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Upper bounds on the average number of colors in the non-equivalent colorings of a graph

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Abstract : A coloring of a graph is an assignment of colors to its vertices such that adjacent vertices have different colors. Two colorings are equivalent if they induce the same partition of the vertex set into color classes. Let $\mathcal{A}(G)$ be the average number of colors in the non-equivalent colorings of a graph G . We give a general upper bound on $\mathcal{A}(G)$ that is valid for all graphs G and a more precise one for graphs G of order n and maximum degree $\Delta(G) \in \{1, 2, n - 2\}$.

Keywords: Graph coloring, average number of colors, graphical Bell number

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1 Introduction

A coloring of a graph G is an assignment of colors to its vertices such that adjacent vertices have different colors. The total number $\mathcal{B}(G)$ of non-equivalent colorings (i.e., with different partitions into color classes) of a graph G is the number of partitions of the vertex set of G whose blocks are stable sets (i.e., sets of pairwise non-adjacent vertices). This invariant has been studied by several authors in the last few years [1, 5, 6, 7, 9, 11] under the name of (graphical) Bell number. It is related to the standard Bell number B_n (sequence A000110 in OEIS [13]) that corresponds to the number of partitions of a set of n elements into non-empty subsets, and is thus obviously the same as the number of non-equivalent colorings of the empty graph or order n (i.e., the graph with n vertices and without any edge).

The 2-Bell number T_n (sequence A005493 in OEIS [13]) is the total number of blocks in all partitions of a set of n elements. Odlyzko and Richmond [12] have studied the average number A_n of blocks in a partition of a set of n elements, which can be defined as $A_n = \frac{T_n}{B_n}$. The corresponding concept in graph theory is the average number $\mathcal{A}(G)$ of colors in the non-equivalent colorings of a graph G . This graph invariant was recently defined in [8]. When constraints (represented by edges in G) impose that certain pairs of elements (represented by vertices) cannot belong to the same block of a partition, $\mathcal{A}(G)$ is the average number of blocks in the partitions that respect all constraints. Clearly, $\mathcal{A}(G) = A_n$ if G is the empty graph of order n .

Lower bounds on $\mathcal{A}(G)$ are studied in [10]. The authors mention that there is no known lower bound on $\mathcal{A}(G)$ which is a function of n and such that there exists at least one graph of order n which reaches it. As we will show, the situation is not the same for the upper bound. Indeed, we show that there is an upper bound on $\mathcal{A}(G)$ which is a function of n and such that there exists at least one graph of order n which reaches it. We also give a sharper upper bound for graphs with maximum degree $\Delta(G) \in \{1, 2, n-2\}$.

In the next section we fix some notations. Section 3 is devoted to properties of $\mathcal{A}(G)$ and basic ingredients that we will use in Section 4 for proving the validity of the upper bounds on $\mathcal{A}(G)$.

2 Notation

For basic notions of graph theory that are not defined here, we refer to Diestel [3]. The order of a graph $G = (V, E)$ is its number $|V|$ of vertices, and the size of G is its number $|E|$ of edges. We write \overline{G} for the complement of G and $G \simeq H$ if G and H are two isomorphic graphs. We denote by K_n (resp. C_n , P_n and \overline{K}_n) the *complete graph* (resp. the *cycle*, the *path* and the *empty graph*) of order n . For a subset W of vertices in G , we write $G[W]$ for the subgraph induced by W . Given two graphs G_1 and G_2 (with disjoint sets of vertices), we write $G_1 \cup G_2$ for the *disjoint union* of G_1 and G_2 . Also, $G \cup pK_1$ is the graph obtained from G by adding p isolated vertices, i.e. $G \cup pK_1 \simeq G \cup \overline{K}_p$.

Let $N(v)$ be the set of vertices adjacent to a vertex v in G . We say that v is *isolated* if $|N(v)| = 0$. We write $\Delta(G)$ for the *maximum degree* of G . A vertex v of a graph G is *simplicial* if the induced subgraph $G[N(v)]$ of G is a clique.

Let u and v be any two vertices in a graph G of order n . We use the following notations:

- $G_{|uv}$ is the graph (of order $n-1$) obtained by identifying (merging) the vertices u and v and, if $uv \in E(G)$, by removing the edge uv ;
- if $uv \in E(G)$, $G - uv$ is the graph obtained by removing the edge uv from G ;
- if $uv \notin E(G)$, $G + uv$ is the graph obtained by adding the edge uv in G ;
- $G - v$ is the graph obtained from G by removing v and all its incident edges.

A *coloring* of a graph G is an assignment of colors to the vertices of G such that adjacent vertices have different colors. The *chromatic number* $\chi(G)$ is the minimum number of colors in a coloring of G .

Two colorings are *equivalent* if they induce the same partition of the vertex set into color classes. Let $S(G, k)$ be the number of non-equivalent colorings of a graph G that use *exactly* k colors. Then, the total number $\mathcal{B}(G)$ of non-equivalent colorings of a graph G is defined by

$$\mathcal{B}(G) = \sum_{k=\chi(G)}^n S(G, k),$$

and the total number $\mathcal{T}(G)$ of color classes in the non-equivalent colorings of a graph G is defined by

$$\mathcal{T}(G) = \sum_{k=\chi(G)}^n kS(G, k).$$

In this paper, we study the average number $\mathcal{A}(G)$ of colors in the non-equivalent colorings of a graph G , that is,

$$\mathcal{A}(G) = \frac{\mathcal{T}(G)}{\mathcal{B}(G)}.$$

For illustration, as shown in Figure 1, there are one non-equivalent coloring of P_4 with 2 colors, three with 3 colors, and one with 4 colors, which gives $\mathcal{B}(P_4) = 5$, $\mathcal{T}(P_4) = 15$ and $\mathcal{A}(P_4) = \frac{15}{5} = 3$.

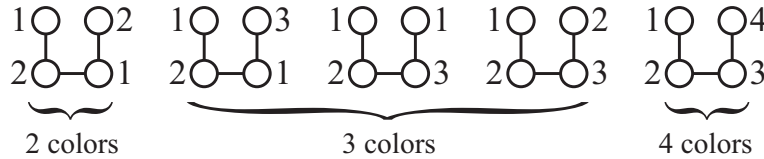


Figure 1: The non-equivalent colorings of P_4

3 Properties of $S(G, k)$ and $\mathcal{A}(G)$

As for several other invariants in graph coloring, the *deletion-contraction* rule (also often called the *Fundamental Reduction Theorem* [4]) can be used to compute $\mathcal{B}(G)$ and $\mathcal{T}(G)$. More precisely, let u and v be any pair of distinct vertices of G . As shown in [6, 11], we have

$$S(G, k) = S(G - uv, k) - S(G|_{uv}, k) \quad \forall uv \in E(G), \quad (1)$$

$$S(G, k) = S(G + uv, k) + S(G|_{uv}, k) \quad \forall uv \notin E(G). \quad (2)$$

It follows that

$$\left. \begin{aligned} \mathcal{B}(G) &= \mathcal{B}(G - uv) - \mathcal{B}(G|_{uv}) \\ \mathcal{T}(G) &= \mathcal{T}(G - uv) - \mathcal{T}(G|_{uv}) \end{aligned} \right\} \quad \forall uv \in E(G), \quad (3)$$

$$\left. \begin{aligned} \mathcal{B}(G) &= \mathcal{B}(G + uv) + \mathcal{B}(G|_{uv}) \\ \mathcal{T}(G) &= \mathcal{T}(G + uv) + \mathcal{T}(G|_{uv}) \end{aligned} \right\} \quad \forall uv \notin E(G). \quad (4)$$

Many properties on $\mathcal{A}(G)$ are proved in [8] and [10]. We mention here some of them that will be useful for proving the validity of the upper bounds on $\mathcal{A}(G)$ given in Section 4.

