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Some Bounds for the Vertex Degree Function Index of Connected Graphs with Given Minimum and Maximum Degrees

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Abstract

This paper gives some bounds for the vertex degree function index $H_f(G)$ in terms of the order and size of a graph G, where G is a simple, finite and connected graph with minimum degree δ and maximum degree Δ. Some families of graphs are also constructed to show that the bounds can be achieved.

1 Introduction

Topological indices (or, chemical indices or graphical indices) play an important role in studying the structures and properties of molecules. Therefore, a lot of papers and books for the extremal values and graphs of topological indices have been published. However, as one can see that the extremal graphs among many graph classes with respect to some topological indices are the same or very similar, namely star or path, etc. Moreover, mathematically the proof methods and techniques are also the same or very similar. So, it is very worthy of finding a unified mathematical method to study a set of topological indices, but not one by one separately. Recently, this kind of approach started; see $[4, 5, 7, 8]$ for examples.

In [9], Yao et al. introduced the *vertex degree function index* $H_f(G)$. Let f be a real value function defined on the vertices of a graph G, and then sum up the values over all the vertices of G, i.e.

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

Some properties about the vertex degree function index have been studied, see [2, 3, 5, 7, 8].

These studies mainly focus on simple, finite and connected graphs. We will give some bounds for the vertex degree function index $H_f(G)$ of graphs with given size and order, as well as minimum degree and maximum degree. We also construct families of graphs which achieve the bounds. As a consequence, results in [1] can be seen as corollaries of ours.

2 Main results

Let G be a simple, finite and connected graph with minimum degree δ and maximum degree $\Delta = \delta + k$, and let size and order of G be m and n, respectively.

We denote by n_r as the number of vertices with degree r in G. Thus,

$$\sum_{i=\delta}^{\delta+k} n_i = n. \tag{2}$$

By the definition of vertex degree function index and $\sum_{i=1}^{n} d(v_i) = 2m$, we have

$$H_f(G) = \sum_{i=\delta}^{\delta+k} n_i f(i), \tag{3}$$

and

$$\sum_{i=\delta}^{\delta+k} i n_i = 2m. \tag{4}$$

Combining Eq.2 and 4, we obtain

$$n_\delta = \frac{1}{k}[(\delta + k)n - 2m - (k-1)n_{\delta+1} - (k-2)n_{\delta+2} - \cdots - n_{\delta+k-1}],$$

and

$$n_{\delta+k} = \frac{1}{k}[2m - \delta n - n_{\delta+1} - 2n_{\delta+2} - \cdots - (k-1)n_{\delta+k-1}].$$

Substituting n_δ and $n_{\delta+k}$ into Eq. 3, we can get

$$\begin{aligned} H_f(G) = &\frac{1}{k}[(\delta+k)f(\delta) - \delta f(\delta+k)]n + \frac{2}{k}(f(\delta+k) - f(\delta))m \\ &+ \sum_{i=1}^{k-1}(f(\delta+i) - \frac{k-i}{k}f(\delta) - \frac{i}{k}f(\delta+k))n_{\delta+i}. \end{aligned}$$

For convenience, we denote

$$\Gamma_f(G) = \sum_{i=1}^{k-1}(f(\delta+i) - \frac{k-i}{k}f(\delta) - \frac{i}{k}f(\delta+k))n_{\delta+i},$$
$$g_i = f(\delta+i) - \frac{k-i}{k}f(\delta) - \frac{i}{k}f(\delta+k), i = 1, 2, \ldots, k-1.$$

Lemma 1. *Let G be a graph with $n_{\delta+1}+n_{\delta+2}+\cdots+n_{\delta+k-1} \geq k-1$. If f is a strictly monotone and strictly convex function, then $\Gamma_f(G) < \min_i\{g_i\}$.*

Proof. Firstly, all $g_i's$ are negative. Then

$$\begin{aligned} &kf(\delta+i) - (k-i)f(\delta) - if(\delta+k) \\ =&(k-i)(f(\delta+i) - f(\delta)) + i(f(\delta+i) - f(\delta+k)). \end{aligned}$$

Since f is a strictly convex function, g_i is less than 0.

