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ORIGINAL PAPER

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 numbers

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, 5–7, 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).

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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 $\mathsf{A}_n = \frac{\mathsf{T}_n}{\mathsf{B}_n}$. 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, $\mathcal{A}(G) = \mathsf{A}_n$ 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 exactly 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 and summarize our contributions. Section 3 is devoted to properties of $\mathcal{A}(G)$ and basic ingredients that we will use in Sect. 4 for proving the validity of the upper bounds on $\mathcal{A}(G)$.

2 Notation and Summary of Contributions

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 $\overline{\mathsf{K}}_n$) 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, and pG is the disjoint union of p copies of G.

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. Given two vertices u and v in a graph G, we use the following notations:

- $G_{|uv}$ is the graph 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* χ(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

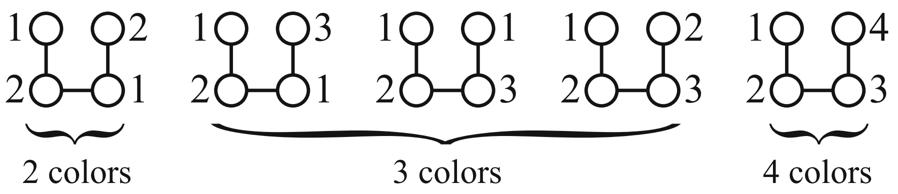

Fig. 1 The non-equivalent colorings of P_4

$\mathcal{B}(G)$ 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 Fig. 1, there are one non-equivalent coloring of P_4 with 2 colors, three with 3 colors, and one with 4 colors, which gives $\mathcal{B}(\mathsf{P}_4) = 5$, $\mathcal{T}(\mathsf{P}_4) = 15$ and $\mathcal{A}(\mathsf{P}_4) = \frac{15}{5} = 3$.

The aim of this paper is to determine a general upper bound on $\mathcal{A}(G)$ that is valid for all graphs G and a sharper one for graphs G of order n and maximum degree $\Delta(G) \in \{1, 2, n-2\}$. More precisely, given a graph G of order n, we show that

- $\mathcal{A}(G) \leq n$, with equality if and only if $G \simeq \mathsf{K}_n$;
- if $\Delta(G) = n-2$ then $\mathcal{A}(G) \leq \frac{n^2-n+1}{n}$, with equality if and only if $G \simeq \mathsf{K}_{n-1} \cup \mathsf{K}_1$;
- if $\Delta(G) = 1$ then $\mathcal{A}(G) \leq \mathcal{A}(\lfloor\frac{n}{2}\rfloor\mathsf{K}_2 \cup (n \bmod 2)\mathsf{K}_1)$, with equality if and only if $G \simeq \lfloor\frac{n}{2}\rfloor\mathsf{K}_2 \cup (n \bmod 2)\mathsf{K}_1$;
- if $\Delta(G) = 2$ then $\mathcal{A}(G) \leq \mathcal{A}(\mathsf{U}_n)$, with equality if and only if $G \simeq \mathsf{U}_n$, where

$$\mathsf{U}_n = \begin{cases} \frac{n}{3}\mathsf{K}_3 & \text{if } n \bmod 3 = 0, \text{ and } n \geq 3, \\ \frac{n-1}{3}\mathsf{K}_3 \cup \mathsf{K}_1 & \text{if } n = 4 \text{ or } n = 7, \\ \frac{n-4}{3}\mathsf{K}_3 \cup \mathsf{C}_4 & \text{if } n \bmod 3 = 1, \text{ and } n \geq 10, \\ \frac{n-5}{3}\mathsf{K}_3 \cup \mathsf{C}_5 & \text{if } n \bmod 3 = 2, \text{ and } n \geq 5. \end{cases}$$

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

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

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

It follows that

$$\left.\begin{array}{l} \mathcal{B}(G) = \mathcal{B}(G-uv) - \mathcal{B}(G_{|uv}) \\ \mathcal{T}(G) = \mathcal{T}(G-uv) - \mathcal{T}(G_{|uv}) \end{array}\right\} \quad \forall uv \in E(G), \tag{3}$$

$$\left.\begin{array}{l} \mathcal{B}(G) = \mathcal{B}(G+uv) + \mathcal{B}(G_{|uv}) \\ \mathcal{T}(G) = \mathcal{T}(G+uv) + \mathcal{T}(G_{|uv}) \end{array}\right\} \quad \forall uv \notin E(G). \tag{4}$$

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 Sect. 4.

