ is a convex function, then among all connected (n, m) -graphs, graphs in $\mathcal{G}(n, m)$ attain the minimum value of $H_f(G)$, where the graph family $\mathcal{G}(n, m)$ is defined in the following Definition 1.5.*

In this paper, we will further study the minimum (maximum) values of $H_f(G)$ among all (n, m) -graphs with the property that f is strictly convex (concave). Moreover,

we will give a same result among all connected (n, m) -graphs. Note that our result Theorem 1.7 will cover the result Theorem 1.4. Before proceeding, we give the definition of our extremal graphs as follows.

Definition 1.5. Given $n \geq 2$ and $1 \leq m \leq n(n-1)/2$, define $\mathcal{G}(n, m)$ to be the family of all (n, m) -graphs G satisfying that $d(v) \in \{\lfloor \frac{2m}{n} \rfloor, \lceil \frac{2m}{n} \rceil\}$ for all $v \in V(G)$.

For an (n, m) -graph G , let $k = \lfloor 2m/n \rfloor$ and $r = 2m - kn \in \{0, 1, \dots, n-1\}$, then G belongs to $\mathcal{G}(n, m)$ if and only if G has r vetices of degree k and $n - r$ vertices of degree $k + 1$. Note that for some given m and n , the graph family $\mathcal{G}(n, m)$ contains both connected and disconnected graphs. We give an example in Figure 1.

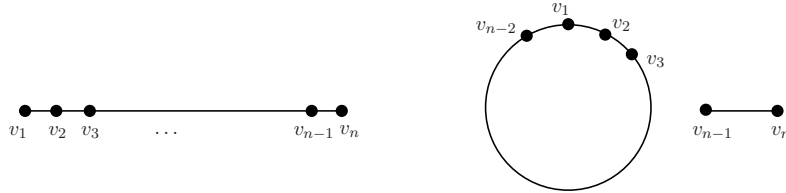


Figure 1. Graphs P_n and $C_{n-2} \cup K_2$ in $\mathcal{G}(n, m)$ for $m = n - 1$ and $n \geq 5$.

Our main results are stated as follows.

Theorem 1.6. Let $n \geq 2$ and G be an (n, m) -graph with $1 \leq m \leq n(n-1)/2$, and let $k = \lfloor 2m/n \rfloor$ and $r = 2m - kn$. If f is a strictly convex function, then it holds that

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

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

We will construct some graphs to show that for $n \leq m \leq n(n-1)/2$, there are connected graphs $G \in \mathcal{G}(n, m)$, and for $m = n - 1$, we have the path $P_n \in \mathcal{G}(n, n - 1)$. Therefore, if we consider only connected (n, m) -graphs, we also have the following result.

Theorem 1.7. Let $n \geq 2$ and G be a connected (n, m) -graph with $n - 1 \leq m \leq n(n-1)/2$, and let $k = \lfloor 2m/n \rfloor$ and $r = 2m - kn$. If f is a strictly convex function, then it holds that

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

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

Our results can cover some previous known results. For example, for the general zeroth-order Randić index ${}^0R_\alpha(G)$, the function $f(x) = x^\alpha$ is strictly convex for $\alpha > 1$. Then we can obtain a lower bound of Randić index ${}^0R_\alpha(G)$ by Theorem 1.6, and moreover, ${}^0R_\alpha(G)$ attains the minimum if and only if $G \in \mathcal{G}(n, m)$.

2 Preliminaries

At first we recall an important inequality, the *Jensen inequality*, which states that

$$\sum_{i=1}^n f(x_i) \geq nf\left(\frac{\sum_{i=1}^n x_i}{n}\right)$$

for any $x_1, x_2, \dots, x_n \in [a, b]$ if f is a convex function on an interval $[a, b]$. Using this inequality, we can get the following lemma.