Proposition 1 ([10]). Let v be a simplicial vertex of degree at least one in a graph G , and let w be one of its neighbors in G . Then $\mathcal{A}(G) > \mathcal{A}(G - vw)$.

Proposition 2 ([10]). Let H_1 and H_2 be any two graphs. If $S(H_1, k)S(H_2, k') \geq S(H_2, k)S(H_1, k')$ for all $k > k'$, the inequality being strict for at least one pair (k, k') , then $\mathcal{A}(G \cup H_1) > \mathcal{A}(G \cup H_2)$ for all graphs G .

Proposition 3 ([8]). Let G, H and F_1, \dots, F_r be $r+2$ graphs, and let $\alpha_1, \dots, \alpha_r$ be r positive numbers such that

- $\mathcal{B}(G) = \mathcal{B}(H) + \sum_{i=1}^r \alpha_i \mathcal{B}(F_i)$
- $\mathcal{T}(G) = \mathcal{T}(H) + \sum_{i=1}^r \alpha_i \mathcal{T}(F_i)$
- $\mathcal{A}(F_i) < \mathcal{A}(H)$ for all $i = 1, \dots, r$.

Then $\mathcal{A}(G) < \mathcal{A}(H)$.

Proposition 4 ([10]). $\mathcal{A}(G \cup C_n) > \mathcal{A}(G \cup P_n)$ for all $n \geq 3$ and all graphs G .

Some graphs G of order $n \leq 9$ will play a special role in the next section. The values $S(G, k)$ of these graphs, with $2 \leq k \leq n$, are given in Table 1. These values lead to the following lemma.

Table 1: Values of $S(G, k)$ for some graphs G of order n and $2 \leq k \leq n$

k	2	3	4	5	6	7	8	9	10
$S(C_3 \cup K_2, k)$	0	6	6	1					
$S(C_4 \cup K_1, k)$	2	7	6	1					
$S(C_5, k)$	0	5	5	1					
$S(2C_3, k)$	0	6	18	9	1				
$S(C_4 \cup K_2, k)$	2	16	25	10	1				
$S(C_5 \cup K_1, k)$	0	15	25	10	1				
$S(C_6, k)$	1	10	20	9	1				
$S(C_3 \cup C_4, k)$	0	18	66	55	14	1			
$S(C_5 \cup K_2, k)$	0	30	90	65	15	1			
$S(C_7, k)$	0	21	70	56	14	1			
$S(C_3 \cup C_5, k)$	0	30	210	285	125	20	1		
$S(2C_4, k)$	2	52	241	296	126	20	1		
$S(C_8, k)$	1	42	231	294	126	20	1		
$S(3C_3, k)$	0	36	540	1242	882	243	27	1	
$S(C_3 \cup C_6, k)$	0	66	666	1351	910	245	27	1	
$S(C_4 \cup C_5, k)$	0	90	750	1415	925	246	27	1	
$S(C_9, k)$	0	85	735	1407	924	246	27	1	
$S(2C_3 \cup C_4, k)$	0	108	1908	5838	5790	2361	433	35	1
$S(2C_5, k)$	0	150	2250	6345	6025	2400	435	35	1

Lemma 5. The following strict inequalities are valid for all graphs G :

- | | |
|--|---|
| (a) $\mathcal{A}(G \cup C_6) < \mathcal{A}(G \cup 2C_3)$ | (b) $\mathcal{A}(G \cup C_7) < \mathcal{A}(G \cup C_3 \cup C_4)$ |
| (c) $\mathcal{A}(G \cup C_8) < \mathcal{A}(G \cup C_3 \cup C_5)$ | (d) $\mathcal{A}(G \cup C_3 \cup K_2) < \mathcal{A}(G \cup C_5)$ |
| (e) $\mathcal{A}(G \cup C_4 \cup K_2) < \mathcal{A}(G \cup 2C_3)$ | (f) $\mathcal{A}(G \cup C_5 \cup K_2) < \mathcal{A}(G \cup C_3 \cup C_4)$ |
| (g) $\mathcal{A}(G \cup C_4 \cup K_1) < \mathcal{A}(G \cup C_5)$ | (h) $\mathcal{A}(G \cup C_5 \cup K_1) < \mathcal{A}(G \cup 2C_3)$ |
| (i) $\mathcal{A}(G \cup 2C_4) < \mathcal{A}(G \cup C_3 \cup C_5)$ | (j) $\mathcal{A}(G \cup C_4 \cup C_5) < \mathcal{A}(G \cup 3C_3)$ |
| (k) $\mathcal{A}(G \cup 2C_5) < \mathcal{A}(G \cup 2C_3 \cup C_4)$. | |

Proof. All these inequalities can be obtained from Proposition 2 by using the values given in Table 1. For example, to check that (a) holds, the 4th and 7th lines of Table 1 allow to check that $S(2C_3, k)S(C_6, k') - S(C_6, k)S(2C_3, k') \geq 0$ for all $k > k'$ and at least one of these values is strictly positive. \square

We now show the validity of four lemmas which will be helpful for proving that $\mathcal{A}(G \cup C_n) < \mathcal{A}(G \cup C_{n-3} \cup C_3)$ for all $n \geq 6$. A direct consequence of this result will be that a graph G that maximizes $\mathcal{A}(G)$ among the graphs with maximum degree 2 cannot contain an induced C_n with $n \geq 6$.

Lemma 6. $S(C_n, k) = (k-1)S(C_{n-1}, k) + S(C_{n-1}, k-1)$ for all $n \geq 4$ and all $k \geq 3$.

Proof. The values in the following table show that the result is true for $n = 4$.

k	2	3	4
$S(C_4, k)$	1	2	1
$S(C_3, k)$	0	1	0

For larger values of n , we proceed by induction. So assume $n \geq 5$, let u be a vertex in C_n , and let v and w be its two neighbors in C_n . Let us analyze the set of non-equivalent colorings of C_n that use exactly k colors:

- there are $(k-1)S(C_{n-2}, k)$ such colorings where v and w have the same color and at least one vertex of $C_n - u$ has the same color as u ;
- there are $S(C_{n-2}, k-1)$ such colorings where v and w have the same color and no vertex on $C_n - u$ has the same color as u ;
- there are $(k-2)S(C_{n-1}, k)$ such colorings where v and w have different colors and at least one vertex of $C_n - u$ has the same color as u ;
- there are $S(C_{n-1}, k-1)$ such colorings where v and w have different colors and no vertex on $C_n - u$ has the same color as u .

