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SHARP BOUNDS FOR THE SUM OF THE SQUARES OF THE DEGREES OF A GRAPH

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Abstract. Let $G = (V, E)$ be a simple graph with n vertices, e edges, and vertex degrees $d_1, d_2, \ldots, d_n$. Let d_1, d_n be the highest and the lowest degree of vertices of G and m_i be the average of the degrees of the vertices adjacent to $v_i \in V$. We prove that

$$\sum_{i=1}^{n} d_i^2 = e\left[\frac{2e}{n-1} + n - 2\right]$$

if and only if G is a star graph or a complete graph or a complete graph with one isolated vertex. We establish the following upper bound for the sum of the squares of the degrees of a graph G:

$$\sum_{i=1}^{n} d_i^2 \leq e\left[\frac{2e}{n-1} + (n-2)\right] - d_1\left[\frac{4e}{n-1} - 2m_1 - \frac{(n+1)}{(n-1)}d_1 + (n-1)\right] ,$$

with equality if and only if G is a star graph or a complete graph or a graph of isolated vertices. Moreover, we present several upper and lower bounds for $\sum_{i=1}^{n} d_i^2$ and determine the extremal graphs which achieve the bounds and apply the inequalities to obtain bounds on the total number of triangles in a graph and its complement.

1. INTRODUCTION

Throughout this paper $G = (V, E)$ will denote a simple undirected graph with n vertices and e edges. In order to avoid trivialities we always assume that $n \geq 2$. Also assume that the vertices are labeled such that $d_1 \geq d_2 \geq \ldots \geq d_n$, where d_i is the degree of the vertex v_i for $i = 1, 2, \ldots, n$. The average of the degrees of the vertices adjacent to v_i is denoted by m_i.

We consider the following problem: find upper and lower bounds for $\sum_{i=1}^{n} d_i^2$ in terms of n, e, d_1 and d_n. We would like the bounds to be sharp, that is, we would like to show the existence of extremal graphs pertaining to the bounds.

We recall some known upper bounds for $\sum_{i=1}^{n} d_i^2$.

1. Székely et al. [11]:

$$\sum_{i=1}^{n} d_i^2 \leq (\sum_{i=1}^{n} \sqrt{d_i})^2. \tag{1}$$

2. D. de Caen [2]:

$$\sum_{i=1}^{n} d_i^2 \leq e(\frac{2e}{n-1} + n - 2). \tag{2}$$

Caen pointed out that (1) and (2) are incomparable. He has also mentioned that the bound (2) is perhaps a bit more useful than (1), since it depends only on n and e rather than on the full-degree sequence.

The rest of the paper is structured as follows. In Section 2, we find out the lower bound for the sum of squares of the degrees of a graph G in terms of n and e. In Section 3, we characterize the graphs for which the equality holds in (2) and also obtain some upper bounds for $\sum\limits_{i=1}^{n} d_i^2$ in terms of n, e, d_1 and d_n. In Section 4, we relate the Laplacian graph eigenvalues to the degree sequence of a graph G. In Section 5, we point out bounds on $t(G) + t(G^c)$, where $t(G)$ denotes the number of triangles in G and G^c is the complement of G. Also we determine the extremal graphs which achieve the bounds on $\sum\limits_{i=1}^{n} d_i^2$.

2. LOWER BOUND FOR $\sum\limits_{i=1}^{n} d_i^2$

In this section we present two lower bounds for $\sum\limits_{i=1}^{n} d_i^2$.

Theorem 2.1. Let G be a simple graph with n vertices, and e edges. Then

$$\sum_{i=1}^{n} d_i^2 \geq 2e(2p+1) - pn(1+p), \text{ where } p = [\tfrac{2e}{n}] \ , \tag{3}$$

and the equality holds if and only if the difference of the degrees of any two vertices of graph G is at most one. Here $[x]$ denotes the greatest positive integer less than or equal to x.

Proof. Consider two vertices, v_i of degree d_i and v_j of degree d_j, where $d_i \geq d_j$. Also let $\sum_{i=1}^{n} d_i^2$ be minimum.

If possible, let $d_i - d_j \geq 2$. Therefore there exists a vertex v_k, which is adjacent to v_i, but not v_j. If we remove the edge $v_k v_i$ and add an edge between the vertices v_k and v_j, then the degree sequence of the new graph is $\overline{d}_1, \overline{d}_2, \ldots, \overline{d}_n$; where $\overline{d}_i = d_i - 1,\ \overline{d}_j = d_j + 1,\ \overline{d}_t = d_t,\ t = 1, 2, \ldots, n;\ t \neq i, j$.
Therefore

$$\begin{aligned} \sum_{i=1}^{n} \overline{d}_i^2 &= \sum_{i=1}^{n} d_i^2 + (d_i - 1)^2 - d_i^2 + (d_j + 1)^2 - d_j^2 \\ &= \sum_{i=1}^{n} d_i^2 - 2(d_i - d_j - 1) \\ &< \sum_{i=1}^{n} d_i^2, \text{ by } d_i \geq d_j + 2, \end{aligned}$$

which is a contradiction as $\sum_{i=1}^{n} d_i^2$ is minimum.