Proposition 1 *([10]) Let v be a simplicial vertex in a graph G. Then $\mathcal{A}(G) > \mathcal{A}(G-v)$.*

Proposition 2 *([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 3 *([10]) $\mathcal{A}(G \cup C_n) > \mathcal{A}(G \cup P_n)$ for all $n \geq 3$ and all graphs G.*

Proposition 4 *([8]) Let G, H and $F_1, \ldots, F_r$ be $r+2$ graphs, and let $\alpha_1, \ldots, \alpha_r$ 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* $i = 1, \ldots, r$.

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

Given two graphs H_1 and H_2, we now give a sufficient condition for $\mathcal{A}(G \cup H_1)$ to be strictly larger than $\mathcal{A}(G \cup H_2)$ for all graphs G.

Proposition 5 *Let H_1 and H_2 be any two graphs such that $S(H_1,k)S(H_2,k') \geq S(H_2,k)S(H_1,k')$ 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.*

Proof We first prove that $\mathcal{B}(G\cup H)=\sum_{k=1}^{n}S(H,k)\mathcal{B}(G\cup \mathsf{K}_k)$ for all graphs H of order n. This is clearly true for $n=1$. For larger values of n we proceed by double induction on the order n and the size m of H.

- If $m=\frac{n(n-1)}{2}$, then $H\simeq \mathsf{K}_n$. Since $S(\mathsf{K}_n,i)=0$ for $i=1,\dots,n-1$ and $S(\mathsf{K}_n,n)=1$, we have $\mathcal{B}(G\cup \mathsf{K}_n)=\sum_{k=1}^{n}S(\mathsf{K}_n,k)\mathcal{B}(G\cup \mathsf{K}_n)$.
- If $m<\frac{n(n-1)}{2}$, then H contains two non-adjacent vertices u and v and we know from Eq. (4) that $\mathcal{B}(G\cup H)=\mathcal{B}(G\cup(H+uv))+\mathcal{B}(G\cup H_{|uv})$. Since $H+uv$ has order n and size $m+1$ and $H_{|uv}$ has order $n-1$, we know by induction that

$$\begin{aligned}\mathcal{B}(G\cup H)&=\sum_{k=1}^{n}S(H+uv,k)\mathcal{B}(G\cup \mathsf{K}_k)+\sum_{k=1}^{n-1}S(H_{|uv},k)\mathcal{B}(G\cup \mathsf{K}_k)\\&=\sum_{k=1}^{n}\big(S(H+uv,k)+S(H_{|uv},k)\big)\mathcal{B}(G\cup \mathsf{K}_k)\\&=\sum_{k=1}^{n}S(H,k)\mathcal{B}(G\cup \mathsf{K}_k).\end{aligned}$$

A similar proof shows that $\mathcal{T}(G\cup H)=\sum_{k=1}^{n}S(H,k)\mathcal{T}(G\cup \mathsf{K}_k)$ for all graphs H of order n. Now let $f(k,k')=S(H_1,k)S(H_2,k')-S(H_2,k)S(H_1,k')$ and assume that H_1 and H_2 are of order n_1 and n_2, respectively. Note that $n_1\geq n_2$ else we would have $n_2>n_1$ and $f(n_2,n_1)=S(H_1,n_2)S(H_2,n_1)-S(H_2,n_2)S(H_1,n_1)=-1<0$. Now,

