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VERTEX-BLOCK ZAGREB INDICES OF GRAPHS

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Abstract. A topological index is a graph invariant applicable in chemistry. The first and second Zagreb indices are topological indices based on the vertex degrees of molecular graphs. For any graph G, the first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of vertices, and the second Zagreb index $M_2(G)$ is equal to the sum of the products of the degrees of pairs of adjacent vertices. A block is a maximal connected graph with no cut-vertices. The vertex-block degree (vb-degree) of a vertex is the number of blocks incident on it. In this paper, we define two new graph invariants, named as the first and second vertex-block Zagreb indices and obtain lower and upper bounds on them in terms of number of vertices, number of blocks and maximum vb-degree of a graph.

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1. Introduction

By a graph $G = (V, E)$ we mean a finite, undirected and simple graph of order $|V| = p$ and size $|E| = q$, where V and E respectively denote the vertex set and the edge set of G. The terminologies and notations used here are as in [11, 20]. The first and second Zagreb indices are topological indices based on vertex degrees of molecular graphs. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of G are defined as follows: $M_1(G) = \sum_{u\in V} d(u)^2$ and $M_2(G) = \sum_{uv\in E} d(u)d(v)$. I. Gutman and N. Trinajstić introduced $M_1(G)$ in 1972 [10], whereas $M_2(G)$ was introduced by I. Gutman et al. in 1975 [9]. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [1, 19]. The main properties of Zagreb indices were summarized in [8, 15]. Also, numerous bounds for $M_1(G)$ and $M_2(G)$ were obtained in [5, 6, 7].

A vertex $v \in V$ is a cut-vertex of a graph G if its removal from G increases the number of components of G. A block is a maximal connected subgraph of G that has no cut-vertices. A block is called a pendant block if it is incident on a single cut-vertex, otherwise it is called a non-pendant block. Let B be a block of a graph G. Then $G - B$ denotes the graph obtained by removing all the edges and non-cut-vertices of B from G. In 2013, P. G. Bhat et al. [2] defined the vertex-block degree (vb-degree) of a vertex. If a block B contains a vertex v then we say that B and v incident to each other. The vb-degree of a vertex v denoted by $d_{vb}(v)$ is the number of blocks incident on v. We denote minimum and maximum vb-degree of vertices of G by $\delta_{vb} = \delta_{vb}(G)$ and $\Delta_{vb} = \Delta_{vb}(G)$, respectively. Note that $\delta_{vb}(G) = 1$, for

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every graph G. The second maximum vb-degree of G is written as $\Delta_{vb_2} = \Delta_{vb_2}(G)$. Surekha [18] proved that, for any connected graph G, $\sum\limits_{u \in V} d_{vb}(u) = p + m - 1$, where p is the order of G and m is the number of blocks in G.

Let $\mathcal{B}(G)$ and $V_c(G)$ denote the set of all blocks and set of all cut-vertices of a graph G, respectively. We denote $|\mathcal{B}(G)| = m$ and $|V_c(G)| = c$. A block-graph $\mathcal{B}_G(G)$ is a graph with vertex set $\mathcal{B}(G)$ and any two vertices in $\mathcal{B}_G(G)$ are adjacent if and only if the corresponding blocks are adjacent in G. A block-walk is a sequence of blocks and cut-vertices, say $B_1, u_1, B_2, u_2, \ldots, B_{m-1}, u_{m-1}, B_m$, beginning and ending with blocks in which each cut-vertex u_i is incident with the blocks B_i and B_{i+1}, $1 \leq i \leq m-1$. A block-walk in which all the cut-vertices are distinct is a block-path. A block-path with m blocks and $m-1$ cut-vertices is denoted as B_{P_m}. Two blocks are said to be adjacent if there is a common cut-vertex incident on them. A block-complete graph denoted by B_{K_m} is a connected graph with m blocks in which every pair of blocks is adjacent. A connected graph G is called as a block-star $B_{m_1, m_2, \ldots, m_c}$ if there exists a block B in G with c cut-vertices such that i^{th} cut-vertex is incident with m_i pendant blocks, where $m_i \in \mathbb{N}$ and $1 \leq i \leq c$.

2. Vertex-Block Zagreb Indices of graphs

We now define two new graph invariants called as the first and second vertex-block Zagreb indices. Let $G = (V, E)$ be a graph. We denote a block $B \in \mathcal{B}(G)$ consisting vertices $u_1, u_2, \ldots, u_k$ by $B = u_1 u_2 \ldots u_k$.