Since v_i and v_j are arbitrary, therefore the difference of any two vertex degrees is at most one. So, some of the vertices have degree p and the remaining vertices (if any) have degree $p+1$, where $p = [\frac{2e}{n}]$. Therefore $(2e - pn)$ vertices have degree $(p+1)$. Hence

$$\text{Min} \sum_{i=1}^{n} d_i^2 \ = \ 2e(2p+1) - pn(1+p),$$

$$\text{i.e.,} \sum_{i=1}^{n} d_i^2 \;\; \geq \;\; 2e(2p+1) - pn(1+p), \;\text{where}\; p = [\tfrac{2e}{n}].$$

Now suppose that the equality holds in (3). Therefore some of the vertices have degree p and the remaining vertices (if any) have degree $p+1$, where $p = [\frac{2e}{n}]$. Hence the difference of the degrees of any two vertices of graph G is at most one.

Conversely, suppose that the difference of the degrees of any two vertices of the graph G be at most one. Then we can easily see that the equality holds in (3).

Lemma 2.2. Let G be a simple graph with n vertices, e edges and let d_1 be the highest vertex degree. If $d_i,\ i = 1, 2, \ldots, n$ is the degree sequence of G, then

$$\sum_{i=1}^{n} d_i^2 \geq (2p+1)(2e-d_1) + d_1^2 + 2(d_1 - n + 1 + t) - p(n-1)(p+1)$$

if $d_1 > n - 1 - t$, and

$$\sum_{i=1}^{n} d_i^2 \geq (2p+1)(2e-d_1) + d_1^2 - p(n-1)(p+1)$$

if $d_1 \leq n - 1 - t$, where $p = [\frac{2(e-d_1)}{(n-1)}]$ and $t = 2(e-d_1) - p(n-1)$.

Proof. Let v_1 be a highest–degree vertex of the graph G. We remove the vertex v_1 and its corresponding edges and denote the resultant graph as G_1. Let $\overline{d}_i,\ i = 1, 2, \ldots, (n-1)$ be the degree sequence of G_1. From Theorem 2.1 we get that the minimum value of $\sum_{i=1}^{n} d_i^2$ is attained in terms of n, e if and only if the difference of the degrees of any two vertices of graph G is at most one. Using this result we conclude that the value of $\sum_{i=1}^{n-1} \overline{d}_i^2$ (in terms of the number of vertices and edges) will be minimum if the value of $\sum_{i=1}^{n} d_i^2$ (in terms of n, e and d_1) is minimum. We have to find the minimum value of $\sum_{i=1}^{n} d_i^2$ in terms of n, e and d_1. For this first we find the minimum value of $\sum_{i=1}^{n-1} \overline{d}_i^2$ in terms of the number of vertices and edges. The graph G_1 has $(n-1)$ vertices and $(e-d_1)$ edges. Using the above Theorem 2.1, we get

$$\sum_{i=1}^{n-1} \overline{d}_i^2 \geq 2(e-d_1)(2p+1) - p(n-1)(1+p), \;\text{where}\; p = [\tfrac{2(e-d_1)}{n-1}],$$

where p is the greatest positive integer less than or equal to $\frac{2(e-d_1)}{n-1}$, and the difference of the degrees of any two vertices of graph G_1 is at most one.

Let $t = 2(e-d_1)-p(n-1)$. Therefore G_1 has t vertices of degree $(p+1)$ and $(n-1-t)$ vertices of degree p.

Now we add the vertex v_1 of degree d_1 and join with edges to the vertices of graph G_1 such that $\sum_{i=1}^{n} d_i^2$ is minimum. So, the vertex v_1 is connected to as many degree p vertices as possible and then to the remaining degree $(p+1)$ vertices till the d_1 degrees are exhausted.

Two cases are (a) $d_1 > n-1-t$, (b) $d_1 \leq n-1-t$.