Secondly, we shall prove that $tg_j < g_i < \frac{g_j}{t}$ for $t \geq k-1$ and $i, j \in \{1, 2, \ldots, k-1\}$. We distinguish the following cases.

Case 1. If $i < j$, then

$$\begin{aligned} &k(tg_i - g_j) \\ =&ti(f(\delta+i) - f(\delta+k)) + t(k-i)(f(\delta+i) - f(\delta)) \\ &- j(f(\delta+j) - f(\delta+k)) - (k-j)(f(\delta+j) - f(\delta)) \\ =&(ti-j)(f(\delta+j) - f(\delta+k)) + [t(k-i) - (k-j)](f(\delta+i) - f(\delta)) \\ &+ [ti + (k-j)](f(\delta+i) - f(\delta+j)) \end{aligned}$$

$$
\begin{aligned}
=&[t(k-i)-(k-j)]\sum_{t_1=1}^{i}(f(\delta+t_1)-f(\delta+t_1-1))\\
&+[ti+(k-j)]\sum_{t_2=i+1}^{j}(f(\delta+t_2-1)-f(\delta+t_2))\\
&+(ti-j)\sum_{t_3=j+1}^{k}(f(\delta+t_3-1)-f(\delta+t_3)).
\end{aligned}
$$

If f is a strictly decreasing function, then for all $t_1 \in \{1,2,\ldots,i\}, t_2 \in \{i+1,i+2,\ldots,j\}, t_3 \in \{j+1,j+2,\ldots,k\}$, we have

$$
\begin{aligned}
&f(\delta+t_1)-f(\delta+t_1-1)<0,\\
&f(\delta+t_2-1)-f(\delta+t_2)>0,\\
&f(\delta+t_3-1)-f(\delta+t_3)>0.
\end{aligned}
$$

Since f is a strictly convex function, we have that for all $t_1 \in \{1,2,\ldots,i\}, t_2 \in \{i+1,i+2,\ldots,j\}, t_3 \in \{j+1,j+2,\ldots,k\}$,

$$|f(\delta+t_1)-f(\delta+t_1-1)|>|f(\delta+t_2-1)-f(\delta+t_2)|>|f(\delta+t_3-1)-f(\delta+t_3)|.$$

Since $t \geq k-1$, the coefficients of the above three summations are all nonnegative and

$$[t(k-i)-(k-j)]i=[ti+(k-j)](j-i)+(ti-j)(k-j).$$

Thus, $tg_i - g_j < 0$.
If f is a strictly increasing function, then for all $t_1 \in \{1,2,\ldots,i\}, t_2 \in \{i+1,i+2,\ldots,j\}, t_3 \in \{j+1,j+2,\ldots,k\}$, we have

$$
\begin{aligned}
&f(\delta+t_1)-f(\delta+t_1-1)>0,\\
&f(\delta+t_2-1)-f(\delta+t_2)<0,\\
&f(\delta+t_3-1)-f(\delta+t_3)<0.
\end{aligned}
$$

Since f is a strictly convex function, we have that for all $t_1 \in \{1,2,\ldots,i\}, t_2$

$\in \{i+1, i+2, \dots, j\}, t_3 \in \{j+1, j+2, \dots, k\}$,

$$|f(\delta+t_1)-f(\delta+t_1-1)| < |f(\delta+t_2-1)-f(\delta+t_2)| < |f(\delta+t_3-1)-f(\delta+t_3)|.$$

Since $t \geq k-1$, the coefficients of the above three summations are all nonnegative and

$$[t(k-i)-(k-j)]i = [ti+(k-j)](j-i)+(ti-j)(k-j).$$

Thus, $tg_i - g_j < 0$.