Definition 2.1. *The first and second vertex-block Zagreb indices denoted by $VBM_1(G)$ and $VBM_2(G)$, respectively are defined as follows:*

$$VBM_1(G) = \sum_{u \in V} d_{vb}(u)^2 \quad \textit{and}$$

$$VBM_2(G) = \sum_{u_1 u_2 \ldots u_k \in \mathcal{B}(G)} [d_{vb}(u_1) d_{vb}(u_2) \ldots d_{vb}(u_k)].$$

2.1. Preliminary results.

Proposition 2.1. *(i) For any block G, $VBM_1(G) = p$ and $VBM_2(G) = 1$.*

(ii) For any block-path B_{P_m} with $m > 1$, $VBM_1(B_{P_m}) = p + 3(m-1)$ and $VBM_2(B_{P_m}) = 4(m-1)$.

(iii) For any block-complete graph B_{K_m}, $VBM_1(B_{K_m}) = p + m^2 - 1$ and $VBM_2(B_{K_m}) = m^2$.

(iv) For any block-star $G = B_{m_1, m_2, \ldots, m_c}$, $VBM_1(G) = p + \sum\limits_{i=1}^{c} [m_i(m_i + 2)]$ and $VBM_2(G) = \sum\limits_{i=1}^{c} m_i(m_i + 1) + \prod\limits_{i=1}^{c} (m_i + 1)$.

Proof. *(ii)* Let $G = B_{P_m}$ be a block-path with $m > 1$. Then

$$\begin{aligned} VBM_1(G) &= \sum_{u \in V_c(G)} d_{vb}(u)^2 + \sum_{u \notin V_c(G)} d_{vb}(u)^2 \\ &= \sum_{u \in V_c(G)} 2^2 + \sum_{u \notin V_c(G)} 1^2 \\ &= 4c + (p - c) \\ &= 4(m-1) + p - (m-1) \\ &= p + 3(m-1). \end{aligned}$$

Since G has exactly 2 pendant blocks and $m-2$ non-pendant blocks, we obtain the following,

$$\begin{aligned} VBM_2(G) &= \sum_{u_1 u_2 \ldots u_k \in \mathcal{B}(G)} [d_{vb}(u_1) d_{vb}(u_2) \ldots d_{vb}(u_k)] \\ &= 2 + 2 + 4(m-2) \\ &= 4(m-1). \end{aligned}$$

(iii) Let $G = B_{K_m}$ be a block-complete graph. Then G has a unique cut-vertex, say u_c with $d_{vb}(u_c) = m$. Now,

$$\begin{aligned} VBM_1(G) &= \sum_{\substack{u \in V(G) \\ u \neq u_c}} d_{vb}(u)^2 + d_{vb}(u_c)^2 \\ &= \sum_{\substack{u \in V(G) \\ u \neq u_c}} 1^2 + m^2 \\ &= p + m^2 - 1. \end{aligned}$$

Further,

$$\begin{aligned} VBM_2(G) &= \sum_{u_1 u_2 \ldots u_k \in \mathcal{B}(G)} [d_{vb}(u_1) d_{vb}(u_2) \ldots d_{vb}(u_k)] \\ &= \sum_{u_1 u_2 \ldots u_k \in \mathcal{B}(G)} m \\ &= m^2. \end{aligned}$$

(iv) Consider a block-star $G = B_{m_1, m_2, \ldots, m_c}$, then G has c cut-vertices and there exists a block $B = v_1 v_2 \ldots v_k$ in G with c cut-vertices such that i^{th} cut-vertex is incident with $m_i + 1$ blocks, where $m_i \in \mathbb{N}$ and $1 \leq i \leq c$. Now,

$$\begin{aligned} VBM_1(G) &= \sum_{u \in V_c(G)} d_{vb}(u)^2 + \sum_{u \notin V_c(G)} d_{vb}(u)^2 \\ &= \sum_{i=1}^{c} (m_i + 1)^2 + (p - c) \\ &= p + \sum_{i=1}^{c} [m_i(m_i + 2)]. \end{aligned}$$