Hence,

$$\begin{aligned}
 S(C_n, k) &= ((k-1)S(C_{n-2}, k) + S(C_{n-2}, k-1)) + (k-2)S(C_{n-1}, k) + S(C_{n-1}, k-1) \\
 &= S(C_{n-1}, k) + (k-2)S(C_{n-1}, k) + S(C_{n-1}, k-1) \\
 &= (k-1)S(C_{n-1}, k) + S(C_{n-1}, k-1).
 \end{aligned}$$

□

Lemma 7. If $n \geq 7$ and $k \leq n$ then

$$S(C_{n-3} \cup C_3, k) = (k-1)S(C_{n-4} \cup C_3, k) + S(C_{n-4} \cup C_3, k-1) - (-1)^n \delta_k$$

where

$$\delta_k = \begin{cases} 6 & \text{if } k = 3, 4, \\ 1 & \text{if } k = 5, \\ 0 & \text{otherwise.} \end{cases}$$

Proof. The values in the following table show that the result is true for $n = 7$.

k	2	3	4	5	6	7
$S(C_4 \cup C_3, k)$	0	18	66	55	14	1
$S(C_3 \cup C_3, k)$	0	6	18	9	1	0

For larger values of n , we proceed by induction. Let u be a vertex in C_{n-3} , and let v and w be its two neighbors. We analyze the set of non-equivalent colorings of $C_{n-3} \cup C_3$ that use exactly k colors:

- there are $(k-1)S(C_{n-5} \cup C_3, k)$ such colorings where v and w have the same color and at least one vertex of $C_{n-3} \cup C_3 - u$ has the same color as u ;
- there are $S(C_{n-5} \cup C_3, k-1)$ such colorings where v and w have the same color and no vertex on $C_{n-3} \cup C_3 - u$ has the same color as u ;
- there are $(k-2)S(C_{n-4} \cup C_3, k)$ such colorings where v and w have different colors and at least one vertex of $C_{n-3} \cup C_3 - u$ has the same color as u ;
- there are $S(C_{n-4} \cup C_3, k-1)$ such colorings where v and w have different colors and no vertex on $C_{n-3} \cup C_3 - u$ has the same color as u .

Hence,

$$\begin{aligned}
S(C_{n-3} \cup C_3, k) &= ((k-1)S(C_{n-5} \cup C_3, k) + S(C_{n-5} \cup C_3, k-1)) \\
&\quad + (k-2)S(C_{n-4} \cup C_3, k) + S(C_{n-4} \cup C_3, k-1) \\
&= (S(C_{n-4} \cup C_3, k) + (-1)^{n-1}\delta_k) \\
&\quad + (k-2)S(C_{n-4} \cup C_3, k) + S(C_{n-4} \cup C_3, k-1) \\
&= (k-1)S(C_{n-4} \cup C_3, k) + S(C_{n-4} \cup C_3, k-1) - (-1)^n\delta_k.
\end{aligned}$$

□

For $n \geq 3$, let Q_n be the graph obtained from P_n by adding an edge between an extremity v of P_n and the vertex at distance 2 from v on P_n .

Lemma 8. If $n \geq 6$ and $k \leq n$ then $S(C_{n-3} \cup C_3, k) = S(Q_n, k) - (-1)^n \rho_k$ where

$$\rho_k = \begin{cases} 2 & \text{if } k = 3, \\ 1 & \text{if } k = 4, \\ 0 & \text{otherwise.} \end{cases}$$

Proof. The values in the following table show that the result is true for $n = 6$.

k	2	3	4	5	6
$S(2C_3, k)$	0	6	18	9	1
$S(Q_6, k)$	0	8	19	9	1

For larger values of n , we proceed by induction. Equations (1) and (2) give

$$\begin{aligned}
S(C_{n-3} \cup C_3, k) &= S(P_{n-3} \cup C_3, k) - S(C_{n-4} \cup C_3, k) \\
&= S(P_{n-3} \cup P_3, k) - S(P_{n-3} \cup P_2, k) - S(C_{n-4} \cup C_3, k) \\
&= S(P_n, k) + S(P_{n-1}, k) - S(P_{n-1}, k) - S(P_{n-2}, k) - S(C_{n-4} \cup C_3, k) \\
&= S(Q_n, k) + S(Q_{n-1}, k) - S(C_{n-4} \cup C_3, k) \\
&= S(Q_n, k) + (-1)^{n-1} \rho_k \\
&= S(Q_n, k) - (-1)^n \rho_k
\end{aligned}$$

□

Lemma 9. The following inequalities are valid for all $n \geq 9$:

- (a) $S(C_n, k) > S(C_n, k-1)$ for all $k \in \{3, 4, 5\}$;
- (b) $S(C_n, k) > 3S(C_{n-1}, k-1)$ for all $k \in \{3, 4, 5, 6\}$;
- (c) $S(C_n, 4) > 8S(C_n, 3)$.

Proof. The values in Table 1 show that the inequalities are satisfied for $n = 9$. For larger values of n , we proceed by induction. Note that (a) and (b) are clearly valid for $k = 3$ since $S(C_n, 3) > 3 \geq \max\{S(C_n, 2), 3S(C_{n-1}, 2)\}$. We may therefore assume $k \in \{4, 5\}$ for (a) and $k \in \{4, 5, 6\}$ for (b). Lemma 6 and the induction hypothesis imply

$$\begin{aligned}
S(C_n, k) &= (k-1)S(C_{n-1}, k) + S(C_{n-1}, k-1) \\
&> (k-2)S(C_{n-1}, k-1) + S(C_{n-1}, k-2) \\
&= S(C_n, k-1).
\end{aligned}$$

Hence (a) is proved. It follows that the following inequality is valid:

$$\begin{aligned}\frac{1}{k-1}S(C_{n-1}, k-1) &= \frac{1}{k-1} \left((k-2)S(C_{n-2}, k-1) + S(C_{n-2}, k-2) \right) \\ &< \frac{1}{k-1} \left((k-1)S(C_{n-2}, k-1) \right) \\ &= S(C_{n-2}, k-1)\end{aligned}$$

which implies

$$\begin{aligned}S(C_n, k) &= (k-1)S(C_{n-1}, k) + S(C_{n-1}, k-1) \\ &> (k-1)S(C_{n-1}, k) \\ &> 3(k-1)S(C_{n-2}, k-1) \\ &> 3S(C_{n-1}, k-1).\end{aligned}$$

Hence (b) is proved. We thus have

$$\begin{aligned}S(C_n, 4) &= 3S(C_{n-1}, 4) + S(C_{n-1}, 3) \\ &> 25S(C_{n-1}, 3) \\ &> \frac{25}{3}S(C_n, 3) \\ &> 8S(C_n, 3).\end{aligned}$$

which proves (c). □

4 Upper bounds on $\mathcal{A}(G)$

We are now ready to give upper bounds on $\mathcal{A}(G)$. The following theorem gives a general upper bound on $\mathcal{A}(G)$ that is valid for all graphs G of order n .

Theorem 10. Let G be a graph of order n , then,

$$\mathcal{A}(G) \leq n,$$

with equality if and only if $G \simeq K_n$.

Proof. Clearly,

$$\mathcal{T}(G) = \sum_{k=1}^n kS(G, k) \leq n \sum_{k=1}^n S(G, k) = n\mathcal{B}(G).$$

Hence, $\mathcal{A}(G) \leq n$, with equality if and only if $S(G, k) = 0$ for all $k < n$, that is if $G \simeq K_n$. □

Since $\Delta(K_n) = n - 1$ we immediately get the following corollary to Theorem 10.