Case 2. If $i > j$, then

$$\begin{aligned} & k(tg_i - g_j) \\ =&[t(k-i)-(k-j)]\sum_{t_1=1}^{j}(f(\delta+t_1)-f(\delta+t_1-1)) \\ &+[t(k-i)+j]\sum_{t_2=j+1}^{i}(f(\delta+t_2)-f(\delta+t_2-1)) \\ &+(ti-j)\sum_{t_3=i+1}^{k}(f(\delta+t_3-1)-f(\delta+t_3)). \end{aligned}$$

Now the proof is done similarly to **Case 1**. Consequently, we can deduce

$$\begin{aligned} \Gamma_f(G) =&\sum_{i=1}^{k-1}(f(\delta+i)-\frac{k-i}{k}f(\delta)-\frac{i}{k}f(\delta+k))n_{\delta+i} \\ \leq&(n_{\delta+1}+n_{\delta+2}+\cdots+n_{\delta+k-1})\max_i\{g_i\} \\ \leq&(k-1)\max_i\{g_i\} \\ <&\min_i\{g_i\}. \end{aligned}$$

■

Theorem 1. *Let G be a graph of order n and size m with minimum degree δ and maximum degree $\Delta = \delta + k$, and let f be a strictly monotone and strictly convex function.*

1 If $n_{\delta+1}+n_{\delta+2}+\cdots+n_{\delta+k-1}\geq k-1$*, then*

$$H_f(G)<\frac{1}{k}[(\delta+k)f(\delta)-\delta f(\delta+k)]n+\frac{2}{k}(f(\delta+k)-f(\delta))m+\min_i\{g_i\}.$$

2 If $2\leq n_{\delta+1}+n_{\delta+2}+\cdots+n_{\delta+k-1}\leq k-2$*, then*

$$\begin{aligned}H_f(G)<&\frac{1}{k}[(\delta+k)f(\delta)-\delta f(\delta+k)]n+\frac{2}{k}(f(\delta+k)-f(\delta))m\\&+\max\{g_1,g_{k-1}\}.\end{aligned}$$

3 If $n_{\delta+1}+n_{\delta+2}+\cdots+n_{\delta+k-1}\leq 1$*, then*

$$\begin{aligned}H_f(G)=&\frac{1}{k}[(\delta+k)f(\delta)-\delta f(\delta+k)]n+\frac{2}{k}(f(\delta+k)-f(\delta))m\\&+\begin{cases}g_in_{\delta+i},\ if\ 2m-\delta n\equiv i\ (mod\ k),\ i=1,2,\ldots,k-1,\\0,\ if\ 2m-\delta n\equiv 0\ (mod\ k).\end{cases}\end{aligned}$$

Moreover, the set of degrees of G *is*

$\{\delta,\Delta,\delta+i\}$ *and only one vertex has a degree* $\delta+i$ *for* $2m-\delta n\equiv i\ (mod\ k)$*,*

$\{\delta,\Delta\}$ *for* $2m-\delta n\equiv 0\ (mod\ k)$*.*

Proof.

1 If $n_{\delta+1}+n_{\delta+2}+\cdots+n_{\delta+k-1}\geq k-1$, then from Lemma 1 the result follows obviously.

2 If $2\leq n_{\delta+1}+n_{\delta+2}+\cdots+n_{\delta+k-1}\leq k-2$, we prove that $\max_i\{g_i\}=\max\{g_1,g_{k-1}\}$.

For $i\in\{1,2,\ldots,k-2\}$, we have

$$\begin{aligned}&k(g_i-g_{i+1})\\=&k(f(\delta+i)-f(\delta))+i(f(\delta)-f(\delta+k))\\&-k(f(\delta+i+1)-f(\delta))-(i+1)(f(\delta)-f(\delta+k))\\=&k(f(\delta+i)-f(\delta+i+1))+(f(\delta+k)-f(\delta)).\end{aligned}$$

Thus $g_i<g_{i+1}$ when $\frac{f(\delta+k)-f(\delta)}{k}<\frac{f(\delta+i+1)-f(\delta+i)}{1}$, and $g_i\geq g_{i+1}$ when $\frac{f(\delta+k)-f(\delta)}{k}\geq\frac{f(\delta+i+1)-f(\delta+i)}{1}$.

