

On Extremal Graphs with Respect to the Atom-Bond Sum Connectivity Index

Swathi Shetty, Billava Ramanna Rakshith*, Sayinath
Udupa Nagara Vinayaka

*Manipal Institute of Technology, Manipal Academy of Higher Education,
Manipal, India*

swathi.dscompl2022@learner.manipal.edu, ranmsc08@yahoo.co.in,
rakshith.br@manipal.edu, sayinath.udupa@manipal.edu

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Abstract

Recently, Ali et al. [1] posed several open problems concerning extremal graphs with respect to the atom-bond sum connectivity index. These problems involve characterizing graphs that attain the maximum *ABS* index within specific graph classes, including: (i) connected graphs with n vertices and p cut-vertices; (ii) connected graphs of order n with vertex k -partiteness $v_k(G) = r$; and (iii) connected bipartite graphs of order n with a fixed vertex connectivity κ . In this paper, we provide complete solutions to all of these problems.

1 Introduction

Throughout the paper, G stands for a graph on n vertices without any loops and multiple-edges. As usual, we denote the vertex set and the edge set of G by $V(G)$ and $E(G)$, respectively. Two adjacent vertices v_i and v_j are represented as $v_i \sim v_j$, or $i \sim j$. The degree of a vertex v_i in G

*Corresponding author.

is denoted as $d_G(v_i)/d(v_i)$. We use the notation $f_G(u, v)$ to denote the quantity $\sqrt{1 - \frac{2}{d_G(u) + d_G(v)}}$. The vertex connectivity κ of G is the cardinality of a minimum vertex cut set. The vertex k -partiteness of G , $v_k(G)$ is the minimum number of vertices whose removal results in a k -partite graph. Topological indices, a well-known class of graph invariants, are numerical values derived from the structure of a graph. In molecular graph theory, these indices are widely used as they often reflect the physicochemical properties of the corresponding molecules. For some recent studies on topological indices, see [4, 6]. The atom-bond sum connectivity index, commonly known as the *ABS* index, is a recently introduced topological invariant that has quickly attracted significant attention. It is defined as

$$ABS(G) = \sum_{uv \in E(G)} \sqrt{1 - \frac{2}{d(u) + d(v)}} = \sum_{uv \in E(G)} f_G(u, v).$$

The chemical relevance of the *ABS* index is explored in [2], while its extremal values and bounds are investigated in [7, 8].

Recently, in the review paper [1], Ali et al. listed known bounds and extremal results related to the *ABS* index. They also stated several new extremal results that follow easily from existing general findings. Furthermore, the authors posed several open problems concerning extremal graphs with respect to the *ABS* index. These problems involve characterizing graphs that attain the maximum *ABS* index within specific graph classes, including: (i) connected graphs with n vertices and p cut-vertices; (ii) connected graphs of order n with vertex k -partiteness $v_k(G) = r$; and (iii) connected bipartite graphs of order n with a fixed vertex connectivity κ . Motivated by these works, in this paper, we provide complete solutions to all of these problems.

2 *ABS* index of graphs with the given number of cut-vertices

Let \mathbb{V}_n^p be the collection of all connected graphs of order n with p number of cut-vertices. We need the following theorem to prove our results in this section.

Theorem 1. [1,9] If G is a graph attaining the maximum ABS index in \mathbb{V}_n^p , then every block of G is a clique and every cut-vertex of G is contained in exactly two blocks.

Lemma 1. Let G be a graph that attains the maximum ABS index in \mathbb{V}_n^p . Then G is either the path graph P_n or it can be formed by attaching one of the end vertices of a path P^i (with a length of at least 1) to a vertex u_i of the complete graph K_{n-p} (with vertex labels u_1, u_2, \dots, u_{n-p}) for $1 \leq i \leq k$, where $1 \leq k \leq n - p$.

Proof. By Theorem 1, every block of G is a clique and every cut-vertex of G is contained in exactly two blocks. Let $H_1 = K_\alpha$ and $H_2 = K_\beta$ be the two largest cliques in G , where $\alpha \geq \beta \geq 2$. Assume that $\beta \geq 3$.

Case 1: Suppose H_1 and H_2 share a common cut-vertex, say x of G . Let y be a vertex of minimum degree in $H_2 \setminus \{x\}$, and z be a vertex of H_2 that is different from the vertices x and y . Let G' be the graph obtained from G by removing all the edges of H_2 which are incident with y except the edge xy , and then joining each vertex of $H_2 \setminus \{x, y\}$ with every vertex in $H_1 \setminus \{x\}$. Then $d_{G'}(u) = d_G(u) + \beta - 2$ for $u \in V(H_1) \setminus \{x\}$, and $d_{G'}(w) = d_G(w) + \alpha - 2$ for $w \in V(H_2) \setminus \{x, y\}$. Also, $d_G(x) = d_{G'}(x) = \alpha + \beta - 2$. Importantly, the cut-vertices of G and G' are essentially the same. Let $\Omega = (E(G) \cap E(G')) \setminus \{xy\}$ and $\Omega_1 = (E(G) \cap E(G')) \setminus \{xy, yy' : y' \sim y, y' \notin V(H_2)\}$. We now consider the following subcases.

Subcase 1.1: The vertex y is not a cut-vertex of G . Then $d_G(y) = \beta - 1$ and $d_{G'}(y) = 1$. Therefore, $ABS(G) - ABS(G')$

$$\begin{aligned} &= \sum_{uw \in \Omega} (f_G(u, w) - f_{G'}(u, w)) + \sum_{w:w \in V(H_2) \setminus \{y\}} f_G(w, y) \\ &- \left(\sum_{u:u \in V(H_1) \setminus \{x\}} \sum_{w:w \in V(H_2) \setminus \{x,y\}} f_{G'}(u, w) \right) - f_{G'}(x, y) \\ &< \sum_{w:w \in V(H_2) \setminus \{y\}} f_G(w, y) \\ &- \sum_{u:u \in V(H_1) \setminus \{x\}} \sum_{w:w \in V(H_2) \setminus \{x,y\}} f_{G'}(u, w). \end{aligned}$$

Since $d_{G'}(u) + d_{G'}(w) > d_G(u) + d_G(y)$ and $|V(H_1)| \geq 3$, $ABS(G) < ABS(G')$, a contradiction.