Corollary 11. Let G be a graph of order n and maximum degree $\Delta(G) = n - 1$. Then, $\mathcal{A}(G) \leq n$, with equality if and only if $G \simeq K_n$.

We now give a more precise upper bound on $\mathcal{A}(G)$ for graphs G of order n and maximum degree $\Delta(G) = n - 2$.

Theorem 12. Let G be a graph of order $n \geq 2$ and maximum degree $\Delta(G) = n - 2$. Then,

$$\mathcal{A}(G) \leq \frac{n^2 - n + 1}{n},$$

with equality if and only if $G \simeq K_{n-1} \cup K_1$.

Proof. Let m be the number of edges in G , and let $x = \frac{n(n-1)}{2} - m = S(G, n-1)$. Then

$$\begin{aligned} \mathcal{T}(G) &= \sum_{k=1}^{n-2} kS(G, k) + x(n-1) + n \\ &\leq (n-1) \sum_{k=1}^{n-2} S(G, k) + x(n-1) + n \\ &= (n-1) \sum_{k=1}^n S(G, k) + 1 \\ &= (n-1)\mathcal{B}(G) + 1. \end{aligned}$$

Hence, $\mathcal{A}(G) \leq n-1 + \frac{1}{\mathcal{B}(G)}$, with possible equality only if $S(G, k) = 0$ for all $k < n-1$. It is proved in [9] that $\mathcal{B}(G) \geq n$, with equality if and only if G is isomorphic to $K_{n-1} \cup K_1$ when $n \neq 4$, and G is isomorphic to $K_3 \cup K_1$ or C_4 when $n = 4$. Since $S(C_4, 2) = 1 > 0$ while $S(K_{n-1} \cup K_1, k) = 0$ for all $k < n-1$, we conclude that $\mathcal{A}(G) \leq n-1 + \frac{1}{n} = \frac{n^2-n+1}{n}$, with equality if and only if $G \simeq K_{n-1} \cup K_1$. \square

The next simple case is when $\Delta(G) = 1$.

Theorem 13. Let G be a graph of order n and maximum degree $\Delta(G) = 1$. Then,

$$\mathcal{A}(G) \leq \mathcal{A}\left(\left\lfloor \frac{n}{2} \right\rfloor K_2 \cup (n \bmod 2)K_1\right)$$

with equality if and only if $G \simeq \left\lfloor \frac{n}{2} \right\rfloor K_2 \cup (n \bmod 2)K_1$.

Proof. If G contains two isolated vertices u and v , we know from Proposition 1 that $\mathcal{A}(G+uv) > \mathcal{A}(G)$. Hence the maximum value of $\mathcal{A}(G)$ is reached when G contains at most one isolated vertex, that is $G \simeq \left\lfloor \frac{n}{2} \right\rfloor K_2 \cup (n \bmod 2)K_1$. \square

We now give a precise upper bound on $\mathcal{A}(G)$ for graphs G with maximum degree 2. We first analyze the impact of the replacement of an induced C_n ($n \geq 6$) by $C_{n-3} \cup C_3$.

Lemma 14. $\mathcal{A}(G \cup C_n) < \mathcal{A}(G \cup C_{n-3} \cup C_3)$ for all $n \geq 6$ and all graphs G .

Proof. We know from Lemma 5 (a), (b) and (c) that the result is true for $n = 6, 7, 8$. We can therefore assume $n \geq 9$.

Let $f_n(k, k') = S(C_{n-3} \cup C_3, k)S(C_n, k') - S(C_n, k)S(C_{n-3} \cup C_3, k')$. Proposition 2 shows that it is sufficient to prove that $f_n(k, k') \geq 0$ for all $k > k'$, the inequality being strict for at least one pair (k, k') . Note that $f_n(n, 2) = 1 > 0$ for n even. Also, $f_n(n, 3) > 0$ for n odd. Indeed, this is true for $n = 9$ since the values in Table 1 give $f_n(9, 3) = 85 - 66 = 19$. For larger odd values of n , we proceed by induction, using Lemmas 6 and 7:

$$\begin{aligned} f_n(n, 3) &= S(C_n, 3) - S(C_{n-3} \cup C_3, 3) \\ &= \left(2S(C_{n-1}, 3) + 1\right) - \left(2S(C_{n-4} \cup C_3, 3) + 6\right) \\ &= \left(4S(C_{n-2}, 3) + 1\right) - \left(2(2S(C_{n-5} \cup C_3, 3) - 6) + 6\right) \\ &= 4S(C_{n-2}, 3) - 4S(C_{n-5} \cup C_3, 3) + 7 \\ &= 4f_{n-2}(n-2, 3) + 7 > 0. \end{aligned}$$

Hence, it remains to prove that $f_n(k, k') \geq 0$ for all $1 \leq k' < k \leq n$. Let us start with the cases where $k' \leq 2$ and/or $k \geq n-1$.

- If $k' \leq 2$ then $f_n(k, k') = S(C_{n-3} \cup C_3, k)S(C_n, k') \geq 0$.
- If $k \geq n-1$ then $S(C_n, k) = S(C_{n-3} \cup C_3, k)$ since
 - $S(C_n, n) = S(C_{n-3} \cup C_3, n) = 1$, and
 - $S(C_n, n-1) = S(C_{n-3} \cup C_3, n-1) = \frac{n^2-3n}{2}$.

Also, it follows from Lemma 8 that $S(C_{n-3} \cup C_3, k') = S(Q_n, k') - (-1)^n \rho_{k'}$ and Equations (1) and (2) give

$$\begin{aligned} S(C_n, k) &= S(P_n, k) - S(C_{n-1}, k) \\ &= (S(Q_n, k) + S(P_{n-1}, k)) - (S(P_{n-1}, k) - S(C_{n-2}, k)) \\ &= S(Q_n, k) + S(C_{n-2}, k). \end{aligned}$$

Altogether, this gives

$$\begin{aligned} f_n(k, k') &= S(C_n, k) \left(S(C_n, k') - S(C_{n-3} \cup C_3, k') \right) \\ &= S(C_n, k) \left((S(Q_n, k') + S(C_{n-2}, k')) - (S(Q_n, k') - (-1)^n \rho_{k'}) \right) \\ &= S(C_n, k) \left(S(C_{n-2}, k') + (-1)^n \rho_{k'} \right). \end{aligned}$$

Hence,

- if n is even and/or $k' \notin \{3, 4\}$, then $f_n(k, k') \geq 0$;
- if n is odd and $k' = 3$ then $f_n(k, k') = S(C_n, k)(S(C_{n-2}, 3) - 2) \geq 0$;
- If n is odd and $k' = 4$ then $f_n(k, k') = S(C_n, k)(S(C_{n-2}, 4) - 1) \geq 0$.