Lemma 2.1. *Let $n \geq 1$, $m \geq 0$ be integers and f be a strictly convex function. Suppose that s_1, s_2, \dots, s_n is a sequence of non-negative integers such that $\sum_{i=1}^n s_i = 2m$. Let $k = \lfloor 2m/n \rfloor$ and $r = 2m - nk$. Then we have*

$$\sum_{i=1}^n f(s_i) \geq rf(k+1) + (n-r)f(k).$$

Proof. If $r = 0$, then by the convexity of f and the *Jensen inequality*, we have

$$\sum_{i=1}^n f(s_i) \geq nf\left(\frac{\sum_{i=1}^n s_i}{n}\right) = nf\left(\frac{2m}{n}\right) = nf(k).$$

It remains to show that the result is true for any $r \in \{1, 2, \dots, n-1\}$. Suppose that $\{s_i\}_{i=1}^n$ is a sequence of integers such that $\sum_{i=1}^n f(s_i)$ is minimal. We claim that $s_i \in \{k, k+1\}$ for all $1 \leq i \leq n$. If the claim does not hold, without loss of generality, suppose that $s_1 \geq s_2 \geq \dots \geq s_n$. Since $1 \leq r \leq n-1$, we have $s_1 \geq k+1$ and $s_n \leq k$. Then, there would be some $s_i \notin \{k, k+1\}$ such that either $s_1 \geq k+2$ or $s_n \leq k-1$. Thus, $s_1 - s_n - 1 \geq 1$. Let $s'_1 = s_1 - 1$, $s'_i = s_i$ for $2 \leq i \leq n-1$ and $s'_n = s_n + 1$. Since $s_1 - s_n - 1 \geq 1$, $s'_1 \neq s_n$ and $s'_n \neq s_1$, it shows that $\{s'_i\}_{i=1}^n$ is a different sequence from

$\{s_i\}_{i=1}^n$. Since f is a strictly convex function, then $f(x+1) - f(x)$ is strictly monotone increasing. So, we would obtain that

$$\sum_{i=1}^n f(s'_i) - \sum_{i=1}^n f(s_i) = [f(s_n + 1) - f(s_n)] - [f(s_1) - f(s_1 - 1)] < 0,$$

which contradicts the minimality of $\sum_{i=1}^n f(s_i)$.

The proof is thus complete. □

We prove Theorem 1.7 by constructing a connected (n, m) -graph G such that $d(v) \in \{\lfloor \frac{2m}{n} \rfloor, \lceil \frac{2m}{n} \rceil\}$ for all $v \in V(G)$. In order to make our construction more consistent and reasonable, we need the following two lemmas.

Lemma 2.2. *Let $\lfloor 2m/n \rfloor = k$ and $r = 2m - nk$, where r is even and $r \neq 0$. Then there is a k -regular graph with n vertices and $m - r/2$ edges, and its complement has a matching with $r/2$ edges.*

Proof. Since r is even, it shows that nk is also even. Note that $r \neq 0$. Then $k < n - 1$. We consider the following three cases.

Case 1. k is even and n is odd.

Consider a graph G_1 with vertex-set $\{v_1, v_2, \dots, v_n\}$ and $v_i \sim v_j$ if and only if $|i - j|$ is congruent modulo n with a number belonging to the set $\{-k/2, -k/2 + 1, \dots, -1, 1, \dots, k/2\}$. Then G_1 is a k -regular graph with $m - r/2$ edges. By the construction of G_1 , there is a matching M_1 in the complement of G_1 with edge-set $\{v_i v_{i+\frac{n-1}{2}} : 1 \leq i \leq (n-1)/2\}$ satisfying $|M_1| = (n-1)/2$. Note that $k/2 < (n-1)/2$. Then these edges do not appear in G_1 . That is, M_1 is a matching with $(n-1)/2$ edges in the complement of G_1 . Since $r \leq n - 1$, G_1 is a required graph.

Case 2. Both k and n are even.

Consider the graph G_1 we constructed above. Then there is a matching M_2 with edge-set $\{v_i v_{i+\frac{n}{2}} : 1 \leq i \leq n/2\}$ in the complement of G_1 . Note that $|M_2| = n/2$ and $r \leq n - 1$. Then G_1 is also a required graph.

Case 3. k is odd and n is even.

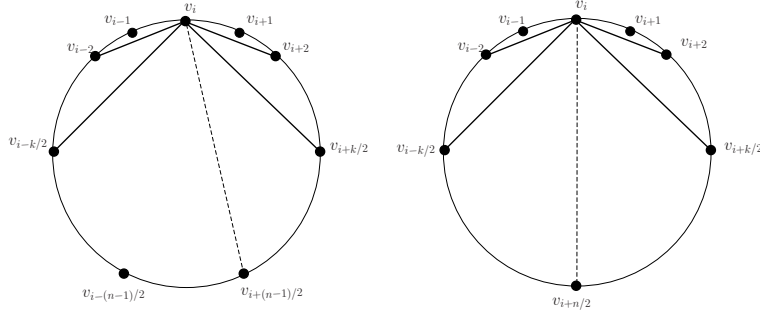


Figure 2. G_1 for k is even.