We have i^{th} cut-vertex of G incident with m_i pendant-blocks, and the product of vb-degrees of vertices of any pendant-block incident with i^{th} cut-vertex is equal to $m_i + 1$. Hence, we obtain

$$\begin{aligned} VBM_2(G) &= d_{vb}(v_1)d_{vb}(v_2)\ldots d_{vb}(v_k) + \sum_{\substack{u_1u_2\ldots u_l \in \mathcal{B}(G) \\ u_1u_2\ldots u_l \neq B}} [d_{vb}(u_1)d_{vb}(u_2)\ldots d_{vb}(u_l)] \\ &= \prod_{i=1}^{c} (m_i + 1) + \sum_{i=1}^{c} m_i(m_i + 1). \end{aligned}$$

□

Remark 2.1. *(i) For any graph G, $VBM_1(G) \leq M_1(G)$ and $VBM_2(G) \leq M_2(G)$.*
(ii) If G is an acyclic graph, then $VBM_1(G) = M_1(G)$ and $VBM_2(G) = M_2(G)$.

Proposition 2.2. [18] *Let G be a connected graph and q_b denotes the number of edges in the block graph $\mathcal{B}_G(G)$. Then, $2q_b = \sum_{u \in V_c(G)} d_{vb}(u)^2 - (m + c - 1)$.*

Theorem 2.1. *For a connected graph G, $VBM_1(G) = 2q_b + (p + m - 1)$.*

Proof. We have,

$$\begin{aligned} VBM_1(G) &= \sum_{u \in V} d_{vb}(u)^2 \\ &= \sum_{u \in V_c(G)} d_{vb}(u)^2 + \sum_{u \notin V_c(G)} d_{vb}(u)^2. \end{aligned} \tag{1}$$

Using Proposition 2.2 in (1), we get

$$\begin{aligned} VBM_1(G) &= 2q_b + (m + c - 1) + \sum_{u \notin V_c(G)} 1^2 \\ &= 2q_b + (m + c - 1) + (p - c) \\ &= 2q_b + (p + m - 1). \end{aligned}$$

□

Remark 2.2. *The first and second vertex-block Zagreb indices $VBM_1(G)$ and $VBM_2(G)$ are incomparable for general graphs. For example, consider the graphs G_1 and G_2 as given in the Figure 1. Note that, $VBM_1(G_1) < VBM_2(G_1)$, whereas $VBM_1(G_2) > VBM_2(G_2)$.*

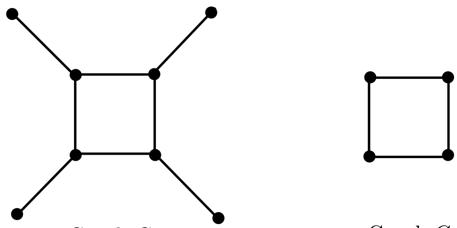

FIGURE 1. Graphs G_1 and G_2

3. Lower and upper bounds on $VBM_1(G)$

In this section, we present some bounds on first vertex-block Zagreb index $VBM_1(G)$ in terms of p, m, Δ_{vb} and Δ_{vb_2}.

Theorem 3.1. *For any connected graph G, $\frac{(p+m-1)^2}{p} \leq VBM_1(G) \leq p{\Delta_{vb}}^2$. Further, equality holds if and only if G is a block.*

Proof. Let $u_1, u_2, \ldots, u_p$ be the vertices of G. By Cauchy-Schwarz inequality, we have

$$\frac{1}{p}\left(\sum_{i=1}^{p} d_{vb}(u_i)\right)^2 \leq \sum_{i=1}^{p} d_{vb}(u_i)^2.$$

Therefore,

$$\frac{(p+m-1)^2}{p} \leq VBM_1(G).$$

Now,

$$VBM_1(G) = \sum_{i=1}^{p} d_{vb}(u_i)^2 \leq \sum_{i=1}^{p} \Delta_{vb}^2 = p\Delta_{vb}^2.$$

Thus, both the lower and upper bounds follows. Further, suppose $\frac{(p+m-1)^2}{p} = VBM_1(G)$. Then $d_{vb}(u_i) = d_{vb}(u_j)$, for all i, j, $1 \leq i, j \leq p$. This implies that, $d_{vb}(u_i) = 1$, for all i, $1 \leq i \leq p$. Therefore, G has no cut-vertices. Since G is connected, G must be a block. Also, if $VBM_1(G) = p{\Delta_{vb}}^2$, then $d_{vb}(u_i) = \Delta_{vb}$, for all i, $1 \leq i \leq p$. This implies that, $d_{vb}(u_i) = 1$, for all i, $1 \leq i \leq p$. Thus, G is a block. Conversely, if G is a block, we have $m = 1$, $\Delta_{vb} = 1$ and $VBM_1(G) = p$. Thus, equality holds. □