Subcase 1.2: The vertex y is a cut-vertex of G . Then $d_G(y) \leq 2\beta - 2$ and $d_{G'}(y) \leq \beta$. Let $u_1 (\neq x)$ be a vertex in H_1 . If $|V(H_2)| \geq 4$, then $V(H_2) \setminus \{x, y, z\} \neq \emptyset$. Let w_1 be a vertex in $V(H_2) \setminus \{x, y, z\}$. Then $ABS(G) - ABS(G')$

$$\begin{aligned}
 &= \sum_{uw \in \Omega_1} (f_G(u, w) - f_{G'}(u, w)) + \sum_{w:w \in V(H_2) \setminus \{y\}} f_G(w, y) - f_{G'}(x, y) \\
 &- \sum_{u:u \in V(H_1) \setminus \{x\}} \sum_{w:w \in V(H_2) \setminus \{x, y\}} f_{G'}(u, w) + \sum_{\substack{y':y' \sim y \\ y' \notin V(H_2)}} (f_G(y, y') - f_{G'}(y, y')) \\
 &< \sum_{w:w \in V(H_2) \setminus \{y\}} f_G(w, y) - \sum_{w:w \in V(H_2) \setminus \{x, y\}} f_{G'}(w, u_1) \\
 &+ \sum_{\substack{y':y' \sim y \\ y' \notin V(H_2)}} f_G(y, y') - \sum_{u:u \in V(H_1) \setminus \{x, u_1\}} f_{G'}(u, z) \\
 &- \sum_{u:u \in V(H_1) \setminus \{x, u_1\}} f_{G'}(u, w_1). \tag{1}
 \end{aligned}$$

Since $|V(H_1)| \geq |V(H_2)| \geq 4$, and $d_{G'}(w) + d_{G'}(u) \geq d_G(w) + d_G(y)$, $d_G(y) + d_G(y')$ for $u \in V(H_1) \setminus \{x\}$, $w \in V(H_2) \setminus \{y\}$, and $y \sim y'$ in G , from equation (1), we get $ABS(G) < ABS(G')$, a contradiction. Otherwise $|V(H_2)| = 3$. In this case, $ABS(G) - ABS(G') <$

$$\begin{aligned}
 &\sum_{w:w \in \{x, z\}} f_G(w, y) - \sum_{u:u \in V(H_1) \setminus \{x\}} f_{G'}(u, z) \\
 &+ \sum_{\substack{y':y' \sim y \\ y' \notin V(H_2)}} f_G(y', y) - \sum_{\substack{y':y' \sim y \\ y' \notin V(H_2)}} f_{G'}(y', y) - f_{G'}(y, x). \tag{2}
 \end{aligned}$$

The sum of the first two terms in (2) is not positive, and it is easy to verify that the sum of the last three terms is negative. Thus, $ABS(G) < ABS(G')$, again a contradiction.

Case 2: Suppose H_1 and H_2 do not share a common cut-vertex. Let x be a cut-vertex of G in H_2 , and let y be a vertex of minimum degree in $H_2 \setminus \{x\}$. Let G' be the graph obtained from G by removing all the edges

of H_2 that are incident with either x or y , except the edge xy , and then joining each vertex of $H_2 \setminus \{x, y\}$ with every vertex in H_1 . Then the cut-vertices of G and G' are essentially the same, and by a similar argument to that of Case 1, we end up with a contradiction.

Thus, $\beta = 2$. Since every block in G is a clique, G is either a path graph P_n or it can be formed by attaching one of the end vertices of a path P^i (with a length of at least 1) to a vertex u_i of the complete graph K_{n-p} (with vertex labels u_1, u_2, \dots, u_{n-p}) for $1 \leq i \leq k$, where $1 \leq k \leq n - p$. ■

Graphs \mathbb{K}_n^p : Let $n \geq 3$ and $0 \leq p \leq n - 2$. If $n \geq 2p$, then \mathbb{K}_n^p is obtained by attaching p pendant vertices to p vertices of the complete graph K_{n-p} . Otherwise ($n < 2p$), the graph \mathbb{K}_n^p is formed by attaching $n - p - 1$ pendant vertices to $n - p - 1$ vertices of K_{n-p} , and then a path of length $2p - n + 1$ is attached to the remaining one vertex of K_{n-p} .

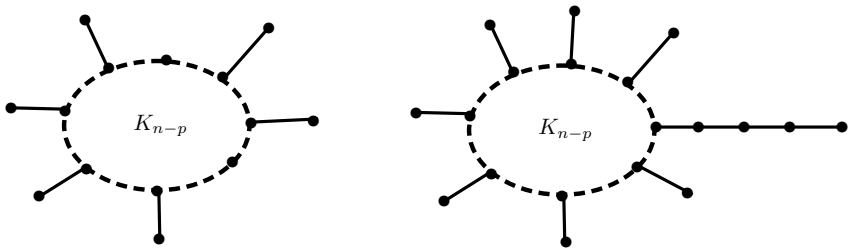


Figure 1. Graphs \mathbb{K}_n^p , for $n \geq 2p$ (left) and $n < 2p$ (right).

Theorem 2. Let $G \in \mathbb{V}_n^p$. Then $ABS(G) \leq ABS(\mathbb{K}_n^p)$, where the equality holds if and only if $G \cong \mathbb{K}_n^p$.