We can therefore assume $3 \leq k' < k \leq n-2$ and we finally prove that

$$f_n(k, k') \geq \begin{cases} 0 & \text{if } k' \geq 6, \\ 7S(C_n, k) & \text{if } k' \in \{3, 4, 5\}. \end{cases}$$

The values in the following table, computed with the help of those for C_9 and $C_6 \cup C_3$ in Table 1, show that this is true for $n = 9$:

(k, k')	(4,3)	(5,3)	(5,4)	(6,3)	(6,4)	(6,5)	(7,3)	(7,4)	(7,5)	(7,6)
$f_9(k, k')$	8100	21973	55923	16366	53466	32046	4589	16239	12369	2520
$7S(C_9, k)$	5145	9849	9849	6468	6468	6468	1722	1722	1722	1722

For larger values of n , we proceed by induction. Lemmas 6 and 7 give

$$\begin{aligned} f_n(k, k') &= S(C_n, k')S(C_{n-3} \cup C_3, k) - S(C_n, k)S(C_{n-3} \cup C_3, k') \\ &= S(C_n, k') \left((k-1)S(C_{n-4} \cup C_3, k) + S(C_{n-4} \cup C_3, k-1) - (-1)^n \delta_k \right) \\ &\quad - S(C_n, k) \left((k'-1)S(C_{n-4} \cup C_3, k') + S(C_{n-4} \cup C_3, k'-1) - (-1)^n \delta_{k'} \right) \\ &= \left((k'-1)S(C_{n-1}, k') + S(C_{n-1}, k'-1) \right) \left((k-1)S(C_{n-4} \cup C_3, k) + S(C_{n-4} \cup C_3, k-1) \right) \\ &\quad - \left((k-1)S(C_{n-1}, k) + S(C_{n-1}, k-1) \right) \left((k'-1)S(C_{n-4} \cup C_3, k') + S(C_{n-4} \cup C_3, k'-1) \right) \\ &\quad + (-1)^n \delta_{k'} S(C_n, k) - (-1)^n \delta_k S(C_n, k') \\ &= (k-1)(k'-1) \left(S(C_{n-1}, k')S(C_{n-4} \cup C_3, k) - S(C_{n-1}, k)S(C_{n-4} \cup C_3, k') \right) \\ &\quad + (k'-1) \left(S(C_{n-1}, k')S(C_{n-4} \cup C_3, k-1) - S(C_{n-1}, k-1)S(C_{n-4} \cup C_3, k') \right) \\ &\quad + (k-1) \left(S(C_{n-1}, k'-1)S(C_{n-4} \cup C_3, k) - S(C_{n-1}, k)S(C_{n-4} \cup C_3, k'-1) \right) \\ &\quad + S(C_{n-1}, k'-1)S(C_{n-4} \cup C_3, k-1) - S(C_{n-1}, k-1)S(C_{n-4} \cup C_3, k'-1) \\ &\quad + (-1)^n \delta_{k'} S(C_n, k) - (-1)^n \delta_k S(C_n, k') \end{aligned}$$

$$\begin{aligned}
&= (k-1)(k'-1)f_{n-1}(k, k') + (k'-1)f_{n-1}(k-1, k') \\
&\quad + (k-1)f_{n-1}(k, k'-1) + f_{n-1}(k-1, k'-1) \\
&\quad + (-1)^n \delta_{k'} S(C_n, k) - (-1)^n \delta_k S(C_n, k').
\end{aligned} \tag{5}$$

Since $\delta_k = 0$ for $k \geq 6$ and $f_{n-1}(k, k') \geq 0$, $f_{n-1}(k-1, k') \geq 0$, $f_{n-1}(k, k'-1) \geq 0$, and $f_{n-1}(k-1, k'-1) \geq 0$ for $k > k'$, we have $f_n(k, k') \geq 0$ for $k > k' \geq 6$.

Therefore, it remains to show that $f_n(k, k') \geq 7S(C_n, k)$ for $k' \in \{3, 4, 5\}$. Let $g_n(k, k') = (-1)^n \delta_{k'} S(C_n, k) - (-1)^n \delta_k S(C_n, k')$. There are 4 possible cases.

Case 1 : $k' \in \{4, 5\}$ and $k \geq k' + 2$.

We have $g_n(k, k') = (-1)^n \delta_{k'} S(C_n, k) \geq -6S(C_n, k)$. Using the induction hypothesis and Lemma 6, Equation (5) gives

$$\begin{aligned}
f_n(k, k') &\geq \left(7(k-1)(k'-1)S(C_{n-1}, k) + 7(k'-1)S(C_{n-1}, k-1)\right) \\
&\quad + \left(7(k-1)S(C_{n-1}, k) + 7S(C_{n-1}, k-1)\right) - 6S(C_n, k) \\
&= 7(k'-1)S(C_n, k) + 7S(C_n, k) - 6S(C_n, k) \\
&= (7k' - 6)S(C_n, k) \\
&> 7S(C_n, k).
\end{aligned}$$

Case 2 : $k' \in \{4, 5\}$ and $k = k' + 1$.

Let us first give a lower bound on $g_n(k, k')$:

- if n is even and $k = 6$, then $g_n(k, k') \geq 0$;
- if n is even and $k = 5$, then $g_n(k, k') \geq -S(C_n, 4)$, and we deduce from Lemma 9 (a) that $g_n(k, k') \geq -S(C_n, 5)$;
- if n is odd, then $g_n(k, k') \geq -\delta_{k'} S(C_n, k) \geq -6S(C_n, k)$.

Hence, whatever n and (k, k') , $g_n(k, k') \geq -6S(C_n, k)$. Since $f_{n-1}(k-1, k') = 0$, using again the induction hypothesis and Lemma 6, we deduce from Equation (5) that

$$\begin{aligned}
f_n(k, k') &\geq \left(7(k-1)(k'-1)S(C_{n-1}, k)\right) + \left(7(k-1)S(C_{n-1}, k) + 7S(C_{n-1}, k-1)\right) - 6S(C_n, k) \\
&= \left(7(k'-1)S(C_n, k) - 7(k'-1)S(C_{n-1}, k-1)\right) + \left(7S(C_n, k)\right) - 6S(C_n, k) \\
&= (7k' - 6)S(C_n, k) - 7(k'-1)S(C_{n-1}, k-1)
\end{aligned}$$

Since $k \leq 6$, Lemma 9 (b) shows that $S(C_{n-1}, k-1) \leq \frac{1}{3}S(C_n, k)$ and we therefore have

$$\begin{aligned}
f_n(k, k') &\geq \left(\frac{14k' - 11}{3}\right) S(C_n, k) \\
&\geq 15S(C_n, k) \\
&> 7S(C_n, k).
\end{aligned}$$

Case 3 : $k' = 3$ and $k \geq 5$.

As in the previous case, we have $g_n(k, k') \geq -6S(C_n, k)$. The induction hypothesis gives $f_{n-1}(k, k') \geq 7S(C_{n-1}, k)$, $f_{n-1}(k-1, k') \geq 7S(C_{n-1}, k-1)$, $f_{n-1}(k, k'-1) \geq 0$, and $f_{n-1}(k-1, k'-1) \geq 0$. Hence, Equation (5) becomes

$$\begin{aligned}
f_n(k, k') &\geq 7(k-1)(k'-1)S(C_{n-1}, k) + 7(k'-1)S(C_{n-1}, k-1) - 6S(C_n, k) \\
&= 7(k'-1)S(C_n, k) - 6S(C_n, k) \\
&= 8S(C_n, k) \\
&> 7S(C_n, k).
\end{aligned}$$

Case 4 : $k' = 3$ and $k = 4$.

