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New Bounds for the First Zagreb Index

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Abstract

The first Zagreb index $M_1(G)$ of a graph G is defined as the sum of squares of the degrees of the vertices. In this paper various bounds for the first Zagreb index are obtained.

1 Introduction

In this paper we are concerned with simple graphs, that is graphs without multiple, directed, or weighted edges, and without self-loops. Let $G = G(V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. Denote by n and m the number of vertices and edges of G, respectively. For $i = 1, 2, \ldots, n$ the degree of a vertex $v_i \in V(G)$ is denoted by d_i and it is defined as the number of edges incident with v_i. We denote by $\Delta = \Delta(G)$ and $\delta = \delta(G)$ the *maximum and the minimum degrees*, respectively, of vertices of G. Topological index is a real number related to a graph. It must be a structural invariant, i.e., it preserves by every graph automorphisms. Among the oldest and most studied topological indices, there are two classical vertex-degree based topological indicesthe *first Zagreb index* and *second Zagreb index*. The Zagreb indices were first introduced by Gutman et al. in [12, 13]; they present an important molecular descriptor closely correlated with many chemical

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properties. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a graph G are defined, respectively, as

$$M_1(G) = \sum_{i=1}^{n} d_i^2 = d_1^2 + d_2^2 + \ldots + d_n^2,$$

and

$$M_2(G) = \sum_{v_i, v_j \in E(G)} d_i d_j.$$

During the past decades, numerous results concerning Zagreb indices have been published, see in [1, 2, 4–7, 17].

In 2004 and 2005, Li et al. [14, 15], introduced the generalized version of the first Zagreb index, defined as

$$Z_p(G) = M_1^p(G) = d_1^p + d_2^p + \ldots + d_n^p$$

where p is a real number. This graph invariant is nowadays known under the name *general first Zagreb index*, and has also been much investigated.

In this paper we focus on the first Zagreb index. In addition, we list known results concerning the bounds of M_1. In [4] the following result that determines the lower bound of M_1 in terms of $m, n, d_1(\Delta)$ and $d_n(\delta)$ was proved.

Theorem 1.1 *[4] Let G be a simple graph with $n \geq 3$ vertices and m edges. Then*

$$M_1 \geq d_1^2 + d_n^2 + \frac{(2m - d_1 - d_n)^2}{n-2},$$

with equality if and only if G is regular or with the property $d_2 = d_3 = \ldots = d_{n-1}$.

The following lower bound of M_1 in terms of parameters n, m, d_1, d_2 and d_n was obtained in [8].

Theorem 1.2 *[8] Let G be a simple graph with $n \geq 3$ vertices and m edges. Then*

$$M_1 \geq d_1^2 + \frac{(2m - d_1)^2}{n-1} + \frac{1}{2}(d_2 - d_n)^2.$$

Equality holds if and only if G is regular graph or with property $d_2 = d_3 = \ldots = d_n$.

In [9] the lower bound for M_1 in terms of n and m was determined.

Theorem 1.3 *[9] Let G be a simple connected graph with n vertices and m edges. Then*

$$M_1 \geq \frac{4m^2}{n}. \tag{1}$$

Equality holds if and only if G is regular.

The *clique number* of a graph G, denoted $\omega(G)$, is the order of a maximum clique of G. Zhou [17] proved the following upper bound for M_1 as a function of $\omega(G)$.

Theorem 1.4 *[17] Let G be a simple graph with n vertices and m edges. Then*

$$M_1 \leq \frac{\omega - 1}{\omega} 2nm.$$

A lower bound for the first Zagreb index in terms of the number of vertices and the clique number is given in [18].

Theorem 1.5 *[18]*

$$M_1 \geq \omega^3 - 2\omega^2 - \omega + 4n - 4$$

with equality holding if and only if G is isomorphic to the kite graph $K_k((n-k)^1)$.

In Section 2 of this paper we derive a lower bound for the first Zagreb index of G which is better than the bound $\frac{4m^2}{n}$, Theorem 2.2. Moreover we give a relation between the first Zagreb index M_1 and the general Zagreb index $Z_4(G)$, Theorem 2.4. The results in Section 3 address the first Zagreb index in terms of n, δ, Δ and ω.