Corollary 3.1. [13] *For a tree T with p vertices and e edges, $M_1(T) \geq \frac{4e^2}{p}$.*

Theorem 3.2. *Let $G = (V, E)$ be a connected graph. Then $VBM_1(G) \leq p + (m-1)[\Delta_{vb}+1]$. Further, equality holds if and only if for any $u \in V$, either $d_{vb}(u) = \Delta_{vb}$ or $d_{vb}(u) = 1$.*

Proof. Let $u_1, u_2, \ldots, u_p$ be the vertices of G.
We have

$$\begin{aligned} VBM_1(G) &= \sum_{i=1}^{p} d_{vb}(u_i)^2 \\ &= \sum_{i=1}^{p} [d_{vb}(u_i)(d_{vb}(u_i) - 1) + d_{vb}(u_i)] \\ &\leq \sum_{i=1}^{p} [\Delta_{vb}(d_{vb}(u_i) - 1) + d_{vb}(u_i)] \\ &= p + (m-1)[\Delta_{vb} + 1]. \end{aligned}$$

Further, equality holds if and only if

$$\sum_{i=1}^{p} (\Delta_{vb} - d_{vb}(u_i))(d_{vb}(u_i) - 1) = 0$$

Note that each term of the above summation is non-negative. Hence, equality holds if and only if for any $u \in V$, either $d_{vb}(u) = \Delta_{vb}$ or $d_{vb}(u) = 1$. □

Lemma 3.1. *(i) (Pólya-Szegö inequality)* [17] *Let* $a = (a_1, a_2, \ldots, a_n)$ *and* $b = (b_1, b_2, \ldots, b_n)$ *be two n-tuples of positive numbers. If* $0 < \gamma \leq a_i \leq A < \infty$ *and* $0 < \beta \leq b_i \leq B < \infty$ *for each* i, $1 \leq i \leq n$, *then* $\sum_{i=1}^{n} {a_i}^2 \sum_{j=1}^{n} {b_j}^2 \leq \frac{(\gamma\beta + AB)^2}{4\gamma\beta AB} \left(\sum_{i=1}^{n} a_i b_i \right)^2$.

(ii) (Ozeki's inequality) [16] *If* $a = (a_1, a_2, \ldots, a_n)$ *and* $b = (b_1, b_2, \ldots, b_n)$ *are two n-tuples of real numbers satisfying* $0 \leq m_1 \leq a_i \leq M_1$ *and* $0 \leq m_2 \leq b_i \leq M_2$ *for every* i, $1 \leq i \leq n$, *then* $\sum_{i=1}^{n} {a_i}^2 \sum_{j=1}^{n} {b_j}^2 - \left(\sum_{i=1}^{n} a_i b_i \right)^2 \leq \frac{n^2}{4} (M_1 M_2 - m_1 m_2)^2$.

Theorem 3.3. *Let G be a connected graph. Then,*

(i) $VBM_1(G) \leq \frac{(1+\Delta_{vb})^2}{4p\Delta_{vb}} (p + m - 1)^2$

(ii) $VBM_1(G) \leq \frac{(p+m-1)^2}{p} + \frac{p}{4}(\Delta_{vb} - 1)^2$.

Further, the equality holds in (i) *and* (ii) *if G is a block.*

Proof. Let $u_1, u_2, \ldots, u_p$ be the vertices of G.
(i) We take $a_i = d_{vb}(u_i)$, $b_i = 1$, for every i, $1 \leq i \leq p$, $\gamma = 1$, $\beta = 1$, $A = \Delta_{vb}$ and $B = 1$ in the Polya-Szego inequality.
Then,

$$\sum_{i=1}^{p} d_{vb}(u_i)^2 \sum_{j=1}^{p} 1^2 \leq \frac{(1 + \Delta_{vb})^2}{4\Delta_{vb}} \left(\sum_{i=1}^{p} d_{vb}(u_i) \right)^2.$$

This implies that,

$$VBM_1(G)p \leq \frac{(1 + \Delta_{vb})^2}{4\Delta_{vb}} (p + m - 1)^2.$$

Thus, the inequality (i) follows.
(ii) We take $a_i = d_{vb}(u_i)$, $b_i = 1$, for every i, $1 \leq i \leq p$, $m_1 = m_2 = M_2 = 1$ and