Since f is strictly convex function, we obtain that the maximum value among all g_i must be g_1 or g_{k-1}. Then

$$\begin{aligned}\Gamma_f(G) =& \sum_{i=1}^{k-1}(f(\delta+i) - \frac{k-i}{k}f(\delta) - \frac{i}{k}f(\delta+k))n_{\delta+i} \\ \leq& (n_{\delta+1} + n_{\delta+2} + \cdots + n_{\delta+k-1}) \max\{g_i\} \\ \leq& 2\max\{g_1, g_{k-1}\} \\ <& \max\{g_1, g_{k-1}\}.\end{aligned}$$

Thus,

$$\begin{aligned}H_f(G) <& \frac{1}{k}[(\delta+k)f(\delta) - \delta f(\delta+k)]n + \frac{2}{k}(f(\delta+k) - f(\delta))m \\ &+ \max\{g_1, g_{k-1}\}.\end{aligned}$$

3 If $n_{\delta+1} + n_{\delta+2} + \cdots + n_{\delta+k-1} \leq 1$, then by Eqs.2 and 4, we have

$$2m - \delta n \equiv n_{\delta+1} + 2n_{\delta+2} + \cdots + (k-1)n_{\delta+k-1} \ (mod\ k).$$

Since $n_{\delta+1} + n_{\delta+2} + \cdots + n_{\delta+k-1} \leq 1$, one can deduce that all $n_i's$ are 0 but at most one is 1. Thus,

$$\begin{aligned}&(n_{\delta+1}, n_{\delta+2}, \ldots, n_{\delta+k-1}) = \\ &\qquad \begin{cases}(0, \ldots, 1_{ith}, \ldots, 0), \ if\ 2m - \delta n \equiv i \ (mod\ k), \\ (0, 0, \ldots, 0), \ if\ 2m - \delta n \equiv 0 \ (mod\ k).\end{cases}\end{aligned}$$

The proof is thus complete. ■

From the third part of the proof of Theorem 1, we can see that the condition 'f be a strictly monotone and strictly convex function' is not necessary for equality in 3 of Theorem 1.

Corollary. *1 Let G be a graph of order n and size m with minimum degree δ and maximum degree $\Delta = \delta + k$, and let f be a strictly monotone and* *strictly convex function. Then we have*

$$H_f(G) \leq \frac{1}{k}[(\delta+k)f(\delta) - \delta f(\delta+k)]n + \frac{2}{k}(f(\delta+k) - f(\delta))m,$$

and the equality holds if and only if the set of degrees of G is $\{\delta, \Delta\}$.

Now we show how to construct a family of graphs which achieve the bounds of Theorem 1. The two construction are inspired by [6].

Construction 1. For $(n_{\delta+1}, n_{\delta+2}, \ldots, n_{\delta+k-1}) = (0, 0, \ldots, 0)$, we do the following constructions:

(1) Input $\{n, m, \Delta, \delta\}$. This quadruple should be graphical, i.e., there exists a simple, connected graph with n vertices, m edges and the set of degrees is $\{\Delta, \delta\}$.

(2) Construct a complete n-partite graph $H = H(V_1, V_2, \ldots, V_n)$, such that the order of V_i is Δ for $i \in \{1, 2, \ldots, \frac{2m-\delta n}{\Delta-\delta}\}$ and the order of V_i is δ for $i \in \{\frac{2m-\delta n}{\Delta-\delta}+1, \frac{2m-\delta n}{\Delta-\delta}+2, \ldots, n\}$.

(3) Find all perfect matchings $\{M_1, M_2, \ldots, M_t\}$ of H.