Consider a graph G_3 with vertex-set $\{v_1, v_2, \dots, v_n\}$ and $v_i \sim v_j$ if and only if $|i - j|$ is congruent modulo n with a number belonging to the set $\{-(k-1)/2, -(k-1)/2 + 1, \dots, -1, 1, \dots, (k-1)/2\}$ or $j = i + n/2$, where $1 \leq i \leq n/2$. By the construction of G_3 , we know that G_3 is a k -regular graph and $G_3 \in G(n, m - r/2)$, and there is a matching M_3 with edge-set $\{v_i v_{i+n/2-1} : 1 \leq i \leq n/2 - 1\}$ satisfying $|M_3| = n/2 - 1$. Note that $k < n - 1$. So we get $(k-1)/2 < n/2 - 1$, which means that M_3 is a matching in the complement of G_3 . Since both r and n are even and $r \leq n - 1$, we have $r \leq n - 2$. Therefore, G_3 is a required graph.

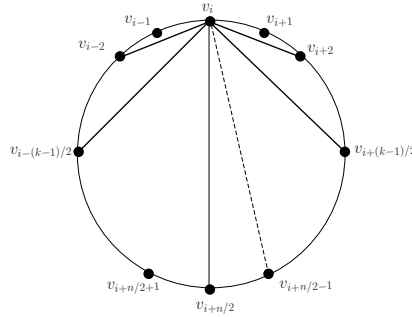


Figure 3. G_3 for k is odd and n is even.

The proof is thus complete. □

Lemma 2.3. *Let $2m = kn + 1$. Then there is a k -regular graph with $n - 1$ vertices and $m - (k + 1)/2$ edges, having a matching with $(n - 1)/2$ edges.*

Proof. Since $2m = nk + 1$, both n and k are odd. From $k < n - 1$, we deduce that $(k + 1)/2 \leq (n - 1)/2$. Consider a k -regular graph G_4 with $n - 1$ vertices as follows: $V(G_4) = \{v_1, v_2, \dots, v_{n-1}\}$ and $v_i \sim v_j$ if and only if $|i - j|$ is congruent modulo $n - 1$ with a number belonging to the set $\{-(k-1)/2, -(k-1)/2 + 1, \dots, -1, 1, \dots, (k-1)/2\}$ or

$j = i + (n-1)/2$, where $1 \leq i \leq (n-1)/2$. Since $2m = kn+1$, we have $2(m - (k+1)/2) = k(n-1)$. That is, G_4 is a k -regular graph and $G_4 \in \mathcal{G}(n-1, m - (k+1)/2)$. Note that $k-1 < n-1$. Then there is a matching M_4 with edge-set $\{v_i v_{i + \frac{n-1}{2}} : 1 \leq i \leq (n-1)/2\}$ in G_4 , such that $|M_4| = (n-1)/2$. Hence, G_4 is a required graph. \square

3 Proofs of Main Results

Now we are ready to give the proofs of our main results Theorems 1.6 and 1.7.

Proof of Theorem 1.6: Since $2m = kn + r$ and $k = \lfloor 2m/n \rfloor$, noticing that $H_f(G) = \sum_{i=1}^n f(d_{v_i})$ and $\sum_{i=1}^n d_{v_i} = 2m$, by Lemma 2.1 we have

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

Moreover, $H_f(G) = rf(k+1) + (n-r)f(k)$ if and only if the (n, m) -graph G has r vertices of degree $k+1$ and $n-r$ vertices of degree k . That is, the equality holds if and only if $G \in \mathcal{G}(n, m)$.

Now, we only need to show $\mathcal{G}(n, m) \neq \emptyset$. That is, there always exist a graph G with degree sequence $\mathbf{d} = (d_1, d_2, \dots, d_n)$ where $d_i = k+1$ and $d_j = k$ for $1 \leq i \leq r$ and $r+1 \leq j \leq n$. In fact, it is easy to see that the degree sequence is graphical simply by verifying the conditions in [7].

Algorithm 1 Find an (n, m) -graph G with degree sequence $\mathbf{d} = (d_1, d_2, \dots, d_n)$ where $d_i = k+1$ and $d_j = k$ for $1 \leq i \leq r$ and $r+1 \leq j \leq n$.