Case (a) $d_1 > n-1-t$.

$$\begin{aligned}
\text{Min} \sum_{i=1}^{n} d_i^2 &= \text{Min} \sum_{i=1}^{n-1} \overline{d}_i^2 + d_1^2 + 2p(n-1-t) + (n-1-t) + (d_1-n+1+t) \\
&\quad [(p+2)^2-(p+1)^2], \\
\text{i.e.,} \sum_{i=1}^{n} d_i^2 &\geq (2p+1)(2e-d_1) + d_1^2 + 2(d_1-n+1+t) - p(n-1)(p+1), \\
\text{where} \qquad & p = [\frac{2(e-d_1)}{(n-1)}] \text{ and } t = 2(e-d_1)-p(n-1).
\end{aligned}$$

Case (b) $d_1 \leq n-1-t$.

$$\begin{aligned}
\text{Min} \sum_{i=1}^{n} d_i^2 &= \text{Min} \sum_{i=1}^{n-1} \overline{d}_i^2 + d_1^2 + d_1(2p+1), \\
\text{i.e.,} \sum_{i=1}^{n} d_i^2 &\geq (2p+1)(2e-d_1) + d_1^2 - p(n-1)(p+1), \\
\text{where} \qquad & p = [\frac{2(e-d_1)}{(n-1)}].
\end{aligned}$$

Remark. The lower bounds obtained from Lemma 2.2 and (3) are the best possible because we can construct a graph for which equality holds.

Theorem 2.3. Let G be a graph with n vertices and e edges. Then

$$\sum_{i=1}^{n} d_i^2 \geq d_1^2 + d_n^2 + \frac{(2e-d_1-d_n)^2}{(n-2)} \,. \tag{4}$$

Moreover, equality in (4) holds if and only if $d_2 = d_3 = \ldots = d_{n-1}$.

Proof. Let us take the degrees $d_2, d_3, \ldots, d_{n-1}$ with associated weights $d_2, d_3, \ldots, d_{n-1}$; then applying A.M. $\geq H.M.$, we get

$$\frac{\sum_{i=2}^{n-1} d_i^2}{\sum_{i=2}^{n-1} d_i} \geq \frac{\sum_{i=2}^{n-1} d_i}{(n-2)},$$

and equality holds if and only if $d_2 = d_3 = \ldots = d_{n-1}$.

Therefore

$$\sum_{i=2}^{n-1} d_i^2 \geq \frac{(\sum_{i=2}^{n-1} d_i)^2}{(n-2)},$$

$$\text{i.e.,} \qquad \sum_{i=1}^{n} d_i^2 \leq d_1^2 + d_n^2 + \frac{(2e - d_1 - d_n)^2}{(n-2)},$$

and equality holds if and only if $d_2 = d_3 = \ldots = d_{n-1}$.

3. UPPER BOUND FOR $\sum\limits_{i=1}^{n} d_i^2$

In this section we give some upper bounds for $\sum_{i=1}^{n} d_i^2$ in terms of n, e, d_1, and d_n. Let N_i be the neighbor set of the vertex $v_i \in V$ and m_1 be the average degree of the highest–degree vertex.

Lemma 3.1. Let G be a graph with degree sequence $d_i,\ i = 1, 2, \ldots, n$ and $\sum_{i=1}^{n} d_i^2$ be maximum. If a vertex v_1 of maximum degree is not adjacent to some vertex v then $d_v = 0$.

Proof. If possible, let $d_v \neq 0$. Now we insert an edge vv_1 and drop an edge vv_2, where v_2 is adjacent to v as $d_v \neq 0$.

The new value of the sum of squares of the vertex degrees is $\sum_{i=1}^{n} d_i^2 = [(d_1 + 1)^2 - d_1^2] - [d_2^2 - (d_2 - 1)^2] = 2(d_1 - d_2 + 1) > 0$, which is a contradiction because $\sum_{i=1}^{n} d_i^2$ was supposed to be maximum.

Hence the result.

Corollary 3.2. Let G be a connected graph with n vertices and e edges. Then the highest degree of G is $(n-1)$ if $\sum_{i=1}^{n} d_i^2$ is maximum.

Theorem 3.3. Let G be a graph with n vertices, e edges and $\sum_{i=1}^{n} d_i^2$ be maximum. Then

$$\begin{array}{rl} (i) & N_i - \{v_j\} = N_j - \{v_i\} \text{ if and only if } d_i = d_j, \\ (ii) & N_i - \{v_j\} \supset N_j - \{v_i\} \text{ if and only if } d_i > d_j, \\ (iii) & d_j < d_i \text{ if } v_i \in N_k \text{ and } v_j \in \{N_k\}^c - \{v_k\}. \end{array}$$

where d_i and d_j are the degrees of any two vertices v_i and v_j , respectively.

Proof. (i) Suppose that $d_i = d_j$.

If possible, let $N_i - \{v_j\} \neq N_j - \{v_i\}$.

Since $d_i = d_j$, there exists at least two vertices, v_s, which is adjacent to v_i but not v_j and v_t, which is adjacent to v_j but not v_i. Let d_s and d_t be the degrees of the vertices v_s and v_t , respectively.