Proof. Suppose G has maximum ABS index. If $G \cong P_n$, then there is nothing to prove. Otherwise, $G \not\cong P_n$, and by Lemma 1, G can be constructed by attaching one of the end vertices of a path P^i (with a length of at least 1) to a vertex u_i of the complete graph K_{n-p} (with vertex labels u_1, u_2, \dots, u_{n-p}) for $1 \leq i \leq k$, where $1 \leq k \leq n - p$ and $1 \leq p \leq n - 3$. Assume that the length of P^1 is at least 2 and $k < n - p$. Consider G' , the graph obtained from G by deleting the pendant vertex of the path P^1 ($w_0(u_1) - w_1 - w_2 - \dots - w_\ell$, $\ell \geq 2$), and then adding a pendant edge to

the vertex u_{n-p} .

$$\begin{aligned} &\text{Now, } ABS(G) - ABS(G') \\ &= \frac{1}{\sqrt{3}} + \sqrt{1 - \frac{2}{d_G(w_{\ell-2}) + 2}} - \sqrt{1 - \frac{2}{d_{G'}(w_{\ell-2}) + 1}} \\ &\quad - \sqrt{1 - \frac{2}{n-p+1}} + (n-p-1) \left(\sqrt{1 - \frac{2}{2(n-p-1)}} - \sqrt{1 - \frac{2}{2(n-p)-1}} \right) \\ &< \frac{1}{\sqrt{2}} - \sqrt{1 - \frac{2}{n-p+1}} \leq 0. \end{aligned}$$

Thus, $ABS(G) < ABS(G')$, a contradiction. Therefore, length of P^i is 1 for $1 \leq i \leq k < n-p$, or $k = n-p$.

If the length of P^i is 1 for $1 \leq i \leq k < n-p$, then we are done. Otherwise, $k = n-p$. Without loss of generality, we can assume that P^1 is of maximum length among all paths P^i . Let G'' be the graph obtained from G by removing the pendant vertex in P^i ($i \neq 1$), and then adding a pendant edge to the pendant vertex in P^1 . Then $ABS(G) = ABS(G'')$ when the length of paths P^1 and P^i are at least 3, and if the length of P^i is 2 and the length of P^1 is at least 2, then $ABS(G) - ABS(G'') = \sqrt{1 - \frac{2}{n-p+2}} - \sqrt{1 - \frac{2}{n-p+1}} + \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \leq \sqrt{\frac{3}{5}} - \sqrt{2} + \frac{1}{\sqrt{3}} < 0$.

That is, $ABS(G) < ABS(G'')$. Hence the length of P^1 is at least 1 and the lengths of P^i is 1 for $2 \leq i \leq n-p$. Proving that $G \cong \mathbb{K}_n^p$. ■

3 *ABS* index and vertex k -partiteness in graphs

A complete multipartite graph with k -partition sets of order n_1, n_2, \dots, n_k is denoted as K_{n_1, n_2, \dots, n_k} . The Turán graph $T(n, k)$ is the complete k -partite graph on n vertices given by $T(n, k) \cong K_{\underbrace{t, t, \dots, t}_{(k-s)}, \underbrace{t+1, t+1, \dots, t+1}_s}$,

where $n = kt + s$ and $s \geq 0$.

We now show that the Turán graph has maximum *ABS* index among all complete k -partite graphs.

Theorem 3. Let G be a complete k -partite graph on n vertices. Then $ABS(G) \leq ABS(T(n, k))$. Equality holds if and only if $G \cong T(n, k)$.

Proof. Let $\Gamma \cong K_{t_1, t_2, \dots, t_k}$ be a complete k -partite graph with maximum ABS index in the class of complete k -partite graphs.

Suppose $|t_i - t_j| \geq 2$ for some $1 \leq i < j \leq k$. Then without loss of generality, we can assume that $t_1 - t_2 \geq 2$. Let $\Gamma' = K_{t_1-1, t_2+1, \dots, t_k}$. By direct calculation, $ABS(\Gamma) - ABS(\Gamma')$

$$\begin{aligned} &= t_1 t_2 \sqrt{1 - \frac{2}{2n - (t_1 + t_2)}} - (t_1 - 1)(t_2 + 1) \sqrt{1 - \frac{2}{2n - (t_1 + t_2)}} \\ &+ \sum_{i=3}^k t_1 t_i \left(\sqrt{1 - \frac{2}{2n - t_1 - t_i}} - \sqrt{1 - \frac{2}{2n - t_i - t_1 + 1}} \right) \\ &+ \sum_{i=3}^k t_2 t_i \left(\sqrt{1 - \frac{2}{2n - t_2 - t_i}} - \sqrt{1 - \frac{2}{2n - t_2 - t_i - 1}} \right) \\ &+ \sum_{i=3}^k t_i \left(\sqrt{1 - \frac{2}{2n - t_i - t_1 + 1}} - \sqrt{1 - \frac{2}{2n - t_i - t_2 - 1}} \right). \end{aligned}$$

Since $t_1 \geq t_2 + 2$, $ABS(\Gamma) - ABS(\Gamma')$

$$\begin{aligned} &< \sum_{i=3}^k t_2 t_i \left(\sqrt{1 - \frac{2}{2n - t_1 - t_i}} - \sqrt{1 - \frac{2}{2n - t_i - t_1 + 1}} \right) \\ &+ \sqrt{1 - \frac{2}{2n - t_2 - t_i}} - \sqrt{1 - \frac{2}{2n - t_2 - t_i - 1}}. \end{aligned} \quad (3)$$

Consider $\zeta(x) = \sqrt{1 - \frac{2}{x - t_i}} - \sqrt{1 - \frac{2}{x - t_i + 1}}$. Employing the first derivative test, we see that the function $\zeta(x)$ is increasing. So, $\zeta(2n - t_2 - 1) \geq \zeta(2n - t_1)$ as $t_1 \geq t_2 + 2$, and thus from inequality (3), $ABS(\Gamma) < ABS(\Gamma')$. This is a contradiction. Hence $\Gamma \cong T(n, k)$. ■

The join of two graphs G_1 and G_2 is obtained from G_1 and G_2 by joining each vertex of G_1 with every vertex in G_2 . It is denoted by $G_1 \vee G_2$. We need the following theorem to prove our next theorem.