$M_1 = \Delta_{vb}$ in the Ozeki's inequality.
Then,

$$\sum_{i=1}^{p} d_{vb}(u_i)^2 \sum_{j=1}^{p} 1^2 - \left(\sum_{i=1}^{p} a_i\right)^2 \leq \frac{p^2}{4}(\Delta_{vb} - 1)^2.$$

This implies that,

$$VBM_1(G)p - (p + m - 1)^2 \leq \frac{p^2}{4}(\Delta_{vb} - 1)^2.$$

Thus,

$$VBM_1(G) \leq \frac{(p + m - 1)^2}{p} + \frac{p}{4}(\Delta_{vb} - 1)^2.$$

Further, the equality holds in (i) and (ii) if G is a block. □

Remark 3.1. *We recall the following facts: Let f be a real valued function defined on an interval I. Then f is strictly convex on I if and only if f'' exists and $f''(x) > 0$, for every $x \in I$. For any positive integer n and strictly convex function f, by Jensen's inequality, we have $f(\sum_{i=1}^{n} \frac{x_i}{n}) \leq \frac{1}{n} \sum_{i=1}^{n} f(x_i)$ and equality holds if and only if $x_1 = x_2 = \cdots = x_k$. Further, if $-f$ is strictly convex, then the above inequality is reversed.*

Theorem 3.4. *For any graph G, $VBM_1(G) \geq p \left(\prod_{u \in V} d_{vb}(u)\right)^{\frac{2}{p}}$. Further, equality holds if and only if G is either a block or a union of blocks.*

Proof. Consider the function $f(x) = log(x)$ on the interval $I = (0, \infty)$. Then $-f(x)$ is a convex function on I. By Jensen's inequality, we have

$$\begin{aligned} log\left(\sum_{u \in V} \frac{d_{vb}(u)^2}{p}\right) &\geq \frac{1}{p} \sum_{u \in V} log\left(d_{vb}(u)^2\right) \\ &= log\left(\prod_{u \in V} d_{vb}(u)\right)^{\frac{2}{p}}. \end{aligned}$$

This implies that,

$$VBM_1(G) \geq p(\prod_{u \in V} d_{vb}(u))^{\frac{2}{p}}.$$

By Jensen's inequality, equality holds if and only if each vertex of G has the same vb-degree if and only if $d_{vb}(u) = 1$, for every $u \in V$ if and only if G is either a block or a union of blocks. □

Lemma 3.2. [3, 12] *Suppose $a = (a_1, a_2, \ldots, a_n)$ and $b = (b_1, b_2, \ldots, b_n)$ are n-tuples of real numbers, then $\left|n \sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i\right| \leq \alpha(n)(A - a)(B - b)$ where a, b, A and B are real constants such that $a \leq a_i \leq A$ and $b \leq b_i \leq B$, for each i, $1 \leq i \leq n$ and, $\alpha(n) = n\lceil\frac{n}{2}\rceil\left(1 - \frac{1}{n}\lceil\frac{n}{2}\rceil\right)$. Equality holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$.*

Theorem 3.5. *Let G be a connected graph. Then, $VBM_1(G) \leq \frac{\alpha(p)(\Delta_{vb}-1)^2+(p+m-1)^2}{p}$. Further, equality holds if and only if G is a block.*

Proof. Let $u_1, u_2, \ldots, u_p$ be the vertices of G. We choose $a_i = b_i = d_{vb}(u_i)$, for every i, $1 \leq i \leq p$, $A = B = \Delta_{vb}$ and $a = b = 1$, in Lemma 3.2, then

$$p\sum_{i=1}^{p} d_{vb}(u_i)^2 - \left(\sum_{i=1}^{p} d_{vb}(u_i)\right)^2 \leq \alpha(p)(\Delta_{vb}-1)^2,$$

that is,

$$pVBM_1(G) - (p+m-1)^2 \leq \alpha(p)(\Delta_{vb}-1)^2.$$

Thus,

$$VBM_1(G) \leq \frac{\alpha(p)(\Delta_{vb}-1)^2 + (p+m-1)^2}{p}.$$

Further, by the Lemma 3.2, equality of the theorem holds if and only if vb-degrees of all vertices of G are equal if and only if G is a block. □