(4) For each matching M_i, construct a graph G_i with vertex set $\{v_1, v_2, \ldots, v_n\}$, and if there are j edges between V_s and V_t in M_i, then connect v_s and v_t by j edges. Then we obtain a family of graphs $\{G_1, G_2, \ldots, G_t\}$, which with n vertices, m edges and the set of degrees is $\{\Delta, \delta\}$.

(5) Delete multigraphs, disconnected graphs and isomorphic graphs from $\{G_1, G_2, \ldots, G_t\}$. Then we obtain a family of simple, connected graphs with n vertices, m edges and the set of degrees is $\{\Delta, \delta\}$.

Construction 2. For $(n_{\delta+1}, n_{\delta+2}, \ldots, n_{\delta+k-1}) = (0, \ldots, 1_{ith}, \ldots, 0)$, we do the following constructions:

(1) Input $\{n, m, \Delta, \delta, \delta+i\}$. This quintuple should be graphical, i.e., there exists a simple, connected graph with n vertices, m edges, the set of degrees is $\{\Delta, \delta, \delta+i\}$ and only one vertex has a degree $\delta+i$.

(2) Construct a complete n-partite graph $H = H(V_1, V_2, \ldots, V_n)$, such that the order of V_i is Δ for $i \in \{1, 2, \ldots, \frac{2m-\delta n-i}{\Delta-\delta}\}$, the order of $V_{\frac{2m-\delta n-i}{\Delta-\delta}+1}$ is $\delta + i$ and the order of V_i is δ for $i \in \{\frac{2m-\delta n-i}{\Delta-\delta} + 2, \frac{2m-\delta n-i}{\Delta-\delta} + 3, \ldots, n\}$.

(3) Find all perfect matchings $\{M_1, M_2, \ldots, M_t\}$ of H.

(4) For each matching M_i, construct a graph G_i with vertex set $\{v_1, v_2, \ldots, v_n\}$, and if there are j edges between V_s and V_t in M_i, then connect v_s and v_t by j edges. Then we obtain a family of graphs $\{G_1, G_2, \ldots, G_t\}$, which with n vertices, m edges, the set of degrees is $\{\Delta, \delta, \delta + i\}$ and only one vertex has a degree $\delta + i$.

(5) Delete multigraphs, disconnected graphs and isomorphic graphs from $\{G_1, G_2, \ldots, G_t\}$. Then we obtain a family of simple, connected graphs with n vertices, m edges, the set of degrees is $\{\Delta, \delta, \delta + i\}$ and only one vertex has a degree $\delta + i$.

Corollary. *2 Let G be a tree with n vertices and maximum degree $\Delta = 1 + k$, and f be a strictly monotone and strictly convex function. Then*

$$H_f(G) \leq \frac{1}{k}[(1+k)f(1) - f(1+k)]n + \frac{2}{k}(f(1+k) - f(1))(n-1),$$

and the equality holds if and only if G is a graph constructed in Construction 1. Particularly, if $\Delta = n - 1$, then the equality holds if and only if G is a star.

Corollary. *3 Let G be a tree with n vertices, and f be a strictly monotone and strictly convex function. Then*

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

and the equality holds if and only if G is a star.

Proof. For convenience, we denote

$$h(\Delta) = \frac{1}{\Delta - 1}[\Delta f(1) - f(\Delta)]n + \frac{2}{\Delta - 1}(f(\Delta) - f(1))m,$$

then,

$$
\begin{aligned}
& h(\Delta)-h(\Delta+1) \\
= & \frac{1}{\Delta-1}[\Delta f(1)-f(\Delta)]n+\frac{2}{\Delta-1}(f(\Delta)-f(1))m \\
& -\frac{1}{\Delta}[(\Delta+1)f(1)-f(\Delta+1)]n-\frac{2}{\Delta}(f(\Delta+1)-f(1))m \\
= & \frac{2(n-1)}{(\Delta-1)\Delta}(\Delta f(\Delta)-(\Delta-1)f(\Delta+1)-f(1)) \\
& -\frac{n}{(\Delta-1)\Delta}(f(1)-(k+1)f(\Delta)+kf(\Delta+1)) \\
= & \frac{1-n}{\Delta(\Delta-1)}(f(1)-(k+1)f(\Delta)+kf(\Delta+1)).
\end{aligned}
$$

Since f is a strictly monotone and strictly convex function, the formula above is less than 0. Thus, $h(n-1)=max_{\Delta}\{h(\Delta)\}$. By Corollaries 1 and 2, we can obtain this result.