Theorem 4. [1,5] If G is a graph possessing the maximum ABS index in the class of connected graphs of order n with vertex k -partiteness at most r ($1 \leq r \leq n - k$). Then there exist k non-negative integers t_1, t_2, \dots, t_k such that $\sum_{i=1}^k t_i = n - r$ and $G \cong K_r \vee K_{t_1, t_2, \dots, t_k}$.

In the following theorem, we identify the graph with maximum ABS index in the class of connected n -order graphs that have fixed vertex k -partiteness $v_k(G)$.

Theorem 5. Let G be a graph of order n with vertex k -partiteness $v_k(G) = r$ ($1 \leq r \leq n - k$). Then $ABS(G) \leq ABS(K_r \vee T(n - r, k))$. Equality holds if and only if $G \cong K_r \vee T(n - r, k)$.

Proof. Let Γ be a graph with maximum ABS index in the class of graphs with k -partiteness $v_k(G) = r$. By Theorem 4, $G \cong K_r \vee K_{t_1, t_2, \dots, t_k}$. Suppose $|t_i - t_j| \geq 2$ for some $1 \leq i \leq j \leq k$. Then without loss of generality, we can assume that $t_1 - t_2 \geq 2$. Let $\Gamma' = K_r \vee K_{t_1-1, t_2+1, \dots, t_k}$. By direct calculation, $ABS(\Gamma) - ABS(\Gamma') =$

$$\begin{aligned} & rt_1 \sqrt{1 - \frac{2}{2n - (t_1 + 1)}} + rt_2 \sqrt{1 - \frac{2}{2n - (t_2 + 1)}} \\ & + \sum_{i=2}^k t_1 t_i \sqrt{1 - \frac{2}{2n - (t_1 + t_i)}} + \sum_{i=3}^k t_2 t_i \sqrt{1 - \frac{2}{2n - (t_2 + t_i)}} \\ & - r(t_1 - 1) \sqrt{1 - \frac{2}{2n - t_1}} - r(t_2 + 1) \sqrt{1 - \frac{2}{2(n - 1) - t_2}} \\ & - (t_1 - 1)(t_2 + 1) \sqrt{1 - \frac{2}{2n - (t_1 + t_2)}} - \sum_{i=3}^k (t_1 - 1)t_i \sqrt{1 - \frac{2}{2n - (t_1 + t_i) + 1}} \\ & - \sum_{i=3}^k (t_2 + 1)t_i \sqrt{1 - \frac{2}{2n - (t_2 + t_i) - 1}}. \end{aligned}$$

Since $t_1 \geq t_2 + 2$, $ABS(\Gamma) - ABS(\Gamma') <$

$$\begin{aligned} & \sum_{i=3}^k t_2 t_i \left(\sqrt{1 - \frac{2}{2n - t_1 - t_i}} - \sqrt{1 - \frac{2}{2n - t_i - t_1 + 1}} + \sqrt{1 - \frac{2}{2n - t_2 - t_i}} \right. \\ & \left. - \sqrt{1 - \frac{2}{2n - t_2 - t_i - 1}} \right) - rt_2 \left(\sqrt{1 - \frac{2}{2n - t_1}} - \sqrt{1 - \frac{2}{2n - t_1 - 1}} \right) \end{aligned}$$

$$\begin{aligned}
& -\sqrt{1 - \frac{2}{2n-1-t_2}} + \sqrt{1 - \frac{2}{2n-t_2-2}} \\
& = \sum_{i=3}^k (t_2 t_i (\zeta(2n-t_1) - \zeta(2n-t_2-1))) - r t_2 (\zeta_1(t_1) - \zeta_1(t_2+1)),
\end{aligned}$$

where $\zeta(x)$ is as defined in Theorem 5 and

$\zeta_1(x) = \sqrt{1 - \frac{2}{2n-x}} - \sqrt{1 - \frac{2}{2n-x-1}}$. Since ζ and ζ_1 are increasing functions, and as $t_1 \geq t_2 + 2$, $\zeta(2n-t_2-1) \geq \zeta(2n-t_1)$ and $\zeta_1(t_1) \geq \zeta_1(t_2+1)$. Thus, $ABS(\Gamma) < ABS(\Gamma')$, a contradiction. This completes the proof of the theorem. \blacksquare

4 *ABS* index of bipartite graphs with given vertex connectivity

In this section, we identify the maximum value of the *ABS* index among the class of connected bipartite graphs with given vertex connectivity. The following graph class is crucial to this section.

Let n_i be a non-negative integer for $i = 1, 2, 3, 4, 5, 6$. The graph $\overline{K}[n_1, n_2, n_3, n_4, n_5, n_6]$ is obtained from the graphs $H_1 = \overline{K}_{n_1}, H_2 = \overline{K}_{n_2}, H_3 = \overline{K}_{n_3}, H_4 = \overline{K}_{n_4}, H_5 = \overline{K}_{n_5}$, and $H_6 = \overline{K}_{n_6}$ by joining each vertex of H_1 (respectively H_3) with every vertex in H_4 and H_5 (respectively H_5 and H_6), and also joining each of vertex of H_2 with every vertex in H_4, H_5 , and H_6 . See Fig. 2.

The class of connected bipartite graphs of order n and vertex connectivity κ is denoted as $\mathcal{BG}_{n,\kappa}$. Also, the subgraph of G induced by a vertex subset S of G is denoted as $G[S]$. The following theorem provides key information about the structure of graphs in $\mathcal{BG}_{n,k}$ that attain the maximum *ABS* index.