Two cases are (a) $d_s \geq d_t$, (b) $d_s < d_t$.

Case (a) $d_s \geq d_t$.

We remove an edge $v_j v_t$ and add an edge between the vertices v_j and v_s. Let the degree sequence of the new graph be $\overline{d}_1, \overline{d}_2, \ldots, \overline{d}_n$; where $\overline{d}_s = d_s + 1,\ \overline{d}_t = d_t - 1,\ \overline{d}_i = d_i,\ i = 1, 2, \ldots, n;\ i \neq s, t$. Then

$$\begin{aligned} \sum_{i=1}^{n} \overline{d}_i^2 &= \sum_{i=1}^{n} d_i^2 + (d_s+1)^2 - d_s^2 + (d_t-1)^2 - d_t^2 \\ &= \sum_{i=1}^{n} d_i^2 + 2(d_s - d_t + 1). \end{aligned}$$

¿From the above relation we get $\sum_{i=1}^{n} \overline{d}_i^2 > \sum_{i=1}^{n} d_i^2$, a contradiction.

Case (b) $d_s < d_t$.

In this case we remove an edge v_iv_s and add an edge between the vertices v_i and v_t. Similarly, we arrive at a contradiction.

Therefore $N_i - \{v_j\} = N_j - \{v_i\}$.

Conversely, let $N_i - \{v_j\} = N_j - \{v_i\}$. Therefore $d_i = d_j$.

(ii) Suppose that $d_i > d_j$.

If possible, let $N_i - \{v_j\} \not\supset N_j - \{v_i\}$. Therefore there exists a vertex v_s, $v_s \in N_j - \{v_i\}$ but $v_s \notin N_i - \{v_j\}$. We remove an edge v_sv_j and add an edge between the vertices v_s and v_i. Then the degree sequence of the new graph is $\overline{d}_i = d_i + 1$, $\overline{d}_j = d_j - 1$, and $\overline{d}_t = d_t$, $i = 1, 2, \ldots, n;\ t \neq i, j$. Then

$$\begin{aligned}\sum_{i=1}^{n} \overline{d}_i^2 &= \sum_{i=1}^{n} d_i^2 + (d_i+1)^2 - d_i^2 + (d_j-1)^2 - d_j^2 \\ &= \sum_{i=1}^{n} d_i^2 + 2(d_i - d_j + 1). \\ &> \sum_{i=1}^{n} d_i^2, \text{ (since } d_i > d_j\text{), a contradiction.}\end{aligned}$$

Therefore $N_i - \{v_j\} \supset N_j - \{v_i\}$.

Conversely, let $N_i - \{v_j\} \supset N_j - \{v_i\}$. Therefore $d_i > d_j$.

(iii) If possible, let $d_j \geq d_i$. Using (i) and (ii), we get $N_i - \{v_j\} \subseteq N_j - \{v_i\}$.

Since $v_i \in N_k$, $v_iv_k \in E$. We have $N_j - \{v_i\} \supseteq N_i - \{v_j\} \supseteq \{v_k\}$. Therefore $v_k \in N_j - \{v_i\}$ implies that $v_jv_k \in E$.

Since $v_j \in \{N_k\}^c - \{v_k\}$, then $v_jv_k \notin E$, a contradiction.

Hence the Theorem.

Lemma 3.4. **[2]** Let G be a simple graph with n vertices and e edges. Then

$$\sum_{i=1}^{n} d_i^2 \leq e\left[\frac{2e}{n-1} + n - 2\right] . \tag{5}$$

Theorem 3.5. Let G be a connected graph with n vertices and e edges. Then

$$\sum_{i=1}^{n} d_i^2 = e\left[\frac{2e}{n-1} + n - 2\right]$$

if and only if G is a star graph or a complete graph.

Proof. If G is a star graph or a complete graph then the equality holds.

Conversely, let

$$\sum_{i=1}^{n} d_i^2 = e\left[\frac{2e}{n-1} + n - 2\right] .$$

When $n = 2$, G is a complete graph of order two as G is a connected graph. Now we are to prove that G is a star graph or a complete graph for $n > 2$. By Lemma 3.4 and the above result, we conclude that $\sum_{i=1}^{n} d_i^2$ is maximum. Using Corollary 3.2 we conclude that the highest degree of G is $n-1$. Now we delete a highest–degree vertex and the corresponding edges from G. Let the degree sequence of G be $d_1 = (n-1)$, d_2, d_3,. . . ,d_n. Therefore the degree sequence of the new graph is $\overline{d}_1 = d_2 - 1$, $\overline{d}_2 = d_3 - 1$,. . . ,$\overline{d}_{n-1} = d_n - 1$.