$$\begin{aligned}\mathcal{A}(G\cup H_1)-\mathcal{A}(G\cup H_2)&=\frac{\sum_{k=1}^{n_1}S(H_1,k)\mathcal{T}(G\cup \mathsf{K}_k)}{\sum_{k=1}^{n_1}S(H_1,k)\mathcal{B}(G\cup \mathsf{K}_k)}-\frac{\sum_{k=1}^{n_2}S(H_2,k)\mathcal{T}(G\cup \mathsf{K}_k)}{\sum_{k=1}^{n_2}S(H_2,k)\mathcal{B}(G\cup \mathsf{K}_k)}\\&=\frac{\sum_{k=1}^{n_1}\sum_{k'=1}^{n_1}f(k,k')\mathcal{T}(G\cup \mathsf{K}_k)\mathcal{B}(G\cup \mathsf{K}_{k'})}{\mathcal{B}(G\cup H_1)\mathcal{B}(G\cup H_2)}.\end{aligned}$$

Since $f(k,k)=0$ for all k and $f(k,k')=-f(k',k)$ for all $k\neq k'$, we deduce

$$\begin{aligned}&\mathcal{A}(G\cup H_1)-\mathcal{A}(G\cup H_2)\\&=\frac{\sum_{k'=1}^{n_1-1}\sum_{k=k'+1}^{n_1}f(k,k')\Big(\mathcal{T}(G\cup \mathsf{K}_k)\mathcal{B}(G\cup \mathsf{K}_{k'})-\mathcal{T}(G\cup \mathsf{K}_{k'})\mathcal{B}(G\cup \mathsf{K}_k)\Big)}{\mathcal{B}(G\cup H_1)\mathcal{B}(G\cup H_2)}.\end{aligned}$$

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

k	2	3	4	5	6	7	8	9	10
$S(\mathsf{C}_3 \cup \mathsf{K}_2, k)$	0	6	6	1					
$S(\mathsf{C}_4 \cup \mathsf{K}_1, k)$	2	7	6	1					
$S(\mathsf{C}_5, k)$	0	5	5	1					
$S(2\mathsf{C}_3, k)$	0	6	18	9	1				
$S(\mathsf{C}_4 \cup \mathsf{K}_2, k)$	2	16	25	10	1				
$S(\mathsf{C}_5 \cup \mathsf{K}_1, k)$	0	15	25	10	1				
$S(\mathsf{C}_6, k)$	1	10	20	9	1				
$S(\mathsf{C}_3 \cup \mathsf{C}_4, k)$	0	18	66	55	14	1			
$S(\mathsf{C}_5 \cup \mathsf{K}_2, k)$	0	30	90	65	15	1			
$S(\mathsf{C}_7, k)$	0	21	70	56	14	1			
$S(\mathsf{C}_3 \cup \mathsf{C}_5, k)$	0	30	210	285	125	20	1		
$S(2\mathsf{C}_4, k)$	2	52	241	296	126	20	1		
$S(\mathsf{C}_8, k)$	1	42	231	294	126	20	1		
$S(3\mathsf{C}_3, k)$	0	36	540	1242	882	243	27	1	
$S(\mathsf{C}_3 \cup \mathsf{C}_6, k)$	0	66	666	1351	910	245	27	1	
$S(\mathsf{C}_4 \cup \mathsf{C}_5, k)$	0	90	750	1415	925	246	27	1	
$S(\mathsf{C}_9, k)$	0	85	735	1407	924	246	27	1	
$S(2\mathsf{C}_3 \cup \mathsf{C}_4, k)$	0	108	1908	5838	5790	2361	433	35	1
$S(2\mathsf{C}_5, k)$	0	150	2250	6345	6025	2400	435	35	1