Theorem 6. [1, 3] Let Γ be a graph with maximum *ABS* index in the class $\mathcal{BG}_{n,\kappa}$. Let S be a minimum vertex cut set of G . If $G - S$ has a non-trivial component, then $G - S$ has exactly two components, namely H_1 and H_2 , such that the graphs $G[S \cup V(H_1)]$ and $G[S \cup V(H_2)]$ are

complete bipartite.

Remark 1. From Theorem 6, a graph that attains the maximum *ABS* index in $\mathcal{BG}_{n,\kappa}$ must be isomorphic to one of the following graphs

- (i) $\overline{\mathcal{K}}[n_1, n_2, n_3, n_4, n_5, n_6]$, where $n_i \geq 1$ for $i = 1, 3, 4, 6$, $n_2 + n_5 = \kappa$, $n_1, n_3 \geq n_5$ and $n_4, n_6 \geq n_2$.
- (ii) $\overline{\mathcal{K}}[0, n_2, n_3, n_4, 0, n_6]$, where $n_3, n_4 \geq 1$, $n_2 = \kappa$ and $n_6 \geq n_2$.
- (iii) $\overline{\mathcal{K}}[n_1, 0, n_3, 0, n_5, n_6]$, where $n_1, n_6 \geq 1$, $n_5 = \kappa$ and $n_3 \geq n_5$.

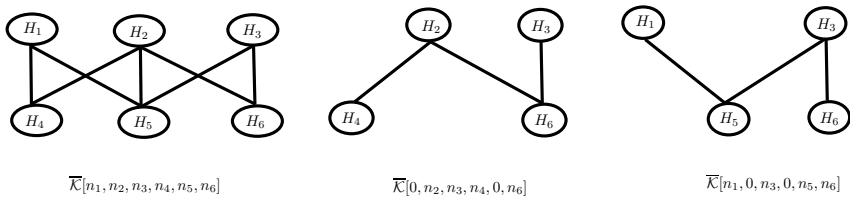


Figure 2. The graphs discussed in Remark 1.

Lemma 2. For the graph $\overline{\mathcal{K}}[n_1, n_2, n_3, n_4, n_5, n_6]$, where $n_i \geq 1$ for $i = 1, 4, 6$, $n_3 \geq 2$, $n_2 + n_5 = \kappa$, $n_1, n_3 \geq n_5$ and $n_4, n_6 \geq n_2$,

$$\overline{\mathcal{K}}[n_1, n_2, n_3, n_4, n_5, n_6] < \overline{\mathcal{K}}[n_1 + n_2 + n_3 - 1, 0, 1, n_4 + n_6 - n_2, n_5 + n_2, 0]$$

Proof. Let $n = n_1 + n_2 + n_3 + n_4 + n_5 + n_6$. Then $\overline{\mathcal{K}}[n_1, n_2, n_3, n_4, n_5, n_6]$

$$\begin{aligned} &= n_1 n_4 \sqrt{1 - \frac{2}{n - n_3 - n_6}} + n_1 n_5 \sqrt{1 - \frac{2}{n - n_6}} + n_2 n_4 \sqrt{1 - \frac{2}{n - n_3}} \\ &+ n_2 n_5 \sqrt{1 - \frac{2}{n}} + n_2 n_6 \sqrt{1 - \frac{2}{n - n_1}} + n_3 n_5 \sqrt{1 - \frac{2}{n - n_4}} \\ &+ n_3 n_6 \sqrt{1 - \frac{2}{n - n_1 - n_4}} \end{aligned} \tag{4}$$

and $\overline{\mathcal{K}}[n_1 + n_2 + n_3 - 1, 0, 1, n_4 + n_6 - n_2, n_5 + n_2, 0]$

$$\begin{aligned}
 &= (n_1 + n_2 + n_3 - 1)(n_4 + n_6 - n_2) \times \sqrt{1 - \frac{2}{n-1}} \\
 &+ (n_1 + n_2 + n_3 - 1)(n_5 + n_2) \sqrt{1 - \frac{2}{n}} + (n_5 + n_2) \sqrt{1 - \frac{2}{n - n_4 - n_6 + n_2}}.
 \end{aligned} \tag{5}$$

From equations (4) and (5),

$\overline{\mathcal{K}}[n_1 + n_2 + n_3 - 1, 0, 1, n_4 + n_6 - n_2, n_5 + n_2, 0] - \overline{\mathcal{K}}[n_1, n_2, n_3, n_4, n_5, n_6] =$

$$\begin{aligned}
 &n_1 n_4 \left(\sqrt{1 - \frac{2}{n-1}} - \sqrt{1 - \frac{2}{n - n_3 - n_6}} \right) + n_1 n_5 \left(\sqrt{1 - \frac{2}{n}} - \sqrt{1 - \frac{2}{n - n_6}} \right) \\
 &+ n_2 n_4 \left(\sqrt{1 - \frac{2}{n-1}} - \sqrt{1 - \frac{2}{n - n_3}} \right) + n_2 n_6 \left(\sqrt{1 - \frac{2}{n-1}} - \sqrt{1 - \frac{2}{n - n_1}} \right) \\
 &+ n_2^2 \left(\sqrt{1 - \frac{2}{n}} - \sqrt{1 - \frac{2}{n-1}} \right) + (n_3 - 1) n_5 \left(\sqrt{1 - \frac{2}{n}} - \sqrt{1 - \frac{2}{n - n_4}} \right) \\
 &+ (n_3 - 1)(n_6 - n_2) \sqrt{1 - \frac{2}{n-1}} + (n_3 - 1) n_2 \sqrt{1 - \frac{2}{n}} \\
 &- (n_3 - 1) n_6 \sqrt{1 - \frac{2}{n - n_1 - n_4}} + (n_3 - 1) n_4 \sqrt{1 - \frac{2}{n-1}} \\
 &+ n_1 n_2 \left(\sqrt{1 - \frac{2}{n}} - \sqrt{1 - \frac{2}{n-1}} \right) + n_1 n_6 \sqrt{1 - \frac{2}{n-1}} \\
 &- n_6 \sqrt{1 - \frac{2}{n - n_1 - n_4}} - n_5 \sqrt{1 - \frac{2}{n - n_4}} + (n_5 + n_2) \sqrt{1 - \frac{2}{n - n_4 - n_6 + n_2}}.
 \end{aligned}$$