2 Results

Let G be a graph with n vertices, m edges and vertex degrees $\Delta = d_1 \geq d_2 \geq \ldots \geq d_n = \delta$. Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ be the eigenvalues of G. The energy of G is defined as

$$E(G) = |\lambda_1| + \ldots + |\lambda_n|.$$

Our first main result involves the parameter $\lambda_1 d_1 + \ldots + \lambda_n d_n$. We start with an easy observation concerning its upper bound.

Proposition 2.1 *Let G be a graph with n vertices and vertex degrees $\Delta = d_1 \geq d_2 \geq \ldots \geq d_n = \delta$. Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ be the eigenvalues of G and let $E(G)$ be its energy. Then*

$$\lambda_1 d_1 + \ldots + \lambda_n d_n \leq \frac{E(G)(\Delta - \delta)}{2}.$$

PROOF. Let $\lambda_1, \ldots, \lambda_p$ be the positive and let $\lambda_{p+1}, \ldots, \lambda_n$ be the negative eigenvalues of G. Since $d_i \leq \Delta$ for each $i = 1, \ldots, p$, we obtain

$$\lambda_1 d_1 + \ldots + \lambda_p d_p \leq (\lambda_1 + \ldots + \lambda_p)\Delta. \tag{2}$$

Similarly, since $d_i \geq \delta$ for each $i = p+1, \ldots, n$, we get

$$\lambda_{p+1} d_{p+1} + \ldots + \lambda_n d_n \leq (\lambda_{p+1} + \ldots + \lambda_n)\delta. \tag{3}$$

Now, from $(\lambda_1 + \ldots + \lambda_p) + (\lambda_{p+1} + \ldots + \lambda_n) = 0$ we get $\lambda_1 + \ldots + \lambda_p = -(\lambda_{p+1} + \ldots + \lambda_n)$ and

$$E(G) = |\lambda_1| + \ldots + |\lambda_n| = (\lambda_1 + \ldots + \lambda_p) - (\lambda_{p+1} + \ldots + \lambda_n) = 2(\lambda_1 + \ldots + \lambda_p). \tag{4}$$

By using (2), (3) and (4) we have

$$\lambda_1 d_1 + \ldots \lambda_n d_n \leq (\lambda_1 + \ldots + \lambda_p)\Delta + (\lambda_{p+1} + \ldots + \lambda_n)\delta =$$

$$= (\lambda_1 + \ldots + \lambda_p)(\Delta - \delta) = \frac{E(G)(\Delta - \delta)}{2}.$$

■

Theorem 2.2 *Let G be a graph with n vertices and m edges. Let $d_1 \geq d_2 \geq \ldots \geq d_n$ be vertex degrees and let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ be the eigenvalues of G. Then*

$$M_1 \geq \frac{4m^2}{n} + \frac{(\lambda_1 d_1 + \ldots + \lambda_n d_n)^2}{2m}. \tag{5}$$

PROOF. The required inequality in (5) is equivalent to the inequality

$$\frac{n}{4m^2} \geq \frac{2m}{2mM_1 - (\lambda_1 d_1 + \ldots + \lambda_n d_n)^2}. \tag{6}$$

By using $d_1^2 + \ldots + d_n^2 = M_1$ and $\lambda_1^2 + \ldots + \lambda_n^2 = 2m$ we get

$$\sum_{i=1}^{n} (2md_i - (\lambda_1 d_1 + \ldots + \lambda_n d_n)\lambda_i)^2 =$$

$$= \sum_{i=1}^{n} (4m^2 d_i^2 - 4md_i(\lambda_1 d_1 + \ldots + \lambda_n d_n)\lambda_i + (\lambda_1 d_1 + \ldots + \lambda_n d_n)^2 \lambda_i^2) =$$

$$= 4m^2 \sum_{i=1}^{n} d_i^2 - 4m(\lambda_1 d_1 + \ldots + \lambda_n d_n) \sum_{i=1}^{n} \lambda_i d_i + (\lambda_1 d_1 + \ldots + \lambda_n d_n)^2 \sum_{i=1}^{n} \lambda_i^2 =$$

$$= 4m^2 M_1 - 4m(\lambda_1 d_1 + \ldots + \lambda_n d_n)^2 + 2m(\lambda_1 d_1 + \ldots + \lambda_n d_n)^2 = 2m(2mM_1 - (\lambda_1 d_1 + \ldots + \lambda_n d_n)^2).$$