Note that if $k > k'$, then $G \cup \mathsf{K}_k$ is obtained from $G \cup \mathsf{K}_{k'}$ by repeatedly adding a simplicial vertex. Hence, we know from Proposition 1 that

$$\begin{aligned} &\mathcal{A}(G \cup \mathsf{K}_k) > \mathcal{A}(G \cup \mathsf{K}_{k'}) \\ &\quad \iff \frac{\mathcal{T}(G \cup \mathsf{K}_k)}{\mathcal{B}(G \cup \mathsf{K}_k)} > \frac{\mathcal{T}(G \cup \mathsf{K}_{k'})}{\mathcal{B}(G \cup \mathsf{K}_{k'})} \\ &\quad \iff \mathcal{T}(G \cup \mathsf{K}_k)\mathcal{B}(G \cup \mathsf{K}_{k'}) - \mathcal{T}(G \cup \mathsf{K}_{k'})\mathcal{B}(G \cup \mathsf{K}_k) > 0. \end{aligned}$$

Since $f(k,k') = S(H_1,k)S(H_2,k') - S(H_1,k')S(H_2,k)$ is positive for all $k > k'$, and strictly positive for at least one such pair, we have $\mathcal{A}(G \cup H_1) - \mathcal{A}(G \cup H_2) > 0$. □

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

Lemma 6 *The following strict inequalities are valid for all graphs G:*

(a) $\mathcal{A}(G \cup \mathrm{C}_6) < \mathcal{A}(G \cup 2\mathrm{C}_3)$ (b) $\mathcal{A}(G \cup \mathrm{C}_7) < \mathcal{A}(G \cup \mathrm{C}_3 \cup \mathrm{C}_4)$
(c) $\mathcal{A}(G \cup \mathrm{C}_8) < \mathcal{A}(G \cup \mathrm{C}_3 \cup \mathrm{C}_5)$ (d) $\mathcal{A}(G \cup \mathrm{C}_3 \cup \mathrm{K}_2) < \mathcal{A}(G \cup \mathrm{C}_5)$
(e) $\mathcal{A}(G \cup \mathrm{C}_4 \cup \mathrm{K}_2) < \mathcal{A}(G \cup 2\mathrm{C}_3)$ (f) $\mathcal{A}(G \cup \mathrm{C}_5 \cup \mathrm{K}_2) < \mathcal{A}(G \cup \mathrm{C}_3 \cup \mathrm{C}_4)$
(g) $\mathcal{A}(G \cup \mathrm{C}_4 \cup \mathrm{K}_1) < \mathcal{A}(G \cup \mathrm{C}_5)$ (h) $\mathcal{A}(G \cup \mathrm{C}_5 \cup \mathrm{K}_1) < \mathcal{A}(G \cup 2\mathrm{C}_3)$
(i) $\mathcal{A}(G \cup 2\mathrm{C}_4) < \mathcal{A}(G \cup \mathrm{C}_3 \cup \mathrm{C}_5)$ (j) $\mathcal{A}(G \cup \mathrm{C}_4 \cup \mathrm{C}_5) < \mathcal{A}(G \cup 3\mathrm{C}_3)$
(k) $\mathcal{A}(G \cup 2\mathrm{C}_5) < \mathcal{A}(G \cup 2\mathrm{C}_3 \cup \mathrm{C}_4)$.

Proof All these inequalities can be obtained from Proposition 5 by using the values given in Table 1. For example, to check that (a) holds, the 4^{th} and 7^{th} lines of Table 1 allow to check that $S(2\mathrm{C}_3, k)S(\mathrm{C}_6, k') - S(\mathrm{C}_6, k)S(2\mathrm{C}_3, k') \geq 0$ for all $k > k'$ and at least one of these values is strictly positive. □