Since $\sqrt{1 - \frac{2}{n-x}} \geq \sqrt{1 - \frac{2}{n-y}}$ for $x \leq y$, we get

$\overline{\mathcal{K}}[n_1 + n_2 + n_3 - 1, 0, 1, n_4 + n_6 - n_2, n_5 + n_2, 0] - \overline{\mathcal{K}}[n_1, n_2, n_3, n_4, n_5, n_6]$

$$\begin{aligned}
 &\geq (n_3 - 1) n_4 \sqrt{1 - \frac{2}{n-1}} + n_1 n_6 \sqrt{1 - \frac{2}{n-1}} - n_6 \sqrt{1 - \frac{2}{n - n_1 - n_4}} \\
 &- n_5 \sqrt{1 - \frac{2}{n - n_4}} + (n_5 + n_2) \sqrt{1 - \frac{2}{n - n_4 - n_6 + n_2}}.
 \end{aligned} \tag{6}$$

Since $n_3 \geq n_5$ and $n_1 \geq n_5$, from equation (6),

$$\begin{aligned} & \overline{\mathcal{K}}[n_1 + n_2 + n_3 - 1, 0, 1, n_4 + n_6 - n_2, n_5 + n_2, 0] - \overline{\mathcal{K}}[n_1, n_2, n_3, n_4, n_5, n_6] \\ & \geq (n_5 - 1)(n_4 + n_6)\sqrt{1 - \frac{2}{n - 1}} - n_5\sqrt{1 - \frac{2}{n - n_4}} \\ & \geq 2(n_5 - 1)\sqrt{1 - \frac{2}{n - 1}} - n_5\sqrt{1 - \frac{2}{n - n_4}} \geq 0 \text{ for } n_5 > 1. \text{ If } n_5 = 1, \text{ then} \\ & \text{from equation (6), we immediately arrive at the desired inequality because} \\ & n_3 \geq 2. \text{ This completes the proof of the lemma.} \quad \blacksquare \end{aligned}$$

Lemma 3. $\overline{\mathcal{K}}[0, n_2, n_3, n_4, 0, n_6] < \overline{\mathcal{K}}[0, n_2, n_3, 1, 0, n_6 + n_4 - 1]$ where $n_3 \geq 1$, $n_4 \geq 2$, $n_6 \geq n_2$ and $n_2 = \kappa$.

Proof. Let $n = n_2 + n_3 + n_4 + n_6$. Then $\overline{\mathcal{K}}[0, n_2, n_3, n_4, 0, n_6]$

$$\begin{aligned} & = n_2(n_4 - 1)\sqrt{1 - \frac{2}{n - n_3}} + n_2\sqrt{1 - \frac{2}{n - n_3}} + n_2n_6\sqrt{1 - \frac{2}{n}} \\ & + n_3n_6\sqrt{1 - \frac{2}{n - n_4}} \end{aligned} \tag{7}$$

and $\overline{\mathcal{K}}[0, n_2, n_3, 1, 0, n_6 + n_4 - 1]$

$$\begin{aligned} & = n_2\sqrt{1 - \frac{2}{n - n_3}} + n_2n_6\sqrt{1 - \frac{2}{n}} + n_2(n_4 - 1)\sqrt{1 - \frac{2}{n}} \\ & + n_3n_6\sqrt{1 - \frac{2}{n - 1}} + n_3(n_4 - 1)\sqrt{1 - \frac{2}{n - 1}}. \end{aligned} \tag{8}$$

From equations (7) and (8), and since $\sqrt{1 - \frac{2}{n - x}} \geq \sqrt{1 - \frac{2}{n - y}}$ for $x \leq y$, we get

$$\begin{aligned} & \overline{\mathcal{K}}[0, n_2, n_3, 1, 0, n_6 + n_4 - 1] - \overline{\mathcal{K}}[0, n_2, n_3, n_4, 0, n_6] \geq n_3(n_4 - 1)\sqrt{1 - \frac{2}{n - 1}} \\ & \geq 0. \quad \blacksquare \end{aligned}$$

The following lemma can be proved using an argument similar to that of Lemma 3.

Lemma 4. $\overline{\mathcal{K}}[n_1, 0, n_3, 0, n_5, n_6] < \overline{\mathcal{K}}[1, 0, n_3 + n_1 - 1, 0, n_5, n_6]$, where $n_6 \geq 1$, $n_1 \geq 2$, $n_5 = \kappa$ and $n_3 \geq n_5$.

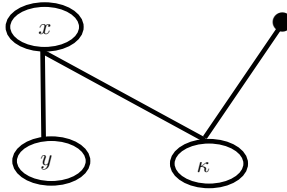


Figure 3. Graph $\bar{K}_\kappa[x, y]$

Let $\bar{K}_\kappa[x, y] = \bar{K}[x, 0, 1, y, \kappa, 0]$ (see Fig 3), where $x \geq 1, y \geq 1$ and $x + y + 1 + \kappa = n$. The following theorem follow from Remark 1 and Lemmas 3, 2 and 4.

Theorem 7. *Let G be a graph with maximum ABS index in $\mathcal{BG}_{n,k}$ and let S be a minimum vertex cut set of G . If $G - S$ has a non-trivial component, then $G \cong K_\kappa[x, y]$ for some positive integers x and y .*

We now proceed to determine the values of x and y for which $ABS(K_\kappa[x, y])$ is maximum.