Therefore

$$\begin{aligned}\sum_{i=1}^{n} d_i^2 &= \sum_{i=1}^{n-1} \overline{d}_i^2 + (n-1)^2 + 4(e-n+1) + (n-1)\\ &= \sum_{i=1}^{n-1} \overline{d}_i^2 + n^2 + 4e - 5n + 4,\end{aligned}$$

i.e., $$e\left[\frac{2e}{n-1} + n - 2\right] \le (e-n+1)\left[\frac{2(e-n+1)}{n-2} + n - 3\right] + n^2 + 4e - 5n + 4,$$

i.e., $$\frac{2e^2}{(n-1)(n-2)} \ge \frac{(n+2)}{(n-2)}e - \frac{n(n-1)}{(n-2)},$$

i.e., $$2e^2 - (n-1)(n+2)e + n(n-1)^2 \ge 0, \text{ by } n > 2,$$

i.e., $$[e-(n-1)][2e - n(n-1)] \ge 0. \tag{6}$$

From (6) we conclude that either $e \le n-1$ or $e \ge \frac{n(n-1)}{2}$. Since G is a connected graph, $n-1 \le e \le \frac{n(n-1)}{2}$. Therefore either $e = n-1$ or $e = \frac{n(n-1)}{2}$. When $e = n-1$, G is a star graph as $d_1 = n-1$. When $e = \frac{n(n-1)}{2}$, G is a complete graph.

Theorem 3.6. Let G be a simple graph with n vertices and e (> 0) edges. Then

$$\sum_{i=1}^{n} d_i^2 = e\left[\frac{2e}{n-1} + n - 2\right]$$

if and only if G is a star graph or a complete graph or a complete graph with one isolated vertex.

Proof. If G is a star graph or a complete graph or a complete graph with one isolated vertex, then the equality holds.

Conversely, let

$$\sum_{i=1}^{n} d_i^2 = e\left[\frac{2e}{n-1} + n - 2\right] .$$

We need to prove that G is a star graph or a complete graph or a complete graph with one isolated vertex.

If G is a connected graph then the theorem is proved by the previous Theorem 3.5. It remains to examine the case when G is a disconnected graph. For a disconnected graph we have to prove that G is a complete graph with one isolated vertex.

Let G be a graph containing two connected components G_1 and G_2 with n_1, n_2 vertices and $e_1(> 0)$, $e_2(> 0)$ edges, respectively. Also let $d_{1i},\ i = 1, 2, \ldots, n_1$ and $d_{2i},\ i = 1, 2, \ldots, n_2$ be the degree sequence of the graphs G_1 and G_2, respectively.

Therefore,

$$\sum_{i=1}^{n_1} d_{1i}^2 \le e_1\left[\frac{2e_1}{n_1-1} + n_1 - 2\right] \tag{7}$$

and
$$\sum_{i=1}^{n_2} d_{2i}^2 \le e_2\left[\frac{2e_2}{n_2-1} + n_2 - 2\right] . \tag{8}$$

We have $2e_1/(n_1-1) \le 2e_1/(n_1+n_2-1)+n_2$ and $2e_2/(n_2-1) \le 2e_2/(n_1+n_2-1)+n_1$.

Therefore

$$\begin{aligned}
\sum_{i=1}^{n} d_i^2 &= \sum_{i=1}^{n_1} d_{1i}^2 + \sum_{i=1}^{n_2} d_{2i}^2 \\
&\leq \frac{2e_1^2}{n_1+n_2-1} + e_1 n_2 + (n_1-2)e_1 + \frac{2e_2^2}{n_1+n_2-1} + e_2 n_1 + (n_2-2)e_2 \\
&\leq \frac{2(e_1+e_2)^2}{n_1+n_2-1} + (n_1+n_2-2)(e_1+e_2) - \frac{4e_1e_2}{n_1+n_2-1} \\
&< \frac{2(e_1+e_2)^2}{n_1+n_2-1} + (n_1+n_2-2)(e_1+e_2). \qquad (9)
\end{aligned}$$

For the disconnected graph G, there are three possibilities: (i) there are at least two isolated vertices, (ii) no isolated vertex, (iii) exactly one isolated vertex.

Case (i): Let k ($k \geq 2$) be the number of isolated vertices in G. Then

$$\sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n-k} d_i^2 \leq e\left[\frac{2e}{n-k-1} + n-k-2\right], \quad \text{by (5).} \qquad (10)$$

We have $\sum\limits_{i=1}^{n} d_i^2 = e[\frac{2e}{n-1} + n - 2]$. From this result and (10), we get $e \geq (n-1)(n-k-1)/2$. But $e \leq (n-k)(n-k-1)/2$. From these two results $k \leq 1$, a contradiction.