Thus we obtain the identity

$$\frac{2m}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}=\sum_{i=1}^{n}\left(\frac{2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}\right)^2. \tag{7}$$

On the other hand, from $\lambda_1+\ldots+\lambda_n=0$ and $d_1+\ldots+d_n=2m$ we get

$$\sum_{i=1}^{n}(2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i)=2m\sum_{i=1}^{n}d_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\sum_{i=1}^{n}\lambda_i=4m^2.$$

Thus

$$\frac{2m}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}=\sum_{i=1}^{n}\frac{1}{2m}\cdot\frac{2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}. \tag{8}$$

The identities in (7) and (8) yield

$$\sum_{i=1}^{n}\left(\frac{2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}\right)^2=\frac{1}{2m}\sum_{i=1}^{n}\frac{2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}. \tag{9}$$

In the end we have

$$\frac{n}{4m^2}-\frac{2m}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}=\sum_{i=1}^{n}\frac{1}{(2m)^2}-\sum_{i=1}^{n}\left(\frac{2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}\right)^2$$

$$=\sum_{i=1}^{n}\frac{1}{(2m)^2}-2\sum_{i=1}^{n}\left(\frac{2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}\right)^2+\sum_{i=1}^{n}\left(\frac{2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}\right)^2$$

$$=\sum_{i=1}^{n}\frac{1}{(2m)^2}-2\cdot\frac{1}{2m}\sum_{i=1}^{n}\frac{2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}+\sum_{i=1}^{n}\left(\frac{2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}\right)^2$$

$$=\sum_{i=1}^{n}\left(\frac{1}{2m}-\frac{2md_i-(\lambda_1d_1+\ldots+\lambda_nd_n)\lambda_i}{2mM_1-(\lambda_1d_1+\ldots+\lambda_nd_n)^2}\right)^2\geq 0.$$

■

Remark 2.3 *Since* $\frac{(\lambda_1d_1+\ldots+\lambda_nd_n)^2}{2m}\geq 0$ *we obtain*

$$M_1\geq\frac{4m^2}{n}+\frac{(\lambda_1d_1+\ldots+\lambda_nd_n)^2}{2m}\geq\frac{4m^2}{n}.$$

If G *is a regular graph, then* $\lambda_1d_1+\ldots+\lambda_nd_n=0$. *In this case* $M_1=\frac{4m^2}{n}$. *Otherwise, if* $\lambda_1d_1+\ldots+\lambda_nd_n\neq 0$, *then the bound in (5) is better than the bound in (1).*

In the following theorem we give a relation between M_1 and $Z_4(G)$. This result follows similar reasoning as Theorem 2.1 in [10].

Theorem 2.4 *Let G be a graph with n vertices, m edges and vertex degrees $\Delta = d_1 \geq d_2 \geq \ldots \geq d_n = \delta$. Then*

$$Z_4(G) \leq \frac{M_1^2}{n} + \frac{8\sqrt{n}\Delta^4}{\delta}\left(\sqrt{M_1} - \frac{2m}{\sqrt{n}}\right). \tag{10}$$

Equality holds if G is a regular graph.

Proof. In [10] was proven that for any two positive real numbers a and b it holds

$$\sqrt{\frac{a}{b}} + \sqrt{\frac{b}{a}} + \frac{ab}{a^2+b^2} \geq \frac{5}{2},$$

that is,

$$a + b \geq \left(2 + \frac{(a-b)^2}{2(a^2+b^2)}\right)\sqrt{ab}. \tag{11}$$

Setting $a = \frac{d_i^2}{M_1}$ and $b = \frac{1}{n}$ in (11) we obtain the following inequality

$$\frac{d_i^2}{M_1} + \frac{1}{n} \geq \left(2 + \frac{(nd_i^2 - M_1)^2}{2(n^2 d_i^4 + M_1^2)}\right)\frac{d_i}{\sqrt{n \cdot M_1}}. \tag{12}$$