Lemma 5. $\bar{K}_\kappa[x + 1, y - 1] > \bar{K}_\kappa[x, y]$, where $x + y + \kappa + 1 = n$ and $y - x - 1 + k \geq 0$.

Proof. $\bar{K}_\kappa[x, y] = xy\sqrt{1 - \frac{2}{n-1}} + xk\sqrt{1 - \frac{2}{n}} + k\sqrt{1 - \frac{2}{n-y}}$

and

$$\bar{K}_\kappa[x + 1, y - 1] = (xy - x + y - 1)\sqrt{1 - \frac{2}{n-1}} + (x + 1)k\sqrt{1 - \frac{2}{n}} + k\sqrt{1 - \frac{2}{n-y+1}}.$$

Therefore,

$$\bar{K}_\kappa[x + 1, y - 1] - \bar{K}_\kappa[x, y] > (y - x - 1 + k)\sqrt{1 - \frac{2}{n-1}} \geq 0. \quad \blacksquare$$

Lemma 6. For n even ($n \geq 8$) and $0 \leq c \leq \frac{n - 2k - 6}{2}$,

$$\bar{K}_\kappa \left[\frac{n}{2} + c, \frac{n - 2k - 2}{2} - c \right] > \bar{K}_\kappa \left[\frac{n}{2} + c + 1, \frac{n - 2k - 2}{2} - c - 1 \right].$$

Proof. Let

$$f(c) = \bar{\mathcal{K}}_\kappa \left[\frac{n}{2} + c, \frac{n-2k-2}{2} - c \right] - \bar{\mathcal{K}}_\kappa \left[\frac{n}{2} + c + 1, \frac{n-2k-2}{2} - c - 1 \right].$$

Then

$$\begin{aligned} f(c) = & 2\sqrt{\frac{n-3}{n-1}}c + \sqrt{\frac{n-3}{n-1}}k - k\sqrt{\frac{n-2}{n}} + k\sqrt{\frac{n+2k-2+2c}{n+2k+2+2c}} \\ & - k\sqrt{\frac{n+2k+2c}{n+2k+4+2c}} + 2\sqrt{\frac{n-3}{n-1}}. \end{aligned}$$

By first derivative test, it is easy to check that the function $f(c)$ is increasing, and thus $f(c) \geq f(0)$.

$$\begin{aligned} \text{Consider } f(0) = & \bar{\mathcal{K}}_\kappa \left[\frac{n}{2}, \frac{n-2k-2}{2} \right] - \bar{\mathcal{K}}_\kappa \left[\frac{n}{2} + 1, \frac{n-2k-2}{2} - 1 \right] = \\ & k\sqrt{\frac{n-3}{n-1}} - k\sqrt{\frac{n-2}{n}} + k\sqrt{\frac{n+2k-2}{n+2k+2}} - k\sqrt{\frac{n+2k}{n+2k+4}} + 2\sqrt{\frac{n-3}{n-1}}. \end{aligned} \tag{9}$$

Claim 1:

$$\sqrt{\frac{n-3}{n-1}} > k\sqrt{\frac{n+2k}{n+2k+4}} - k\sqrt{\frac{n+2k-2}{n+2k+2}}. \tag{10}$$

Squaring both sides of inequality (10), we get

$$\begin{aligned} 2k^2\sqrt{\frac{n+2k-2}{n+2k+2}}\sqrt{\frac{n+2k}{n+2k+4}} & > 2k^2 - \frac{4k^2}{n+2k+2} - \frac{4k^2}{n+2k+4} \\ & - 1 + \frac{2}{n-1}. \end{aligned}$$

$$\begin{aligned} \text{Now, } & \left(2k^2\sqrt{\frac{n+2k-2}{n+2k+2}}\sqrt{\frac{n+2k}{n+2k+4}} \right)^2 - \left(2k^2 - \frac{4k^2}{n+2k+2} \right. \\ & \left. - \frac{4k^2}{n+2k+4} - 1 + \frac{2}{n-1} \right)^2 \\ = & \frac{1}{(n+2k+2)^2(n+2k+4)^2(n-1)^2} \times \end{aligned}$$

$$\left[(64n^2 - 256n + 192)k^6 + (128n^3 - 256n^2 - 640n + 768)k^5 + (96n^4 - 1072n^2 + 352n + 560)k^4 + (32n^5 + 64n^4 - 448n^3 - 416n^2 + 1312n - 1056)k^3 + (4n^6 + 16n^5 - 76n^4 - 192n^3 + 632n^2 + 368n - 2256)k^2 + (-8n^5 - 24n^4 + 152n^3 + 408n^2 - 720n - 1728)k - n^6 - 6n^5 + 11n^4 + 108n^3 + 44n^2 - 480n - 576 \right] > 0. \text{ Thus Claim 1 is true.}$$

In similar lines to Claim 1, we get,

$$\sqrt{\frac{n-3}{n-1}} > k\sqrt{\frac{n-2}{n}} - k\sqrt{\frac{n-3}{n-1}}. \tag{11}$$

Thus from equations (9), (10) and (11), $f(0) > 0$. Hence $f(c) > 0$. Proving the inequality. ■

The following lemma can be proved using an argument similar to that of Lemma 6.

Lemma 7. For n odd ($n \geq 7$) and $0 \leq c \leq \frac{n-2k-5}{2}$,

$$\bar{\mathcal{K}}_\kappa \left[\frac{n-1}{2} + c, \frac{n-2k-1}{2} - c \right] > \bar{\mathcal{K}}_\kappa \left[\frac{n-1}{2} + c + 1, \frac{n-2k-1}{2} - c - 1 \right].$$

Theorem 8. (i) If n is even, then $\mathcal{K}_\kappa[x, y] \leq \mathcal{K}_\kappa \left[\frac{n}{2}, \frac{n-2k-2}{2} \right]$. Equality holds if and only if $x = \frac{n}{2}$ and $y = \frac{n-2k-2}{2}$.