We now show the validity of four lemmas which will be helpful for proving that $\mathcal{A}(G \cup \mathrm{C}_n) < \mathcal{A}(G \cup \mathrm{C}_{n-3} \cup \mathrm{C}_3)$ 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 7 $S(\mathrm{C}_n, k) = (k-1)S(\mathrm{C}_{n-1}, k) + S(\mathrm{C}_{n-1}, k-1)$ *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
$S(\mathrm{C}_4, k)$	1	2	1
$S(\mathrm{C}_3, k)$	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 $(k-1)S(\mathrm{C}_{n-2}, k)$ such colorings where v and w have the same color and at least one vertex of $\mathrm{C}_n - u$ has the same color as u;
- There are $S(\mathrm{C}_{n-2}, k-1)$ such colorings where v and w have the same color and no vertex on $\mathrm{C}_n - u$ has the same color as u;
- There are $(k-2)S(\mathrm{C}_{n-1}, k)$ such colorings where v and w have different colors and at least one vertex of $\mathrm{C}_n - u$ has the same color as u;
- There are $S(\mathrm{C}_{n-1}, k-1)$ such colorings where v and w have different colors and no vertex on $\mathrm{C}_n - u$ has the same color as u.

Hence,

$$\begin{aligned} S(\mathrm{C}_n, k) &= \Big((k-1)S(\mathrm{C}_{n-2}, k) + S(\mathrm{C}_{n-2}, k-1)\Big) \\ &\quad + (k-2)S(\mathrm{C}_{n-1}, k) + S(\mathrm{C}_{n-1}, k-1) \\ &= S(\mathrm{C}_{n-1}, k) + (k-2)S(\mathrm{C}_{n-1}, k) + S(\mathrm{C}_{n-1}, k-1) \\ &= (k-1)S(\mathrm{C}_{n-1}, k) + S(\mathrm{C}_{n-1}, k-1). \end{aligned}$$

□

Lemma 8 *If $n \geq 7$ and $k \leq n$ then*

$$S(\mathrm{C}_{n-3} \cup \mathrm{C}_3, k) = (k-1)S(\mathrm{C}_{n-4} \cup \mathrm{C}_3, k) + S(\mathrm{C}_{n-4} \cup \mathrm{C}_3, k-1) - (-1)^n \delta_k$$

where

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

Proof The values in Table 1 show that the result is true for $n = 7$. 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 $\mathrm{C}_{n-3} \cup \mathrm{C}_3$ that use exactly k colors:

- There are $(k-1)S(\mathrm{C}_{n-5} \cup \mathrm{C}_3, k)$ such colorings where v and w have the same color and at least one vertex of $\mathrm{C}_{n-3} \cup \mathrm{C}_3 - u$ has the same color as u;
- There are $S(\mathrm{C}_{n-5} \cup \mathrm{C}_3, k-1)$ such colorings where v and w have the same color and no vertex on $\mathrm{C}_{n-3} \cup \mathrm{C}_3 - u$ has the same color as u;
- There are $(k-2)S(\mathrm{C}_{n-4} \cup \mathrm{C}_3, k)$ such colorings where v and w have different colors and at least one vertex of $\mathrm{C}_{n-3} \cup \mathrm{C}_3 - u$ has the same color as u;
- There are $S(\mathrm{C}_{n-4} \cup \mathrm{C}_3, k-1)$ such colorings where v and w have different colors and no vertex on $\mathrm{C}_{n-3} \cup \mathrm{C}_3 - u$ has the same color as u.

Hence,

$$\begin{aligned} S(\mathsf{C}_{n-3} \cup \mathsf{C}_3, k) &= \Big((k-1)S(\mathsf{C}_{n-5} \cup \mathsf{C}_3, k) + S(\mathsf{C}_{n-5} \cup \mathsf{C}_3, k-1)\Big) \\ &\quad + (k-2)S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k) + S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k-1) \\ &= \Big(S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k) + (-1)^{n-1}\delta_k\Big) \\ &\quad + (k-2)S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k) + S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k-1) \\ &= (k-1)S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k) + S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k-1) - (-1)^n \delta_k. \end{aligned}$$