From (12) we deduce

$$\frac{1}{M_1}\sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n}\frac{1}{n} \geq \frac{2}{\sqrt{n \cdot M_1}}\sum_{i=1}^{n} d_i + \sum_{i=1}^{n}\frac{(nd_i^2 - M_1)^2}{2(n^2 d_i^4 + M_1^2)}\frac{d_i}{\sqrt{n \cdot M_1}}. \tag{13}$$

Since $\sum_{i=1}^{n} d_i^2 = M_1$ and $\sum_{i=1}^{n} d_i = 2m$, the inequality in (13) becomes

$$2 \geq \frac{4m}{\sqrt{n \cdot M_1}} + \frac{1}{\sqrt{n \cdot M_1}}\sum_{i=1}^{n}\frac{(nd_i^2 - M_1)^2}{2(n^2 d_i^4 + M_1^2)} d_i.$$

Since $d_i \leq \Delta$ for each $i = 1, 2, \ldots, n$ we have $M_1 \leq n\Delta^2$. Therefore $\frac{1}{n^2 d_i^4 + M_1^2} \geq \frac{1}{2n^2\Delta^4}$. The previous inequality is equivalent to

$$\sqrt{M_1} \geq \frac{2m}{\sqrt{n}} + \frac{\delta}{8\sqrt{n}\Delta^4}\sum_{i=1}^{n}(d_i^2 - \frac{M_1}{n})^2 = \frac{2m}{\sqrt{n}} + \frac{\delta}{8\sqrt{n}\Delta^4}\left(Z_4(G) - \frac{M_1^2}{n}\right).$$

Thus we have

$$Z_4(G) \leq \frac{M_1^2}{n} + \frac{8\sqrt{n}\Delta^4}{\delta}\left(\sqrt{M_1} - \frac{2m}{\sqrt{n}}\right).$$

The inequality (10) becomes equality if in (11) holds equality. It is possible when $a = b$, which implies $M_1 = nd_i^2$ for each $i = 1, \ldots, n$. These identities occur only if $d_1 = \ldots = d_n$, that is, if G is a regular graph. ■

Remark 2.5 *From the inequality between quadratic and arithmetic mean for the numbers* $d_1^2, \ldots, d_n^2$ *it follows*

$$Z_4(G) = d_1^4 + \ldots + d_n^4 \geq \frac{(d_1^2 + \ldots + d_n^2)^2}{n} = \frac{M_1^2}{n}.$$

Hence

$$Z_4(G) \in \left[\frac{M_1^2}{n}, \frac{M_1^2}{n} + \frac{8\sqrt{n}\Delta^4}{\delta}\left(\sqrt{M_1} - \frac{2m}{\sqrt{n}}\right)\right].$$

3 New bounds for M_1 for graphs with given clique number

As shown by Caro [3] and Wei [19], the degree sequence $d_1, d_2, \ldots, d_n$ of a graph G of order n gives rise to a lower bound on the clique number ω of G:

$$\omega(G) \geq \frac{1}{n-d_1} + \frac{1}{n-d_2} + \ldots + \frac{1}{n-d_n}. \tag{14}$$

Taking advantage of this result, in the next result we obtain a lower bound for M_1 in terms of n, m and ω.

Theorem 3.1 *Let G be a graph with n vertices, m edges and clique number ω. Then*

$$M_1 \geq 4mn + \frac{n^3}{w^2} - n^3.$$

Equality holds if and only if G is a regular graph of degree k and $\omega = \frac{n}{n-k}$.

Proof. Using the inequality between quadratic and harmonic mean for the positive numbers $n-d_1, n-d_2, \ldots, n-d_n$ we have

$$\sqrt{\frac{(n-d_1)^2 + (n-d_2)^2 + \ldots + (n-d_n)^2}{n}} \geq \frac{n}{\frac{1}{n-d_1} + \frac{1}{n-d_2} + \ldots + \frac{1}{n-d_n}}. \tag{15}$$