(ii) If n is odd, then $\mathcal{K}_\kappa[x, y] \leq \mathcal{K}_\kappa \left[\frac{n-1}{2}, \frac{n-2k-1}{2} \right]$. Equality holds if and only if $x = \frac{n-1}{2}$ and $y = \frac{n-2k-1}{2}$.

Proof. By Lemmas 5 and 6,

$$\mathcal{K}_\kappa[\kappa, n-2\kappa-1] < \mathcal{K}_\kappa[\kappa+1, n-2\kappa-2] < \dots < \mathcal{K}_\kappa \left[\frac{n}{2}, \frac{n-2\kappa-2}{2} \right] \tag{12}$$

and

$$\mathcal{K}_\kappa \left[\frac{n}{2}, \frac{n-2\kappa-2}{2} \right] > \mathcal{K}_\kappa \left[\frac{n}{2} + 1, \frac{n-2\kappa-2}{2} - 1 \right] > \dots > \mathcal{K}_\kappa [n-\kappa-2, 1]. \tag{13}$$

Thus, from equations (12) and (13), we get the desired result. Proof of (ii) follows from Lemmas 5 and 7 in a similar manner to that of (i). ■

Remark 2. Let G be a graph with maximum ABS index in $\mathcal{BG}_{n,\kappa}$ and let S be a minimum vertex cut set of G . If $G - S$ is an empty graph, then S is a partition set of G and $G \cong K_{\kappa,n-\kappa}$ (because addition of an edge increases ABS index).

The main result of this section is presented below.

Theorem 9. *Let $G \in \mathcal{BG}_{n,\kappa}$ with $n \geq 7$.*

1. For $\kappa \in \left\{ \frac{n-2}{2}, \frac{n-1}{2}, \frac{n}{2} \right\}$, $ABS(G) \leq \kappa(n-\kappa)\sqrt{1-\frac{2}{n}}$. Equality holds if and only if $G \cong K_{\kappa,n-\kappa}$.
2. For n even and $1 \leq k \leq \frac{n-4}{2}$,

$$ABS(G) \leq \frac{n(n-2k-2)}{4} \sqrt{1-\frac{2}{n-1}} + \frac{nk}{2} \sqrt{1-\frac{2}{n}} + k \sqrt{1-\frac{4}{2k+n+2}}.$$

Equality holds if and only if $G \cong \overline{\mathcal{K}}_{\kappa} \left[\frac{n}{2}, \frac{n-2k-2}{2} \right]$.

3. For n odd and $1 \leq k \leq \frac{n-3}{2}$,

$$ABS(G) \leq \frac{(n-1)(n-2k-1)}{4} \sqrt{1-\frac{2}{n-1}} + \frac{(n-1)k}{2} \sqrt{1-\frac{2}{n}} + k \sqrt{1-\frac{4}{2k+n+1}}.$$

Equality holds if and only if $G \cong \overline{\mathcal{K}}_{\kappa} \left[\frac{n-1}{2}, \frac{n-2k-1}{2} \right]$.

Proof. Let $G \in \mathcal{BG}_{n,\kappa}$ with maximum ABS index and let S be a minimum vertex cut set of G . Let $\kappa \in \left\{ \frac{n-1}{2}, \frac{n}{2} \right\}$. If $G - S$ has a non-trivial component, then by Theorem 7, $G \cong \overline{\mathcal{K}}_{\kappa}[x, y]$ with $x \geq 1$ and $y \geq \kappa$. So, $|G| = x + y + \kappa + 1 > n$, a contradiction. Hence $G - S$ is an empty graph, and so by Remark 2, $G \cong \mathcal{K}_{\kappa,n-\kappa}$.

Let $\kappa = \frac{n-2}{2}$. Then from Remark 2 and by Theorems 7 and 8, we get,

$$G \cong K_{\frac{n-2}{2}, \frac{n+2}{2}} \text{ or } \bar{\mathcal{K}}_{\kappa} \left[\frac{n-2}{2}, 1 \right]. \text{ Since } ABS \left(K_{\frac{n-2}{2}, \frac{n+2}{2}} \right) > ABS \left(\bar{\mathcal{K}}_{\kappa} \left[\frac{n-2}{2}, 1 \right] \right), G \cong K_{\frac{n-2}{2}, \frac{n+2}{2}}. \text{ Assume that } 1 \leq k \leq \frac{n-3}{2}.$$

If n is even, then from Remark 2 and by Theorems 7 and 8, $G \cong K_{\kappa, n-\kappa}$ or $G \cong \bar{\mathcal{K}}_{\kappa} \left[\frac{n}{2}, \frac{n-2k-2}{2} \right]$. Since $ABS \left(\bar{\mathcal{K}}_{\kappa} \left[\frac{n}{2}, \frac{n-2k-2}{2} \right] \right)$

$$\geq ABS \left(\bar{\mathcal{K}}_{\kappa} [n-k-2, 1] \right) > ABS \left(K_{\kappa, n-\kappa} \right), G \cong \bar{\mathcal{K}}_{\kappa} \left[\frac{n}{2}, \frac{n-2k-2}{2} \right].$$

Otherwise n is odd. Similar to the case n is even, we get

$$G \cong \bar{\mathcal{K}}_{\kappa} \left[\frac{n-1}{2}, \frac{n-2k-1}{2} \right]. \quad \blacksquare$$

5 Conclusion

This work characterizes graphs with the maximum ABS index in the following classes: (i) connected graphs with n vertices and p cut-vertices; (ii) connected graphs of order n with a vertex k -partiteness $v_k(G) = r$; and (iii) connected bipartite graphs of order n with a fixed vertex connectivity κ . This study provides solutions to some of the many open problems proposed in [1]. Several open extremal problems related to this index require further investigation in future research.

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