Case (ii): Let there are no isolated vertices in G. In this case let there be p connected components in G. Therefore there is at least one edge in each component of G. Using (9) we conclude that $\sum\limits_{i=1}^{n} d_i^2 < e[\frac{2e}{n-1} + (n-2)]$, a contradiction.

Case (iii): Let G contain only one isolated vertex. Then

$$\sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n-1} d_i^2 \leq e\left[\frac{2e}{n-2} + n-3\right], \text{ by (5).} \qquad (11)$$

We have $\sum\limits_{i=1}^{n} d_i^2 = e[\frac{2e}{n-1} + n - 2]$. Using this result and (11), we get $e \geq (n-1)(n-2)/2$. But $e \leq (n-1)(n-2)/2$. Therefore $e = (n-1)(n-2)/2$, that is, G is a complete graph with one isolated vertex.

Hence the theorem.

Theorem 3.7. Let G be a simple graph with degree sequence $d_1,\ d_2, \ldots,\ d_n$. Then

$$\sum_{i=1}^{n} d_i^2 \leq e(e+1). \tag{12}$$

Proof. We show that if (12) holds for the graph G with n vertices and e edges then it also holds for the new graph G_1, constructed by joining any two non-adjacent vertices, v_r and v_s, by an edge. Therefore

$$d_r + d_s \leq e\ . \tag{13}$$

G_1 has n vertices and $e+1$ edges with degree sequence $\overline{d}_1, \overline{d}_2, \ldots, \overline{d}_n$. Therefore $\overline{d}_r = d_r + 1$, $\overline{d}_s = d_s + 1$, and $\overline{d}_i = d_i,\ i = 1, 2, \ldots, n;\ i \neq r, s$.

We have

$$\begin{aligned} \sum_{i=1}^{n} \overline{d}_i^2 &= \sum_{i=1}^{n} d_i^2 + 2(d_r + d_s + 1) \\ &\leq e(e+1) + 2(e+1), \text{ by (13)} \\ &= (e+1)(e+2). \end{aligned}$$

Therefore (12) holds for graph G_1. Also for the star graph $S_{1,n-1}$ of order n, the equality in (12) holds. The inequality in (12) also holds for the graph constructed by adding an isolated vertex to the graph G. Any graph G can be constructed by starting with the star graph S_{1,d_1} (d_1, the highest degree) and making required constructions (addition of edges and vertices) at each step of which (12) holds true. Hence the theorem is proved for any graph G.

Theorem 3.8. Let G be a connected graph with n vertices and e edges. Then

$$\sum_{i=1}^{n} d_i^2 \leq 2en - n(n-1)d_n + 2e(d_n - 1), \tag{14}$$

where d_n is the lowest degree. Moreover, the equality holds if and only if G is a star graph or a regular graph.

Proof. We have $\sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} d_i m_i$, where m_i is the average degree of the adjacent vertices of the vertex $v_i \in V$.

We have $d_i m_i \leq 2e - d_i - (n - d_i - 1)d_n$ and the equality holds if and only if $d_i = n-1$ or vertex v_i is not adjacent to the d_n degree vertices. Using this result, we get

$$\begin{aligned}\sum_{i=1}^{n} d_i^2 &\leq \sum_{i=1}^{n} [2e - d_i - (n - d_i - 1)d_n] \\ &= 2en - n(n-1)d_n + 2e(d_n - 1).\end{aligned}$$

Suppose now that equality in (14) holds. Then either $d_i = n - 1$ or $d_j = d_n$, for all $v_i \in V$, $v_i v_j \notin E$, which implies that either (a) G is a star graph or (b) G is a regular graph.

Conversely, it is easy to verify that equality in (14) holds for a star graph or a regular graph.

Theorem 3.9 Let G be a graph with n vertices and e edges. Then

$$\sum_{i=1}^{n} d_i^2 \leq e\left[\frac{2e}{n-1} + n - 2\right] - d_1\left[\frac{4e}{n-1} - 2m_1 - \frac{(n+1)}{(n-1)}d_1 + (n-1)\right], \tag{15}$$

where d_1 is the highest degree and m_1 is the average degree of the vertices adjacent to the highest degree vertex. Moreover, equality in (15) holds if and only if G is a star graph or a complete graph or a graph of isolated vertices.

Proof. Let v_1 be the highest–degree vertex of degree d_1. Two cases are: (i) $d_1 = n-1$, (ii) $d_1 < n - 1$.

Case (i): $d_1 = n - 1$.
In this case $m_1 = \frac{2e-n+1}{n-1}$. The inequality (15) reduces to

$$\sum_{i=1}^{n} d_i^2 \leq e\left[\frac{2e}{n-1} + n - 2\right], \tag{16}$$

which is true by (5).