We have $g_n(k, k') = (-1)^n 6S(C_n, k) - (-1)^n 6S(C_n, k')$ and we know from Lemma 9 (a) that $S(C_n, 4) > S(C_n, 3)$. Hence, $g_n(4, 3) \geq -6(S(C_n, k) - S(C_n, k'))$. Using the induction hypothesis, Equation (5) gives

$$\begin{aligned} f_n(k, k') &\geq -7(k-1)(k'-1)S(C_{n-1}, k) - 6(S(C_n, k) - S(C_n, k')) \\ &= 42S(C_{n-1}, k) - 6(S(C_n, k) - S(C_n, k')). \end{aligned}$$

We therefore conclude from Lemmas 6 and 9 (c) that

$$\begin{aligned} f_n(4, 3) &\geq \frac{42}{3}(S(C_n, 4) - S(C_n, 3)) - 6(S(C_n, 4) - S(C_n, 3)) \\ &= 8(S(C_n, 4) - S(C_n, 3)) \\ &> 8\left(S(C_n, 4) - \frac{1}{8}S(C_n, 4)\right) \\ &= 7S(C_n, 4). \end{aligned}$$

□

It is easy to check that

- $\mathcal{A}(K_3 \cup K_1) = \frac{13}{4} > 3 = \mathcal{A}(C_4)$, and
- $\mathcal{A}(2K_3 \cup K_1) = \frac{778}{175} > \frac{684}{154} = \mathcal{A}(K_3 \cup C_4)$.

Hence, $\mathcal{A}((p+1)K_3 \cup K_1) > \mathcal{A}(pK_3 \cup C_4)$ for $p = 0, 1$. We next prove that this inequality is reversed for larger values of p , that is $\mathcal{A}((p+1)K_3 \cup K_1) < \mathcal{A}(pK_3 \cup C_4)$ for $p \geq 2$. Proposition 2 is of no help for this proof since, whatever p , there are pairs (k, k') for which $S((p+1)K_3 \cup K_1, k)S(pK_3 \cup C_4, k') > S(pK_3 \cup C_4, k)S((p+1)K_3 \cup K_1, k')$, and other pairs for which the inequality is reversed. Also, it is not true that

$$\mathcal{A}((p+1)K_3 \cup K_1) - \mathcal{A}(pK_3 \cup K_1) > \mathcal{A}(pK_3 \cup C_4) - \mathcal{A}((p-1)K_3 \cup C_4)$$

which would have given a simple proof by induction on p . The only way we have found to prove the desired result is to explicitly calculate $\mathcal{A}((p+1)K_3 \cup K_1)$ and $\mathcal{A}(pK_3 \cup C_4)$. This is what we do next, with the help of two lemmas.

Lemma 15. If G is a graph of order n , then

$$\begin{aligned} \mathcal{B}(G \cup K_2) &= \sum_{k=1}^n (k^2 + k + 1)S(G, k), \\ \mathcal{T}(G \cup K_2) &= \sum_{k=1}^n (k^3 + k^2 + 3k + 2)S(G, k), \\ \mathcal{B}(G \cup K_3) &= \sum_{k=1}^n (k^3 + 2k + 1)S(G, k), \\ \mathcal{T}(G \cup K_3) &= \sum_{k=1}^n (k^4 + 5k^2 + 4k + 3)S(G, k). \end{aligned}$$

Proof. As observed in [9],

$$S(G \cup K_r, k) = \sum_{i=0}^r \binom{k-i}{r-i} \binom{r}{i} (r-i)! S(G, k-i). \quad (6)$$

For $r = 2$, this gives $S(G \cup K_2, k) = k(k-1)S(G, k) + 2(k-1)S(G, k-1) + S(G, k-2)$. Hence,

$$\mathcal{B}(G \cup K_2) = \sum_{k=1}^{n+2} S(G \cup K_2, k)$$

$$\begin{aligned}
&= \sum_{k=1}^{n+2} \left(k(k-1)S(G, k) + 2(k-1)S(G, k-1) + S(G, k-2) \right) \\
&= \sum_{k=1}^n k(k-1)S(G, k) + \sum_{k=1}^n 2kS(G, k) + \sum_{k=1}^n S(G, k) \\
&= \sum_{k=1}^n (k^2 + k + 1)S(G, k)
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{T}(G \cup K_2) &= \sum_{k=1}^{n+2} kS(G \cup K_2, k) \\
&= \sum_{k=1}^{n+2} \left(k^2(k-1)S(G, k) + 2k(k-1)S(G, k-1) + kS(G, k-2) \right) \\
&= \sum_{k=1}^n k^2(k-1)S(G, k) + \sum_{k=1}^n 2(k+1)kS(G, k) + \sum_{k=1}^n (k+2)S(G, k) \\
&= \sum_{k=1}^n (k^3 + k^2 + 3k + 2)S(G, k).
\end{aligned}$$

The values for $\mathcal{B}(G \cup K_3)$ and $\mathcal{T}(G \cup K_3)$ are computed in a similar way. \square

Lemma 16. If G is a graph of order n , then,

$$\begin{aligned}
\mathcal{B}(G \cup K_3 \cup K_1) &= \sum_{k=1}^n (k^4 + k^3 + 5k^2 + 6k + 4)S(G, k), \\
\mathcal{T}(G \cup K_3 \cup K_1) &= \sum_{k=1}^n (k^5 + k^4 + 9k^3 + 15k^2 + 21k + 13)S(G, k).
\end{aligned}$$

Proof. Let $G' = G \cup K_3$. Equation (6) gives $S(G' \cup K_1, k) = kS(G', k) + S(G', k-1)$. Hence, it follows from Lemma 15 that

$$\begin{aligned}
\mathcal{B}(G \cup K_3 \cup K_1) &= \sum_{k=1}^{n+4} \left(kS(G', k) + S(G', k-1) \right) \\
&= \sum_{k=1}^{n+3} kS(G', k) + \sum_{k=1}^{n+3} S(G', k) \\
&= \mathcal{T}(G') + \mathcal{B}(G') \\
&= \sum_{k=1}^n \left((k^4 + 5k^2 + 4k + 3) + (k^3 + 2k + 1) \right) S(G, k) \\
&= \sum_{k=1}^n (k^4 + k^3 + 5k^2 + 6k + 4)S(G, k).
\end{aligned}$$

Equation (6) gives

$$\begin{aligned}
\sum_{k=1}^{n+3} k^2 S(G', k) &= \sum_{k=1}^n k^2 \left(k(k-1)(k-2)S(G, k) \right) + \sum_{k=1}^{n+1} k^2 \left(3(k-1)(k-2)S(G, k-1) \right) \\
&\quad + \sum_{k=1}^{n+2} k^2 \left(3(k-2)S(G, k-2) \right) + \sum_{k=1}^{n+3} k^2 S(G, k-3)
\end{aligned}$$

$$\begin{aligned}
&= \sum_{k=1}^n k^3(k-1)(k-2)S(G, k) + \sum_{k=1}^n 3(k+1)^2k(k-1)S(G, k) \\
&\quad + \sum_{k=1}^n 3(k+2)^2kS(G, k) + \sum_{k=1}^n (k+3)^2S(G, k) \\
&= \sum_{k=1}^n \left(k^3(k-1)(k-2) + 3(k+1)^2k(k-1) + 3(k+2)^2k + (k+3)^2 \right) S(G, k) \\
&= \sum_{k=1}^n (k^5 + 8k^3 + 10k^2 + 15k + 9)S(G, k).
\end{aligned}$$