Lemma 3.3. [14] *Let $a = (a_1, a_2, \ldots, a_n)$ and $b = (b_1, b_2, \ldots, b_n)$ be two n-tuples of real numbers. Then $\sum\limits_{i=1}^{n} {a_i}^2 \sum\limits_{j=1}^{n} {b_j}^2 - \left(\sum\limits_{i=1}^{n} a_i b_i\right)^2 = \sum\limits_{1\leq i<j\leq n} (a_i b_j - a_j b_i)^2$.*

Theorem 3.6. *Let G be a connected graph with $p > 2$ vertices. Then, $VBM_1(G) \geq {\Delta_{vb}}^2 + \frac{(p+m-\Delta_{vb}-1)^2}{p-1} + \frac{2(p-2)}{(p-1)^2}(\Delta_{vb_2}-1)^2$. Further, equality holds if and only if G is either a block or block-complete graph.*

Proof. Let $u_1, u_2, \ldots, u_p$ be vertices of G such that $d_{vb}(u_1) \geq d_{vb}(u_2) \geq \cdots \geq d_{vb}(u_p)$. We take $n = p-1$, $a_i = d_{vb}(u_{i+1})$ and $b_i = 1$, for every i, $1 \leq i \leq n$ in Lemma 3.3. Then we get,

$$\sum_{i=2}^{p} d_{vb}(u_i)^2 \sum_{j=2}^{p} 1^2 - \left(\sum_{i=2}^{p} d_{vb}(u_i)\right)^2 = \sum_{2\leq i<j\leq p} \left(d_{vb}(u_i) - d_{vb}(u_j)\right)^2.$$

This implies that,

$$(p-1)\left[VBM_1(G) - {\Delta_{vb}}^2\right] - (p+m-1-\Delta_{vb})^2 = \sum_{2\leq i<j\leq p} \left(d_{vb}(u_i) - d_{vb}(u_j)\right)^2. \tag{2}$$

Consider,

$$\sum_{2\le i<j\le p} |d_{vb}(u_i)-d_{vb}(u_j)| = (p-2)d_{vb}(u_2) - \sum_{i=3}^{p} d_{vb}(u_i) + \sum_{3\le i<j\le p-1} |d_{vb}(u_i)-d_{vb}(u_j)| + \sum_{i=3}^{p-1} d_{vb}(u_i) - (p-3)d_{vb}(u_p)$$

$$= (p-2)[d_{vb}(u_2)-d_{vb}(u_p)] + \sum_{3\le i<j\le p-1} |d_{vb}(u_i)-d_{vb}(u_j)|$$

$$\ge (p-2)[\Delta_{vb_2}-1]. \tag{3}$$

By power-mean inequality [4], we have

$$\left(\frac{\sum_{2\le i<j\le p} (d_{vb}(u_i)-d_{vb}(u_j))^2}{[(p-1)(p-2)]/2}\right)^{\frac{1}{2}} \ge \frac{\sum_{2\le i<j\le p} |d_{vb}(u_i)-d_{vb}(u_j)|}{[(p-1)(p-2)]/2}$$

with equality if and only if $|d_{vb}(u_i)-d_{vb}(u_j)| = |d_{vb}(u_l)-d_{vb}(u_k)|$, for every $2 \le i,j,l,k \le p$.
Then,

$$\sum_{2\le i<j\le p} (d_{vb}(u_i)-d_{vb}(u_j))^2 \ge \frac{2}{(p-1)(p-2)} \left(\sum_{2\le i<j\le p} |d_{vb}(u_i)-d_{vb}(u_j)|\right)^2 \tag{4}$$

with equality if and only if $d_{vb}(u_2) = d_{vb}(u_3) = \cdots = d_{vb}(u_p)$.
Now, from (3),

$$\sum_{2\le i<j\le p} (d_{vb}(u_i)-d_{vb}(u_j))^2 \ge \frac{2}{(p-1)(p-2)}(p-2)^2(\Delta_{vb_2}-1)^2 = \frac{2(p-2)}{(p-1)}(\Delta_{vb_2}-1)^2.$$

Using (2), from the above, we get

$$(p-1)\left[VBM_1(G)-{\Delta_{vb}}^2\right] \ge (p+m-1-\Delta_{vb})^2 + \frac{2(p-2)}{(p-1)}(\Delta_{vb_2}-1)^2.$$

Thus,

$$VBM_1(G) \ge {\Delta_{vb}}^2 + \frac{(p+m-\Delta_{vb}-1)^2}{p-1} + \frac{2(p-2)}{(p-1)^2}(\Delta_{vb_2}-1)^2. \tag{5}$$

Now, suppose that the equality holds in (5). Then the equality hold in (3) and (4). From the equality in (3) and (4), we get $d_{vb}(u_2) = d_{vb}(u_3) = \cdots = d_{vb}(u_p) = 1$. If $\Delta_{vb} = 1$, then G is a block. Otherwise, if $\Delta_{vb} > 1$, then G has exactly one cut-vertex. Hence, G is a block-complete graph. Conversely, if G is a block or block-complete graph, clearly the equality holds in (5).