Input: $E^{(0)} = \emptyset$, $\mathbf{d}^{(0)'} = \mathbf{d}$ and $V^{(0)'} = (v_1^{(0)'}, v_2^{(0)'}, \dots, v_n^{(0)'})$.

Output: An (n, m) -graph $G = (V^{(l)}, E^{(l-1)})$ with degree sequence $\mathbf{d} = (d_1, d_2, \dots, d_n)$ where $d_i = k+1$ and $d_j = k$ for $1 \leq i \leq r$ and $r+1 \leq j \leq n$.

1: **Set** $l = 1$.

2: Find a permutation σ , such that $\sigma \mathbf{d}^{(l-1)'} = (d_1^{(l)}, d_2^{(l)}, \dots, d_n^{(l)})$ is non-increasing for $\mathbf{d}^{(l-1)'} = (d_1^{(l-1)'}, d_2^{(l-1)'}, \dots, d_n^{(l-1)'})$. Denote $\sigma V^{(l-1)'} = (v_1^{(l)}, v_2^{(l)}, \dots, v_n^{(l)}) = V^{(l)}$.

3: **if** $d_1^{(l)} \neq 0$ **then**

4: **Set** $E^{(l)} = E^{(l-1)} \cup \{v_1^{(l)} v_j^{(l)} | j = 2, 3, \dots, d_1^{(l)} + 1\}$ and $\mathbf{d}^{(l)'} = (0, d_2^{(l)} - 1, \dots, d_{d_1^{(l)}+1}^{(l)} - 1, d_{d_1^{(l)}+2}^{(l)}, \dots, d_n^{(l)})$.

5: **else** go to 7.

6: **Set** $l = l + 1$ and go to 2.

7: **return** $G = (V^{(l)}, E^{(l-1)})$.

By choosing different permutations σ in Algorithm 1, we can obtain some (n, m) -graphs $G \in \mathcal{G}(n, m)$ which minimize the value of $H_f(G)$. However, from [15] we can get the following algorithm, which can generate all graphs of $\mathcal{G}(n, m)$.

Algorithm 2 Find all (n, m) -graphs with degree sequence $\mathbf{d} = (d_1, d_2, \dots, d_n)$ where $d_i = k + 1$ and $d_j = k$ for $1 \leq i \leq r$ and $r + 1 \leq j \leq n$.

Input: n, m and $\mathbf{d} = (d_1, d_2, \dots, d_n)$ where $d_i = k + 1$ and $d_j = k$ for $1 \leq i \leq r$ and $r + 1 \leq j \leq n$.

Output: $\mathcal{G}(n, m)$ for any given n and m .

- 1: Construct a complete n -partite graph $H = (P_1, P_2, \dots, P_n)$, such that each P_i for $1 \leq i \leq r$ has $k + 1$ vertices and each P_j for $r + 1 \leq j \leq n$ has k vertices.
 - 2: Find all perfect matchings in H , denoted by $\{M_1, M_2, \dots, M_l\}$.
 - 3: **Set** $\mathcal{G}(n, m) = \emptyset$ and $s = 1$.
 - 4: **while** $s \leq l$ **do**
 - 5: Construct a new graph G_s with vertex-set $\{p_1, p_2, \dots, p_n\}$ and $p_i \sim p_j$ if and only if there is an edge between P_i and P_j in M_s .
 - 6: **if** G_s does not have multiple edges and $G_s \not\cong G$ for any $G \in \mathcal{G}(n, m)$ **then**
 - 7: **Set** $\mathcal{G}(n, m) = \mathcal{G}(n, m) \cup \{G_s\}$.
 - 8: **else** $\mathcal{G}(n, m) = \mathcal{G}(n, m)$.
 - 9: **Set** $s = s + 1$ and go to 4.
 - 10: **return** $\mathcal{G}(n, m)$.
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□

Note that to check that $G_s \not\cong G$ for any $G \in \mathcal{G}(n, m)$ is a very hard nut to crack. Although this algorithm can be used to generate all graphs of $\mathcal{G}(n, m)$, it cannot guarantee the existence of any graph in $\mathcal{G}(n, m)$.

Proof of Theorem 1.7: By the proof of Theorem 1.6, we only need to show that there is a connected (n, m) -graph belonging to $\mathcal{G}(n, m)$ for any given n and m such that $n - 1 \leq m \leq n(n - 1)/2$.