□

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 9 *If $n \geq 6$ and $k \leq n$ then $S(\mathrm{C}_{n-3} \cup \mathrm{C}_3, k) = S(\mathrm{Q}_n, k) - (-1)^n \rho_k$ where*

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

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

k	2	3	4	5	6
$S(2\mathsf{C}_3, k)$	0	6	18	9	1
$S(\mathsf{Q}_6, k)$	0	8	19	9	1

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

$$\begin{aligned} &S(\mathsf{C}_{n-3} \cup \mathsf{C}_3, k) \\ &\quad = S(\mathsf{P}_{n-3} \cup \mathsf{C}_3, k) - S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k) \\ &\quad = S(\mathsf{P}_{n-3} \cup \mathsf{P}_3, k) - S(\mathsf{P}_{n-3} \cup \mathsf{P}_2, k) - S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k) \\ &\quad = S(\mathsf{P}_n, k) + S(\mathsf{P}_{n-1}, k) - S(\mathsf{P}_{n-1}, k) - S(\mathsf{P}_{n-2}, k) - S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k) \\ &\quad = S(\mathsf{Q}_n, k) + S(\mathsf{Q}_{n-1}, k) - S(\mathsf{C}_{n-4} \cup \mathsf{C}_3, k) \\ &\quad = S(\mathsf{Q}_n, k) - (-1)^n \rho_k. \end{aligned}$$

□

Lemma 10 *The following inequalities are valid for all $n \geq 9$:*

(a) $S(\mathsf{C}_n, k) > S(\mathsf{C}_n, k-1)$ *for all* $k \in \{3, 4, 5\}$*;*
(b) $S(\mathsf{C}_n, k) > 3S(\mathsf{C}_{n-1}, k-1)$ *for all* $k \in \{3, 4, 5, 6\}$*;*
(c) $S(\mathsf{C}_n, 4) > 8S(\mathsf{C}_n, 3)$.

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 $S(\mathsf{C}_n, 3) > 3 \geq \max\{S(\mathsf{C}_n, 2)), 3S(\mathsf{C}_{n-1}, 2)\}$. We may therefore assume $k \in \{4, 5\}$ for (a) and $k \in \{4, 5, 6\}$ for (b). Lemma 7 and the induction hypothesis imply

$$\begin{aligned} S(\mathsf{C}_n, k) &= (k-1)S(\mathsf{C}_{n-1}, k) + S(\mathsf{C}_{n-1}, k-1) \\ &> (k-2)S(\mathsf{C}_{n-1}, k-1) + S(\mathsf{C}_{n-1}, k-2) \\ &= S(\mathsf{C}_n, k-1). \end{aligned}$$

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

$$\begin{aligned} \frac{1}{k-1} S(\mathsf{C}_{n-1}, k-1) &= \frac{1}{k-1}\Big((k-2)S(\mathsf{C}_{n-2}, k-1) + S(\mathsf{C}_{n-2}, k-2)\Big) \\ &< \frac{1}{k-1}\Big((k-1)S(\mathsf{C}_{n-2}, k-1)\Big) \\ &= S(\mathsf{C}_{n-2}, k-1) \end{aligned}$$

which implies

$$\begin{aligned} S(\mathsf{C}_n, k) &= (k-1)S(\mathsf{C}_{n-1}, k) + S(\mathsf{C}_{n-1}, k-1) \\ &> (k-1)S(\mathsf{C}_{n-1}, k) \\ &> 3(k-1)S(\mathsf{C}_{n-2}, k-1) \\ &> 3S(\mathsf{C}_{n-1}, k-1). \end{aligned}$$

Hence (b) is proved. We thus have

$$\begin{aligned} S(\mathsf{C}_n, 4) &= 3S(\mathsf{C}_{n-1}, 4) + S(\mathsf{C}_{n-1}, 3) \\ &> 25S(\mathsf{C}_{n-1}, 3) \\ &> \frac{25}{3}S(\mathsf{C}_n, 3) \\ &> 8S(\mathsf{C}_n, 3) \end{aligned}$$

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 11 *Let G be a graph of order n, then,*

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

with equality if and only if $G \simeq \mathsf{K}_n$.