Theorem 3.7. *Let B_{P_m} and B_{K_m} be the block-path and block-complete graphs, respectively with p vertices and m blocks of same order. If G is a connected graph with p vertices and m blocks of same order, then $VBM_1(B_{P_m}) \leq VBM_1(G) \leq VBM_1(B_{K_m})$.*

Proof. Let G be a connected graph with p vertices and m blocks of same order. We prove the result by induction on m. If $m = 1$ or $m = 2$, we have $VBM_1(B_{P_m}) = VBM_1(G) = VBM_1(B_{K_m})$. When $m = 3$, we have B_{P_3} and B_{K_3} are the only connected graphs with same number of vertices and 3 blocks of same order. This implies that, either $G = B_{P_3}$ or $G = B_{K_3}$. Further, we have $VBM_1(B_{P_3}) = p+6 < p+8 = VBM_1(B_{K_3})$. Hence, the result holds. If $m = 4$, we have $VBM_1(B_{P_4}) = p + 9$ and $VBM_1(B_{K_4}) = p + 15$. Now, consider a connected graph G with p vertices and 4 blocks of same order, different from B_{P_4} and B_{K_4}. Then G has exactly 3 pendant blocks. Then we have the following two cases.
Case-i: If two pendant blocks of G are adjacent to each other. Then $VBM_1(G) = 3^2 + 2^2 + (p-2) = p + 11$.
Case-ii: If no pendant blocks of G are adjacent with each other. Then $VBM_1(G) = 2^2 + 2^2 + 2^2 + (p-3) = p + 9$.
In both cases, we have $VBM_1(B_{P_4}) \leq VBM_1(G) \leq VBM_1(B_{K_4})$.
Assume that $m > 4$ and the result is true for $m-1$. Now, we prove the result for m. Let G be a connected graph with p vertices and m blocks of same order. Consider B_{P_m} and B_{K_m} with p vertices and m blocks of same order. Let $\{u_1, u_2, \ldots, u_p\}$, $\{v_1, v_2, \ldots, v_p\}$ and $\{w_1, w_2, \ldots, w_p\}$ be the set of all vertices of B_{P_m}, G and B_{K_m}, respectively. Let $\mathcal{B}(G) = \{B_1, B_2, \ldots, B_m\}$, $\mathcal{B}(B_{P_m}) = \{B'_1, B'_2, \ldots, B'_m\}$ and $\mathcal{B}(B_{K_m}) = \{B''_1, B''_2, \ldots, B''_m\}$. We take $|B_i| = |B'_i| = |B''_i| = k$, for every i, $1 \leq i \leq m$. Without loss of generality, we assume that $B_1 = \{v_1, v_2, \ldots, v_k\}$, $B'_1 = \{u_1, u_2, \ldots, u_k\}$ and $B''_1 = \{w_1, w_2, \ldots, w_k\}$ are pendant blocks of G, B_{P_m} and B_{K_m}, respectively such that v_k, u_k and w_k are cut-vertices. Now, by the induction assumption, we have $VBM_1(B_{P_m} - B'_1) \leq VBM_1(G - B_1) \leq VBM_1(B_{K_m} - B''_1)$.
Note that,

$$VBM_1(G - B_1) = (d_{vb}(v_k) - 1)^2 + \sum_{i=k+1}^{p} d_{vb}(u_i)^2.$$

This implies that,

$$\begin{aligned} VBM_1(G) &= \sum_{i=1}^{p} d_{vb}(u_i)^2 \\ &= (k-1) + VBM_1(G - B_1) + 2d_{vb}(v_k) - 1. \end{aligned}$$