If $m = n - 1$ we have the path $P_n \in \mathcal{G}(n, n - 1)$, which is connected, as required.

If $n \leq m \leq n(n - 1)/2$, then $k = \lfloor \frac{2m}{n} \rfloor \geq 2$. Noticing that $2m = kn + r$, we distinguish the following three cases to discuss.

Case 1. $r = 0$, *i.e.*, $2m = nk$.

In this case, we need to find a connected k -regular (n, m) -graph. From the condition

[2] for a sequence to be graphical, we know that a k -regular graph with n vertices exists if and only if $n \geq k + 1$ and nk is even. Noticing that $m \leq n(n - 1)/2$, there must be a k -regular (n, m) -graph which satisfies $2m = nk$. Moreover, it is easy to know that there also exists a connected k -regular (n, m) -graph G which satisfies $2m = nk$. That is, $G \in \mathcal{G}(n, m)$ and G is connected.

Case 2. r is even and $r \neq 0$.

From $2m = nk + r$, we obtain $2(m - r/2) = kn$. By Lemma 2.2, there is a k -regular graph H^* with n vertices and $m - r/2$ edges, and its complement has a matching M^* with $r/2$ edges. Adding all $r/2$ edges that appear in M^* to the graph H^* , we then get a new graph, called G . One can see that $G \in \mathcal{G}(n, m)$ and $H_f(G) = rf(k + 1) + (n - r)f(k)$. That is, $G \in \mathcal{G}(n, m)$. From our construction, there is an n -cycle $v_1v_2 \dots v_nv_1$ in G , and so G is also connected.

Case 3. r is odd.

Note that $k < n - 1$. First, we show that it is true for $r = 1$. By Lemma 2.3, there is a k -regular graph $H^{**} \in G(n - 1, m - (k + 1)/2)$, which contains a matching M^{**} with $(k + 1)/2$ edges. Deleting all $(k + 1)/2$ edges in M^{**} from H^{**} and adding a new vertex such that this vertex is adjacent to all $k + 1$ vertices of M^{**} , we get a graph $G \in G(n, m)$, which satisfies $H_f(G) = f(k + 1) + (n - 1)f(k)$. By our construction, the graph G is also connected.

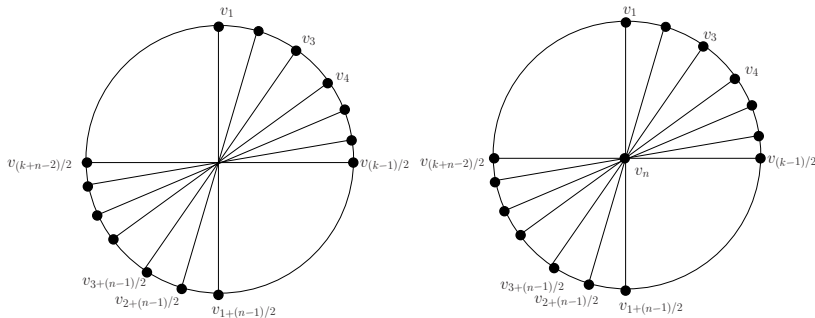


Figure 4. H^{**} and G for $r = 1$.

It remains to show that the result is true for $r \geq 3$ and r is odd. The equality can be written as $2(m - (r - 1)/2) = nk + 1$. By Lemma 2.3, there is a k -regular graph $D_1 \in G(n - 1, m - (k + r)/2)$, which contains a matching N_1 with $(k + 1)/2$ edges.