From (15) and $\omega = \omega(G) \geq \frac{1}{n-d_1} + \frac{1}{n-d_2} + \ldots + \frac{1}{n-d_n}$ we have

$$\sqrt{\frac{n^3 - 4mn + M_1}{n}} \geq \frac{n}{w}$$

which leads to

$$M_1 \geq 4mn + \frac{n^3}{w^2} - n^3.$$

The equality in (15) holds if and only if $n - d_1 = \ldots = n - d_n$, that is, if and only if $d_1 = d_2 = \ldots = d_n = k$. Moreover, equality in the inequality $\omega \geq \frac{1}{n-d_1} + \frac{1}{n-d_2} + \ldots + \frac{1}{n-d_n}$ holds if $\omega = \frac{n}{n-k}$. ■

Similarly as in the previous result, we derive a lower bound for the first Zagreb index in terms of n, m, ω and Δ.

Theorem 3.2 *Let G be a graph with n vertices, m edges, clique number ω and maximum degree Δ. Then*

$$M_1 \geq 2n(2m-\Delta)+\Delta^2+\frac{(n-1)^3}{\left(w-\frac{1}{n-\Delta}\right)^2}-n^2(n-1).$$

Equality holds if $d_2=\ldots=d_n=\frac{2m-\Delta}{n-1}$ and $\omega=\frac{1}{n-\Delta}+\frac{(n-1)^2}{n^2-n-2m+\Delta}$.

PROOF. We proceed similarly as in the previous proof. Using the inequality between quadratic and harmonic mean for the positive numbers $n-d_2,\ldots,n-d_n$ we have

$$\sqrt{\frac{(n-d_2)^2+\ldots+(n-d_n)^2}{n-1}} \geq \frac{n-1}{\frac{1}{n-d_2}+\ldots+\frac{1}{n-d_n}}. \tag{16}$$

From (16) and $\omega-\frac{1}{n-d_1} \geq \frac{1}{n-d_2}+\ldots+\frac{1}{n-d_n}$ we have

$$\sqrt{\frac{(n-1)n^2-2n(2m-\Delta)+M_1-\Delta^2}{n-1}} \geq \frac{n-1}{w-\frac{1}{n-\Delta}}$$

which leads to the required inequality.

The inequality (16) becomes equality if $n-d_2=\ldots=n-d_n$, that is, if $d_2=\ldots=d_n=\frac{2m-\Delta}{n-1}$. The equality in $\omega-\frac{1}{n-d_1} \geq \frac{1}{n-d_2}+\ldots+\frac{1}{n-d_n}$ holds when $\omega=\frac{1}{n-\Delta}+\frac{(n-1)^2}{n^2-n-2m+\Delta}$. ■

A graph which does not contain triangles is called *triangle-free graph.* In [16] Zhou obtained the following bound:

Theorem 3.3 *[16] Let G be a triangle free (n,m)-graph. Then*

$$M_1(G) \leq mn \tag{17}$$

and equality holds if and only if G is a complete bipartite graph.

Based on Theorem 3.3 we are in a position to obtain an upper bound for M_1 for triangle-free graphs in terms of n and Δ.

Theorem 3.4 *Let G be a triangle-free graph with n vertices and maximum degree Δ. Then*

$$M_1 \leq \frac{n(n^2-n+\Delta)}{2}-\frac{n(n-1)^2(n-\Delta)}{4(n-\Delta)-2}. \tag{18}$$

PROOF. Since G is a triangle-free graph we get $\omega \leq 2$. From the inequality (14) we obtain

$$2-\frac{1}{n-\Delta} \geq \frac{1}{n-d_2}+\ldots+\frac{1}{n-d_n}.$$

By applying Cauchy-Schwarz inequality to the numbers $\frac{1}{n-d_2}, \dots, \frac{1}{n-d_n}$ we have

$$\frac{2(n-\Delta)-1}{n-\Delta} = 2 - \frac{1}{n-\Delta} \geq \frac{(1+1+\ldots+1)^2}{n-d_2+\ldots+n-d_n} = \frac{(n-1)^2}{n(n-1)-(2m-\Delta)}. \qquad (19)$$

From (19) we obtain

$$m \leq \frac{n^2-n+\Delta}{2} - \frac{(n-\Delta)(n-1)^2}{4(n-\Delta)-2}.$$

The bound in (18) follows directly from (17). ∎

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