Now,

$$\begin{aligned} VBM_1(B_{P_m}) &= p + 3(m-1) \\ &= VBM_1(B_{P_m} - B'_1) + k + 2 \\ &\leq VBM_1(G - B_1) + k + 2 \\ &= VBM_1(G) + 4 - 2d_{vb}(v_k) \\ &\leq VBM_1(G) \end{aligned}$$

and

$$\begin{aligned} VBM_1(G) &= (k-1) + VBM_1(G - B_1) + 2d_{vb}(v_k) - 1 \\ &\leq (k-1) + VBM_1(B_{K_m} - B_1'') + 2d_{vb}(v_k) - 1 \\ &= (k-1) + (m-1)^2 + p - k + 2d_{vb}(v_k) - 1 \\ &= VBM_1(B_{K_m}) - 2m + 2d_{vb}(v_k) \\ &\leq VBM_1(B_{K_m}) - 2m + 2m \\ &= VBM_1(B_{K_m}). \end{aligned}$$

Hence the result follows. □

Corollary 3.2. [8] *If T_n is an n-vertex tree, different from the star S_n and path P_n, then $M_1(P_n) \leq M_1(T_n) \leq M_1(S_n)$.*

4. Lower and upper bound on $VBM_2(G)$

In this section, we give a lower and upper bound on second vertex-block Zagreb index $VBM_2(G)$ in terms of p, m and Δ_{vb}.

Lemma 4.1. [13] *For positive real numbers $x_1, x_2, \ldots, x_n$ the following inequality holds: $x_1 log(x_1) + x_2 log(x_2) + \cdots + x_n log(x_n) \geq (x_1 + x_2 + \cdots + x_n) log\left(\frac{x_1+x_2+\cdots+x_n}{n}\right)$. Equality holds if and only if all x_i are equal.*

Theorem 4.1. *For any connected graph G, $m\left(\frac{p+m-1}{p}\right)^{\left(\frac{p+m-1}{m}\right)} \leq VBM_2(G) \leq m{\Delta_{vb}}^p$. Further, equality holds if and only if G is a block.*

Proof. Let $u_1, u_2, \ldots, u_p$ be the vertices of G.
Consider,

$$\frac{VBM_2(G)}{m} = \frac{\sum\limits_{u_1u_2\ldots u_k \in \mathcal{B}(G)} [d_{vb}(u_1)d_{vb}(u_2)\ldots d_{vb}(u_k)]}{m}.$$

By the arithmetic and geometric mean inequality, we have

$$\begin{aligned} \frac{VBM_2(G)}{m} &\geq \sqrt[m]{\prod_{u_1u_2\ldots u_k \in \mathcal{B}(G)} [d_{vb}(u_1)d_{vb}(u_2)\ldots d_{vb}(u_k)]} \\ &= \sqrt[m]{\prod_{i=1}^{p} d_{vb}(u_i)^{d_{vb}(u_i)}}. \end{aligned}$$

Since $d_{vb}(u_i) \geq 1$, we take the logarithm of both sides to get

$$log\left(\frac{VBM_2(G)}{m}\right) \geq \frac{1}{m}\sum_{i=1}^{p} d_{vb}(u_i) log(d_{vb}(u_i)).$$

Now, by Lemma 4.1, we have

$$log\left(\frac{VBM_2(G)}{m}\right) \geq \frac{1}{m}\sum_{i=1}^{p} d_{vb}(u_i) log\left(\frac{\sum\limits_{i=1}^{p} d_{vb}(u_i)}{p}\right)$$
$$= \frac{1}{m}(p+m-1) log\left(\frac{p+m-1}{p}\right).$$

Hence,

$$VBM_2(G) \geq m\left(\frac{p+m-1}{p}\right)^{\left(\frac{p+m-1}{m}\right)}. \tag{6}$$

Thus, the lower bound follows.
By the property of arithmetic and geometric mean inequality and, by Lemma 4.1, equality holds in (6) if and only if $d_{vb}(u_1) = d_{vb}(u_2) = \cdots = d_{vb}(u_p)$ if and only if G is a block.
To prove the upper bound, consider

$$\begin{aligned} VBM_2(G) &= \sum_{u_1u_2\ldots u_k \in \mathcal{B}(G)} [d_{vb}(u_1)d_{vb}(u_2)\ldots d_{vb}(u_k)] \\ &\leq \sum_{u_1u_2\ldots u_k \in \mathcal{B}(G)} {\Delta_{vb}}^k \\ &\leq m{\Delta_{vb}}^p. \end{aligned}$$

Further, equality holds if and only if G is a block. □

Corollary 4.1. [13] *Let T be a tree with p vertices and m edges, then $M_2(T) \geq \frac{4m^3}{p^2}$.*

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