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 $G \simeq \mathsf{K}_n$. □

Since $\Delta(\mathsf{K}_n) = n - 1$ we immediately get the following corollary to Theorem 11.

Corollary 12 *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* $G \simeq \mathrm{K}_n$.

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 13 *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 $G \simeq \mathrm{K}_{n-1} \cup \mathrm{K}_1$.

Proof We have

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

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 $\mathsf{K}_{n-1} \cup \mathsf{K}_1$ when $n \neq 4$, and G is isomorphic to $\mathsf{K}_3 \cup \mathsf{K}_1$ or C_4 when $n = 4$. Since $S(\mathsf{C}_4, 2) = 1 > 0$ while $S(\mathsf{K}_{n-1} \cup \mathsf{K}_1, k) = 0$ 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 $G \simeq \mathsf{K}_{n-1} \cup \mathsf{K}_1$. □

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

Theorem 14 *Let G be a graph of order n and maximum degree $\Delta(G) = 1$. Then,*

$$\mathcal{A}(G) \leq \mathcal{A}(\lfloor \frac{n}{2} \rfloor \mathrm{K}_2 \cup (n \bmod 2)\mathrm{K}_1)$$

with equality if and only if $G \simeq \lfloor \frac{n}{2} \rfloor \mathrm{K}_2 \cup (n \bmod 2)\mathrm{K}_1$.

Proof If G contains two isolated vertices u and v, we know from Proposition 2 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 $G \simeq \lfloor \frac{n}{2} \rfloor \mathsf{K}_2 \cup (n \bmod 2)\mathsf{K}_1$. □

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 $\mathsf{C}_{n-3} \cup \mathsf{C}_3$.

Lemma 15 $\mathcal{A}(G \cup \mathrm{C}_n) < \mathcal{A}(G \cup \mathrm{C}_{n-3} \cup \mathrm{C}_3)$ *for all $n \geq 6$ and all graphs G.*

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

Let $f_n(k,k') = S(\mathrm{C}_{n-3} \cup \mathrm{C}_3, k)S(\mathrm{C}_n, k') - S(\mathrm{C}_n, k)S(\mathrm{C}_{n-3} \cup \mathrm{C}_3, k')$. Proposition 5 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 7 and 8:

$$\begin{aligned} f_n(n,3) &= S(\mathsf{C}_n,3) - S(\mathsf{C}_{n-3} \cup \mathsf{C}_3,3) \\ &= \Big(2S(\mathsf{C}_{n-1},3)+1\Big) - \Big(2S(\mathsf{C}_{n-4} \cup \mathsf{C}_3,3)+6\Big) \\ &= \Big(4S(\mathsf{C}_{n-2},3)+1\Big) - \Big(2\big(2S(\mathsf{C}_{n-5} \cup \mathsf{C}_3,3)-6\big)+6\Big) \\ &= 4S(\mathsf{C}_{n-2},3) - 4S(\mathsf{C}_{n-5} \cup \mathsf{C}_3,3)+7 \\ &= 4f_{n-2}(n-2,3)+7 > 0. \end{aligned}$$

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 where $k \geq n-1$.

- If $k' \leq 2$ then $f_n(k,k') = S(\mathsf{C}_{n-3} \cup \mathsf{C}_3, k)S(\mathsf{C}_n, k') \geq 0$.
- If $k \geq n-1$ then $S(\mathsf{C}_n, k) = S(\mathsf{C}_{n-3} \cup \mathsf{C}_3, k)$ since
  - $S(\mathsf{C}_n, n) = S(\mathsf{C}_{n-3} \cup \mathsf{C}_3, n) = 1$, and
  - $S(\mathsf{C}_n, n-1) = S(\mathsf{C}_{n-3} \cup \mathsf{C}_3, n-1) = \frac{n^2-3n}{2}$.