Hence, using again Lemma 15, we get

$$\begin{aligned}
\mathcal{T}(G \cup K_3 \cup K_1) &= \sum_{k=1}^{n+4} \left(k^2 S(G', k) + k S(G', k-1) \right) \\
&= \sum_{k=1}^{n+3} k^2 S(G', k) + \sum_{k=1}^{n+3} (k+1) S(G', k) \\
&= \sum_{k=1}^{n+3} k^2 S(G', k) + \mathcal{T}(G') + \mathcal{B}(G') \\
&= \sum_{k=1}^n \left((k^5 + 8k^3 + 10k^2 + 15k + 9) + (k^4 + 5k^2 + 4k + 3) + (k^3 + 2k + 1) \right) S(G, k) \\
&= \sum_{k=1}^n (k^5 + k^4 + 9k^3 + 15k^2 + 21k + 13) S(G, k).
\end{aligned}$$

□

We are now ready to compare $\mathcal{A}(pK_3 \cup C_4)$ with $\mathcal{A}((p+1)K_3 \cup K_1)$.

Theorem 17.

- $\mathcal{A}(pK_3 \cup C_4) < \mathcal{A}((p+1)K_3 \cup K_1)$ if $p = 0, 1$ and
- $\mathcal{A}(pK_3 \cup C_4) > \mathcal{A}((p+1)K_3 \cup K_1)$ if $p \geq 2$.

Proof. We have already mentioned that

- $\mathcal{A}(K_3 \cup K_1) = \frac{13}{4} > 3 = \mathcal{A}(C_4)$, and
- $\mathcal{A}(2K_3 \cup K_1) = \frac{778}{175} > \frac{684}{154} = \mathcal{A}(K_3 \cup C_4)$.

Hence, it remains to prove that $\mathcal{A}(pK_3 \cup C_4) > \mathcal{A}((p+1)K_3 \cup K_1)$ for all $p \geq 2$. So assume $p \geq 2$ and let

$$f(p) = \mathcal{T}(pK_3 \cup C_4)\mathcal{B}((p+1)K_3 \cup K_1) - \mathcal{B}(pK_3 \cup C_4)\mathcal{T}((p+1)K_3 \cup K_1).$$

Since

$$\mathcal{A}(pK_3 \cup C_4) - \mathcal{A}((p+1)K_3 \cup K_1) = \frac{f(p)}{\mathcal{B}(pK_3 \cup C_4)\mathcal{B}((p+1)K_3 \cup K_1)},$$

we have to prove that $f(p) > 0$. Note that Equations (1) and (2) give

$$\begin{aligned}
S(G \cup C_4, k) &= S(G \cup P_4, k) - S(G \cup K_3, k) \\
&= S(G \cup Q_4, k) + S(G \cup P_3, k) - S(G \cup K_3, k) \\
&= \left(S(G \cup K_3 \cup K_1, k) - S(G \cup K_3, k) \right) \\
&\quad + \left(S(G \cup K_3, k) + S(G \cup K_2, k) \right) - S(G \cup K_3, k) \\
&= S(G \cup K_3 \cup K_1, k) - S(G \cup K_3, k) + S(G \cup K_2, k),
\end{aligned}$$

which implies

$$\begin{aligned}\mathcal{B}(G \cup C_4) &= \mathcal{B}(G \cup K_3 \cup K_1) - \mathcal{B}(G \cup K_3) + \mathcal{B}(G \cup K_2), \text{ and} \\ \mathcal{T}(G \cup C_4) &= \mathcal{T}(G \cup K_3 \cup K_1) - \mathcal{T}(G \cup K_3) + \mathcal{T}(G \cup K_2).\end{aligned}$$

Hence, with $G = pK_3$, we get

$$\begin{aligned}f(p) &= \mathcal{T}(G \cup C_4)\mathcal{B}(G \cup K_3 \cup K_1) - \mathcal{T}(G \cup K_3 \cup K_1)\mathcal{B}(G \cup C_4) \\ &= \left(\mathcal{T}(G \cup K_3 \cup K_1) - \mathcal{T}(G \cup K_3) + \mathcal{T}(G \cup K_2)\right)\mathcal{B}(G \cup K_3 \cup K_1) \\ &\quad - \mathcal{T}(G \cup K_3 \cup K_1)\left(\mathcal{B}(G \cup K_3 \cup K_1) - \mathcal{B}(G \cup K_3) + \mathcal{B}(G \cup K_2)\right) \\ &= \mathcal{B}(G \cup K_3 \cup K_1)\left(\mathcal{T}(G \cup K_2) - \mathcal{T}(G \cup K_3)\right) \\ &\quad - \mathcal{T}(G \cup K_3 \cup K_1)\left(\mathcal{B}(G \cup K_2) - \mathcal{B}(G \cup K_3)\right).\end{aligned}$$

Since $S(G, k) = 0$ for $k < 3$, we deduce from Lemmas 15 and 16 that

$$\begin{aligned}f(p) &= \sum_{k=1}^n a_k S(G, k) \sum_{k=1}^n b_k S(G, k) - \sum_{k=1}^n c_k S(G, k) \sum_{k=1}^n d_k S(G, k) \\ &= \sum_{k=3}^n \sum_{k'=3}^n (a_k b_{k'} - c_k d_{k'}) S(G, k) S(G, k') \\ &= \sum_{k=3}^n (a_k b_k - c_k d_k) S^2(G, k)\end{aligned}\tag{7}$$

$$+ \sum_{k'=3}^{n-1} \sum_{k=k'+1}^n (a_k b_{k'} - c_k d_{k'} + a_{k'} b_k - c_{k'} d_k) S(G, k) S(G, k')\tag{8}$$

where

$$\begin{aligned}a_k &= k^4 + k^3 + 5k^2 + 6k + 4, \\ b_k &= (k^3 + k^2 + 3k + 2) - (k^4 + 5k^2 + 4k + 3) \\ &= -k^4 + k^3 - 4k^2 - k - 1, \\ c_k &= k^5 + k^4 + 9k^3 + 15k^2 + 21k + 13, \text{ and} \\ d_k &= (k^2 + k + 1) - (k^3 + 2k + 1) \\ &= -k^3 + k^2 - k.\end{aligned}$$

It is therefore sufficient to prove that the sums defined at (7) and (8) are strictly positive.

- Let $g(k) = a_k b_k - c_k d_k = k^6 + k^5 - 5k^4 - 19k^3 - 19k^2 + 3k - 4$. It can be checked that $g(k) > 0$ for all $k > 3$. Note that Equation (6) gives

$$\begin{aligned}S(G, 3) &= S(pK_3, 3) = 6S((p-1)K_3, 3) \\ &< 18S(p-1)K_3, 3) + 24S((p-1)K_3, 4) \\ &= S((p)K_3, 4) = S(G, 4).\end{aligned}$$

Since $g(3) = -112$ and $g(4) = 2328$, we have $g(3)S^2(G, 3) + g(4)S^2(G, 4) > 0$, which implies

$$\sum_{k=3}^n (a_k b_k - c_k d_k) S^2(G, k) = g(3)S^2(G, 3) + g(4)S^2(G, 4) + \sum_{k=5}^n g(k)S^2(G, k) > 0.$$

Hence, the sum in (7) is strictly positive.