Case (ii): $d_1 < n-1$.

In this case all the vertices those are not adjacent to the vertex v_1 are adjacent to the vertex v_1. Denote the new graph by G_1. Also let $\overline{d}_i,\ i = 1, 2, \ldots, n$ be the degrees of G_1.

By Lemma 3.4 on G_1,

$$\sum_{i=1}^{n} \overline{d}_i^2 \le (e+n-d_1-1)\left[\frac{2(e+n-d_1-1)}{n-1} + n - 2\right]. \tag{17}$$

Now, $$\sum_{i=1}^{n} \overline{d}_i^2 - \sum_{i=1}^{n} d_i^2 = (n-1)^2 - d_1^2 + 2[2e - d_1 m_1 - d_1] + (n - d_1 - 1),$$

i.e., $$\sum_{i=1}^{n} d_i^2 \le e\left[\frac{2e}{n-1} + n - 2\right] - d_1\left[\frac{4e}{n-1} - 2m_1 - \frac{(n+1)}{(n-1)} d_1 + (n-1)\right].$$

Suppose that equality in (15) holds. Then the equality holds in either (16) or (17). Using Theorem 3.5 we conclude that G is either a star graph or a complete graph if the equality holds in (16). Since the graph G_1 is connected, using Theorem 3.5, G_1 is a star graph or a complete graph if the equality holds in (17). Since $d_1 < n-1$, G is a graph of isolated vertices if the equality holds in (17). Hence G is a star graph or a complete graph or a graph of isolated vertices.

Conversely, it is easy to verify that equality in (15) holds for a star graph, a complete graph, and a graph of isolated vertices.

Corollary 3.10 Let G be a graph with n vertices and e edges. Then

$$\sum_{i=1}^{n} d_i^2 \le e\left[\frac{2e}{n-1} + n - 2\right] - d_1\left[\frac{4e}{n-1} - 2d_1 - \frac{(n+1)}{(n-1)} d_1 + (n-1)\right].$$

Moreover, equality holds if and only if G is a complete graph or a graph of isolated vertices.

Remark. In the case of trees, the upper bound (15) is always better than D. Caen's bound, but it is not always so for any graph.

4. LAPLACIAN EIGENVALUE WITH DEGREE SEQUENCE

Let $A(G)$ be the adjacency matrix of G and let $D(G)$ be the diagonal matrix of vertex degrees. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. Clearly, $L(G)$ is a real symmetric matrix. From this fact and Geršgorin's theorem, it follows that its eigenvalues are non-negative real numbers. Moreover, since its rows sum to 0, 0 is the smallest eigenvalue of $L(G)$. The spectrum of G is

$$S(G) = (\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)),$$

where $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G) = 0$ are the eigenvalues of $L(G)$ arranged in non-increasing order.

We have

$$\sum_{i=1}^{n}(2e - d_i)d_i = 2\sum_{i\neq j} d_i d_j,$$

$$\text{and} \qquad \sum_{i=1}^{n}(2e - \lambda_i)\lambda_i = 2\sum_{i\neq j} \lambda_i \lambda_j.$$

Since

$$\sum_{i=1}^{n} d_i = \sum_{i=1}^{n} \lambda_i \ ,$$

from the above two relations follows,

$$\sum_{i=1}^{n} \lambda_i^2 - \sum_{i=1}^{n} d_i^2 = 2\sum_{i\neq j} d_i d_j - 2\sum_{i\neq j} \lambda_i \lambda_j \ .$$

From matrix theory is known that the sum of the product of two eigenvalues of $L(G)$ is given by $\sum_{i\neq j} \lambda_i \lambda_j = \sum_{i\neq j} d_i d_j - e$.

Therefore

$$\sum_{i=1}^{n} \lambda_i^2 = \sum_{i=1}^{n} d_i^2 + 2e \ ,$$

that is,

$$\sum_{i=1}^{n} \lambda_i^2 = \sum_{i=1}^{n} d_i(d_i + 1) \ .$$

Lemma 4.1. Let G be a graph. If we remove an edge v_iv_j then the maximum possible drop in eigenvalue λ_k of $L(G)$ is $\frac{d_i+d_j+2}{\lambda_k}$, where d_i and d_j are the degrees of the vertices v_i and v_j , respectively.

Proof. We have

$$\sum_{i=1}^{n-1} \lambda_i^2 = \sum_{i=1}^{n} d_i^2 + 2e\ .$$

Also we know that if we remove an edge from the graph then the Laplacian eigenvalues of the graph are non-increasing.