The proof is thus complete. ■

If f is a strictly monotone and strictly concave function, we can get the corresponding results.

Lemma 2. *Let G be a graph with $n_{\delta+1}+n_{\delta+2}+\cdots+n_{\delta+k-1}\geq k-1$. If f is a strictly monotone and strictly concave function, then $\Gamma_f(G)>\max_i\{g_i\}$.*

Theorem 2. *Let G be a graph of order n and size m with minimum degree δ and maximum degree $\Delta=\delta+k$, and let f be a strictly monotone and strictly concave function.*

1 *If $n_{\delta+1}+n_{\delta+2}+\cdots+n_{\delta+k-1}\geq k-1$, then*

$$H_f(G)>\frac{1}{k}[(\delta+k)f(\delta)-\delta f(\delta+k)]n+\frac{2}{k}(f(\delta+k)-f(\delta))m+\max_i\{g_i\}.$$

2 *If $2\leq n_{\delta+1}+n_{\delta+2}+\cdots+n_{\delta+k-1}\leq k-2$, then*

$$
\begin{aligned}
H_f(G)>&\frac{1}{k}[(\delta+k)f(\delta)-\delta f(\delta+k)]n+\frac{2}{k}(f(\delta+k)-f(\delta))m \\
&+\min\{g_1,g_{k-1}\}.
\end{aligned}
$$

3 If $n_{\delta+1} + n_{\delta+2} + \cdots + n_{\delta+k-1} \leq 1$, *then*

$$H_f(G) = \frac{1}{k}[(\delta+k)f(\delta) - \delta f(\delta+k)]n + \frac{2}{k}(f(\delta+k) - f(\delta))m$$
$$+ \begin{cases} g_i n_{\delta+i}, \ if \ 2m - \delta n \equiv i \ (mod\ k), \ i = 1, 2, \ldots, k-1, \\ 0, \ if \ 2m - \delta n \equiv 0 \ (mod\ k). \end{cases}$$

Moreover, the degree set of G *is*

$\{\delta, \Delta, \delta+i\}$ *and only one vertex has a degree* $\delta+i$ *if* $2m - \delta n \equiv i \ (mod\ k)$,

$\{\delta, \Delta\}$ *if* $2m - \delta n \equiv 0 \ (mod\ k)$.

Corollary. *4 Let* G *be a graph of order* n *and size* m *with minimum degree* δ *and maximum degree* $\Delta = \delta + k$, *and let* f *be a strictly monotone and strictly concave function. Then we have*

$$H_f(G) \geq \frac{1}{k}[(\delta+k)f(\delta) - \delta f(\delta+k)]n + \frac{2}{k}(f(\delta+k) - f(\delta))m,$$

and the equality holds if and only if the degree set of G *is* $\{\delta, \Delta\}$.

Corollary. ***5*** *Let* G *be a tree with* n *vertices and maximum degree* $\Delta = 1+k$, *and let* f *be a strictly monotone and strictly concave function. Then*

$$H_f(G) \geq \frac{1}{k}[(1+k)f(1) - f(1+k)]n + \frac{2}{k}(f(1+k) - f(1))(n-1),$$

and the equality holds if and only if G *is a graph constructed in Construction 1. Particularly, if* $\Delta = n-1$, *the equality holds if and only if* G *is a star.*

Corollary. ***6*** *Let* G *be a tree with* n *vertices, and* f *be a strictly monotone and strictly concave function. Then*

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

and the equality holds if and only if G *is a star.*

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