- Let $h(k', k) = a_k b_{k'} - c_k d_{k'} + a_{k'} b_k - c_{k'} d_k$. By definition of a_k, b_k, c_k and d_k we obtain

$$\begin{aligned} h(k', k) &= (k^3 - k^2 + k)k'^5 \\ &\quad - (2k^4 - k^3 + 10k^2 + 6k + 5)k'^4 \\ &\quad + (k^5 + k^4 + 20k^3 + 7k^2 + 35k + 16)k'^3 \\ &\quad - (k^5 + 10k^4 - 7k^3 + 70k^2 + 35k + 34)k'^2 \\ &\quad + (k^5 - 6k^4 + 35k^3 - 35k^2 + 30k + 3)k' \\ &\quad - 5k^4 + 16k^3 - 34k^2 + 3k - 8. \end{aligned}$$

Let us make a change of variable. More precisely, we substitute k' by $i + 3$ and k by $j + i + 4$. Since $k' \geq 3$ and $k \geq k' + 1$, we get $i \geq 0$ and $j \geq 0$. It is a tedious but easy exercise to check that with these new variables, $h(k', k) = h(i+3, j+i+4) = h'(i, j)$ with

$$\begin{aligned} h'(i, j) &= (j^2 + 2j + 3)i^6 + (3j^3 + 25j^2 + 47j + 63)i^5 \\ &\quad + (3j^4 + 52j^3 + 243j^2 + 437j + 533)i^4 \\ &\quad + (j^5 + 37j^4 + 338j^3 + 1154j^2 + 2017j + 2267)i^3 \\ &\quad + (8j^5 + 161j^4 + 997j^3 + 2713j^2 + 4692j + 4873)i^2 \\ &\quad + (22j^5 + 290j^4 + 1258j^3 + 2729j^2 + 4784j + 4443)i \\ &\quad + 21j^5 + 172j^4 + 440j^3 + 575j^2 + 1112j + 602. \end{aligned}$$

Since $i \geq 0, j \geq 0$, and all coefficients in $h'(i, j)$ are positive, we conclude that $h'(i, j) = h(k', k) > 0$ for $3 \leq k' < k \leq n$.

Hence, the sum $\sum_{k'=3}^{n-1} \sum_{k=k'+1}^n h(k', k) S(G, k) S(G, k')$ in (8) is strictly positive. \square

We are now ready to prove the main result of this section. Let U_n ($n \geq 3$) be the following graph.

$$U_n = \begin{cases} \frac{n}{3} K_3 & \text{if } n \bmod 3 = 0, \text{ and } n \geq 3, \\ \frac{n-1}{3} K_3 \cup K_1 & \text{if } n = 4 \text{ or } n = 7, \\ \frac{n-4}{3} K_3 \cup C_4 & \text{if } n \bmod 3 = 1, \text{ and } n \geq 10, \\ \frac{n-5}{3} K_3 \cup C_5 & \text{if } n \bmod 3 = 2, \text{ and } n \geq 5. \end{cases}$$

Theorem 18. If G is a graph of order $n \geq 3$ and maximum degree $\Delta(G) = 2$, then,

$$\mathcal{A}(G) \leq \mathcal{A}(U_n),$$

with equality if and only if $G \simeq U_n$.

Proof. Since $\Delta(G) = 2$, G is a disjoint union of cycles and paths. Now, suppose that G maximizes \mathcal{A} among all graphs of maximum degree 2. Then at most one connected component of G is a path. Indeed, if $G \simeq G' \cup P_k \cup P_{k'}$, then Equations (3) and (4) give $\mathcal{B}(G' \cup P_k \cup P_{k'}) = \mathcal{B}(G' \cup P_{k+k'}) + \mathcal{B}(G' \cup P_{k+k'-1})$ and $\mathcal{T}(G' \cup P_k \cup P_{k'}) = \mathcal{T}(G' \cup P_{k+k'}) + \mathcal{T}(G' \cup P_{k+k'-1})$. Moreover, we know from Proposition 1 that $\mathcal{A}(G' \cup P_{k+k'-1}) < \mathcal{A}(G' \cup P_{k+k'})$. Hence, Proposition 3 implies that $\mathcal{A}(G) = \mathcal{A}(G' \cup P_k \cup P_{k'}) < \mathcal{A}(G' \cup P_{k+k'})$. Since $(G' \cup P_{k+k'})$ is of order n and maximum degree 2, this contradicts the hypothesis that G maximizes \mathcal{A} .

We know from Lemma 4 that replacing a path P_k of order $k \geq 3$ by a cycle C_k strictly increases $\mathcal{A}(G)$. Moreover, Lemma 14 shows that replacing a cycle C_k of order $k \geq 6$ by $C_{k-3} \cup K_3$ increases $\mathcal{A}(G)$. Hence G is a disjoint union of copies of K_3, C_4 and C_5 and eventually one path that is either K_1 or K_2 .

Considering Lemma 5, we know from (d), (e) and (f) that G does not contain K_2 , and from (g)-(k) that at most one connected component of G is not a K_3 . Hence, if $n \bmod 3 = 0$ then $G \simeq \frac{n}{3} K_3$ and if $n \bmod 3 = 2$ then $G \simeq \frac{n-5}{3} K_3 \cup C_5$. Finally, Theorem 17 shows that $G \simeq \frac{n-1}{3} K_3 \cup K_1$ if $n = 4$ or 7 , and $G \simeq \frac{n-4}{3} K_3 \cup C_4$ if $n \bmod 3 = 1$ and $n \geq 10$. \square

5 Concluding remarks

We have given a general upper bound on $\mathcal{A}(G)$ that is valid for all graphs G , and a more precise one for graphs of order n and maximum degree $\Delta(G) \in \{1, 2, n-2\}$. Note that there is no known lower bound on $\mathcal{A}(G)$ which is a function of n and such that there exists at least one graph of order n which reaches it.

The problem of finding a tight upper bound for graphs with maximum degree in $\{3, \dots, n-3\}$ remains open. Since all graphs of order n and maximum degree $\Delta(G) \in \{1, n-2, n-1\}$ that maximize $\mathcal{A}(G)$ are isomorphic to $\left\lfloor \frac{n}{\Delta(G)+1} \right\rfloor K_{\Delta(G)+1} \cup K_{n \bmod (\Delta(G)+1)}$ (but this is not always true for $\Delta(G) = 2$), one could be tempted to think that this is also true when $3 \leq \Delta(G) \leq n-3$. We have checked this statement by enumerating all graphs having up to 11 vertices, using *PHOEG* [2]. We have thus determined that there is only one graph of order $n \leq 11$ and $\Delta(G) \neq 2$ (among more than a billion), namely $\overline{C}_6 \cup K_4$, for which such a statement is wrong. Indeed, $\mathcal{A}(\overline{C}_6 \cup K_4) = 5.979 > 5.967 = \mathcal{A}(2K_4 \cup K_2)$, which shows that $2K_4 \cup K_2$ does not maximize $\mathcal{A}(G)$ among all graphs of order 10 and maximum degree 3.

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