Deleting all $(k+1)/2$ edges in N_1 from D_1 and adding a new vertex such that this vertex is adjacent to all $k+1$ vertices of N_1 , we get a graph $D_2 \in G(n, m - (r-1)/2)$ and $H_f(D_2) = f(k+1) + (n-1)f(k)$. If $r-1 \leq k+1$, we can add any $(r-1)/2$ edges in N_1 to D_2 . Thus, we find a graph $G \in G(n, m)$ satisfying $H_f(G) = rf(k+1) + (n-r)f(k)$. If $r-1 > k+1$, we denote $s = r - k - 2$. Notice that $2(m - (r-1)/2) = nk + 1$. Since r is odd, then both n and k are odd. That is, both $n-1$ and $k+r$ are even. From the construction we give above, in fact, by the proof of Case 3 in Lemma 2.2, there is a k -regular graph $D_3 \in G(n-1, m - (k+r)/2)$, whose complement has a matching N_2 with $(n-3)/2$ edges. Note that $s = r - k - 2 \leq n - 3 - 2 = n - 5 < n - 3$. So we can add any $s/2$ edges in matching N_2 to D_3 . In this way, we obtain a graph D_4 with $n-1$ vertices and $m - (k+1)$ edges. Moreover, it has s vertices of degree $k+1$ and $n-1-s$ vertices of degree k . Add a new vertex to D_4 such that the new vertex is adjacent to any $k+1$ of the remaining $n-1-s$ vertices. It does works since $n-1-s = n-1 - (r-k-2) \geq n-1 - (n-2-k-2) = k+3$. Hence, we get a graph $G \in G(n, m)$ satisfying $H_f(G) = rf(k+1) + (n-r)f(k)$. It is easy to see from our construction that G is also connected. That is, there is a connected graph $G \in \mathcal{G}(n, m)$ when r is odd.

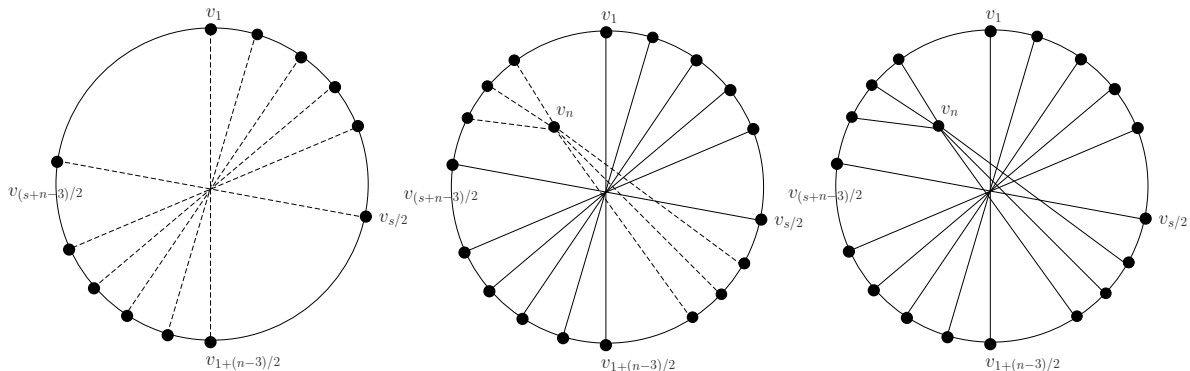


Figure 5. Graphs for $r \geq 3$ and $r - 1 > k + 1$.

The above proof can guarantee the existence of connected graphs in $\mathcal{G}(n, m)$. The following Algorithm 3 (similar to Algorithm 2) can be used to find all connected graphs in $\mathcal{G}(n, m)$.

Algorithm 3 Find all connected (n, m) -graphs with degree sequence $\mathbf{d} = (d_1, d_2, \dots, d_n)$ where $d_i = k + 1$ and $d_j = k$ for $1 \leq i \leq r$ and $r + 1 \leq j \leq n$.

Input: n, m and $\mathbf{d} = (d_1, d_2, \dots, d_n)$ where $d_i = k + 1$ and $d_j = k$ for $1 \leq i \leq r$ and $r + 1 \leq j \leq n$.

Output: All connected graphs in $\mathcal{G}(n, m)$ for any given n and m , denoted by $\mathcal{G}^*(n, m)$.

- 1: Construct a complete n -partite graph $H = (P_1, P_2, \dots, P_n)$, such that each P_i for $1 \leq i \leq r$ has $k + 1$ vertices and each P_j for $r + 1 \leq j \leq n$ has k vertices.
 - 2: Find all perfect matchings in H , denoted by $\{M_1, M_2, \dots, M_l\}$.
 - 3: **Set** $\mathcal{G}^*(n, m) = \emptyset$ and $s = 1$.
 - 4: **while** $s \leq l$ **do**
 - 5: Construct a new graph G_s with vertex-set $\{p_1, p_2, \dots, p_n\}$ and $p_i \sim p_j$ if and only if there is an edge between P_i and P_j in M_s .
 - 6: **if** G_s is **connected** with no multiple edges and $G_s \not\cong G$ for any $G \in \mathcal{G}^*(n, m)$ **then**
 - 7: **Set** $\mathcal{G}^*(n, m) = \mathcal{G}^*(n, m) \cup \{G_s\}$.
 - 8: **else** $\mathcal{G}^*(n, m) = \mathcal{G}^*(n, m)$.
 - 9: **Set** $s = s + 1$ and go to 4.
 - 10: **return** $\mathcal{G}^*(n, m)$.
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□

Note that although this algorithm can be used to generate all connected graphs of $\mathcal{G}(n, m)$, it cannot guarantee the existence of any connected graph in $\mathcal{G}(n, m)$.