Let $\triangle\lambda_k$ be the drop of the k-th eigenvalue λ_k of $L(G)$. Then, $\sum_{k=1}^{n-1}(\lambda_k - \triangle\lambda_k)^2 = \sum_{k=1}^{n} d_k^2 - 2(d_i+d_j) + 2e$.

From these two results, we get

$$\begin{aligned}
&\sum_{k=1}^{n-1} \lambda_k^2 - \sum_{k=1}^{n-1}(\lambda_k - \triangle\lambda_k)^2 = 2(d_i+d_j),\\
\text{i.e., } & 2\sum_{k=1}^{n-1} \lambda_k\triangle\lambda_k - \sum_{k=1}^{n-1}(\triangle\lambda_k)^2 = 2(d_i+d_j),\\
\text{i.e., } & \sum_{k=1}^{n-1} \lambda_k\triangle\lambda_k \le d_i+d_j+2, \text{ by } \textstyle\sum_{k=1}^{n}(\triangle\lambda_k)^2 \le 4,\\
\text{i.e., } & \triangle\lambda_k \le \frac{d_i+d_j+2}{\lambda_k}, \quad k = 1, 2, \ldots, (n-1).
\end{aligned}$$

Example 4.2. Consider a graph G depicted in the Fig. 1.

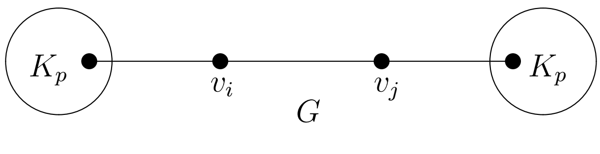

Fig. 1

In G, v_i and v_j are two adjacent vertices connected by edges to one vertex each of the two complete graphs of order p. Therefore the highest degree of G is p. If we remove an edge v_iv_j then using Lemma 4.1 the largest eigenvalue can drop by a maximum of $\frac{6}{\lambda_1}$, where λ_1 is the largest eigenvalue of G. Therefore

$$\begin{aligned}
& \triangle\lambda_1 \leq \frac{6}{\lambda_1}, \\
\text{i.e.,} \quad & \lambda_1^{'} = \lambda_1 - \triangle\lambda_1 \geq \lambda_1 - \frac{6}{\lambda_1}, \\
\text{i.e.,} \quad & p+1 \geq \lambda_1 - \frac{6}{\lambda_1}, \ (\text{since } \lambda_1^{'} = p+1), \\
\text{i.e.,} \quad & \lambda_1 \leq \frac{(p+1)+\sqrt{(p+1)^2+24}}{2},
\end{aligned}$$

which is an upper bound for λ_1 of the graph G. Also this bound gives a better result than the other bounds (Section 1, [3]) for $p > 4$.

Lemma 4.3. **[10]** If G is a simple connected graph, then

$$\lambda_1(G) \leq d_n + \frac{1}{2} + \sqrt{(d_n - \frac{1}{2})^2 + \sum_{i=1}^{n} d_i(d_i - d_n)}\ .$$

Equality holds if and only if G is a star graph [see [1], p. 283] or a regular bipartite graph.

In [7] is shown that for a connected graph G with $n > 1$, $\lambda_1 \geq d_1 + 1$. Moreover, equality holds if and only if $d_1 = n - 1$.

Theorem 4.4. Let G be a simple connected graph with n vertices and e edges. Then

$$\sum_{i=1}^{n} d_i^2 \geq (d_1 - d_n)^2 + d_1 + d_n(2e - d_n), \tag{18}$$

Euality in (18) holds if and only if G is a star graph.

Proof. We have $\lambda_1(G) \geq d_1 + 1$, where d_1 is the highest degree of G. From Lemma 4.3 and using this result, we get

$$\sum_{i=1}^{n} d_i^2 \geq (d_1 - d_n)^2 + d_1 + d_n(2e - d_n)\ .$$

Moreover, we can easily determine that the equality holds in (18) if and only if G is a star graph.

5. APPLICATION

Let $t(G)$ denote the number of triangles in G. It was first observed by Goodman [4] that $t(G) + t(G^c)$, where G^c denotes the complement of G, is determined by the degree sequence:

$$t(G) + t(G^c) = \frac{1}{2} \sum_{v_i \in V} [d_i - \frac{(n-1)}{2}]^2 + \frac{n(n-1)(n-5)}{24}. \tag{19}$$

Goodman [5] raised the question of finding a best possible upper bound of the form $t(G)+t(G^c) \leq B(n,e)$, and he conjectured an expression for $B(n,e)$. This conjecture was proved recently by Olpp [8]. Moreover, the expression of $B(n,e)$ is rather complicated. We remark that two lower bounds and the four upper bounds on $t(G) + t(G^c)$ follows from (3), (4) and (12), (14), (15), (17), respectively.

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