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References

- [1] A. Ali, I. Gutman, H. Saber, A. M. Alanazi, On bond incident degree indices of (n, m) -graphs, *MATCH Commun. Math. Comput. Chem.* **87**(2022) 89-96.
- [2] J. A. Bondy, U. S. R. Murty, *Graph Theory*, GTM No.244, Springer, Berlin, 2008.
- [3] S. M. Cioaba, Sums of powers of the degrees of a graph, *Discr. Math.* **306**(2008) 959–1964.

- [4] R. Cruz, J. Rada, The path and the star as extremal values of vertex-degree-based topological indices among trees, *MATCH Commun. Math. Comput. Chem.* **82**(3)(2019) 715-732.
- [5] I. Gutman, Degree-based topological indices, *Croat. Chem. Acta* **86**(4)(2013) 351-361.
- [6] I. Gutman, B. Furtula, *Novel Molecular Structure Descriptors - Theory and Applications I and II*, Mathematical Chemistry Monographs, Nos. 8 and 9, University of Kragujevac, Kragujevac, Serbia, 2010.
- [7] V. Havel, A remark on the existence of finite graphs, *Casopis Pest. Mat.* **6**(2)(1995) 161-179.
- [8] Y. Hu, Y. Shi, X. Li, T. Xu, On molecular graphs with smallest and greatest zeroth-order general Randić index, *MATCH Commun. Math. Comput. Chem.* **54**(2)(2005) 425-434.
- [9] Y. Hu, Y. Shi, X. Li, T. Xu, Connected graphs with minimum and maximum zeroth-order general Randić index, *Discr. Appl. Math.* **155**(2007) 1044-1054.
- [10] Z. Hu, L. Li, X. Li, D. Peng, Extremal graphs for topological index defined by a degree-based edge-weight function, accepted for publication in *MATCH Commun. Math. Comput. Chem.*
- [11] R. Lang, X. Li, S. Zhang, Inverse problem for the Zagreb index of molecular graphs, *Appl. Math. J. Chinese Univ. Ser.A* **4**(2003) 487-493.
- [12] X. Li, I. Gutman, *Mathematical Aspects of Randić-Type Molecular Structure Descriptors*, Mathematical Chemistry Monographs, No.1, University of Kragujevac, Kragujevac, Serbia, 2006.
- [13] X. Li, J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54**(1)(2005) 195-208.
- [14] N. Linial, E. Rozenman, An extremal problem on degree sequences of graphs, *Graph. Comb.* **18**(2002) 573-582.

- [15] M. Molloy, B. Reed, A critical point for random graphs with a given degree sequence, *Random Struct. Algorithm.* **80**(1955) 477-480.
- [16] J. Rada, R. Cruz, Vertex-degree-based topological indices over graphs, *MATCH Commun. Math. Comput. Chem.* **72**(3)(2014) 603-616.
- [17] G. Su, M. Meng, L. Cui, Z. Chen, X. Lan, The general zeroth-order Randić index of maximal outerplanar graphs and trees with k maximum degree vertices, *Science Asia* **43**(2017) 387.
- [18] I. Tomescu, Properties of connected (n, m) -graphs extremal relatively to vertex degree function index for convex functions, *MATCH Commun. Math. Comput. Chem.* **85**(2)(2021) 285-294.
- [19] I. Tomescu, Graphs with given cyclomatic number extremal relatively to vertex degree function index for convex functions, *MATCH Commun. Math. Comput. Chem.* **87**(1)(2022) 109-114.
- [20] N. Trinajstić, *Chemical Graph Theory*, Sec. Ed., CRC Press, Inc., 1992.
- [21] D. Vukičević, J. Durdević, Bond additive modeling 10. Upper and lower bounds of bond incident degree indices of catacondensed fluoranthenes, *Chem. Phys. Lett.* **515**(2011) 186-189.