  Also, it follows from Lemma 9 that $S(\mathsf{C}_{n-3} \cup \mathsf{C}_3, k') = S(\mathsf{Q}_n, k') - (-1)^n \rho_{k'}$ and Eqs. (1) and (2) give

$$\begin{aligned} S(\mathsf{C}_n,k') &= S(\mathsf{P}_n,k') - S(\mathsf{C}_{n-1},k') \\ &= \big(S(\mathsf{Q}_n,k') + S(\mathsf{P}_{n-1},k')\big) - \big(S(\mathsf{P}_{n-1},k') - S(\mathsf{C}_{n-2},k')\big) \\ &= S(\mathsf{Q}_n,k') + S(\mathsf{C}_{n-2},k'). \end{aligned}$$

  Altogether, this gives

$$\begin{aligned} f_n(k,k') &= S(\mathsf{C}_n,k)\Big(S(\mathsf{C}_n,k') - S(\mathsf{C}_{n-3} \cup \mathsf{C}_3,k')\Big) \\ &= S(\mathsf{C}_n,k)\Big(\big(S(\mathsf{Q}_n,k') + S(\mathsf{C}_{n-2},k')\big) - \big(S(\mathsf{Q}_n,k') - (-1)^n \rho_{k'}\big)\Big) \\ &= S(\mathsf{C}_n,k)\Big(S(\mathsf{C}_{n-2},k') + (-1)^n \rho_{k'}\Big). \end{aligned}$$

  Hence,

  - if n is even then $f_n(k,k') \geq 0$;
  - if n is odd and $k' \notin \{3,4\}$ then $f_n(k,k') \geq 0$;
  - if n is odd and $k' = 3$ then $f_n(k,k') = S(\mathsf{C}_n,k)(S(\mathsf{C}_{n-2},3)-2) \geq 0$;
  - if n is odd and $k' = 4$ then $f_n(k,k') = S(\mathsf{C}_n,k)(S(\mathsf{C}_{n-2},4)-1) \geq 0$.

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

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

The values in the following table, computed with the help of those for C_9 and $\mathsf{C}_6 \cup \mathsf{C}_3$ 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
$7S(\mathsf{C}_9, k)$	5145	9849	9849	6468	6468	6468	1722	1722	1722	1722

For larger values of n, we proceed by induction. Lemmas 7 and 8 give

$$\begin{aligned}
f_n(k,k') &= S(\mathsf{C}_n,k')S(\mathsf{C}_{n-3}\cup\mathsf{C}_3,k) - S(\mathsf{C}_n,k)S(\mathsf{C}_{n-3}\cup\mathsf{C}_3,k') \\
&= S(\mathsf{C}_n,k')\Big((k-1)S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k)+S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k-1)-(-1)^n\delta_k\Big) \\
&\quad -S(\mathsf{C}_n,k)\Big((k'-1)S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k')+S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k'-1)-(-1)^n\delta_{k'}\Big) \\
&= \Big((k'-1)S(\mathsf{C}_{n-1},k')+S(\mathsf{C}_{n-1},k'-1)\Big)\Big((k-1)S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k)+S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k-1)\Big) \\
&\quad -\Big((k-1)S(\mathsf{C}_{n-1},k)+S(\mathsf{C}_{n-1},k-1)\Big)\Big((k'-1)S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k')+S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k'-1)\Big) \\
&\quad +(-1)^n\delta_{k'}S(\mathsf{C}_n,k)-(-1)^n\delta_k S(\mathsf{C}_n,k') \\
&= (k-1)(k'-1)\Big(S(\mathsf{C}_{n-1},k')S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k)-S(\mathsf{C}_{n-1},k)S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k')\Big) \qquad (5)\\
&\quad +(k'-1)\Big(S(\mathsf{C}_{n-1},k')S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k-1)-S(\mathsf{C}_{n-1},k-1)S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k')\Big) \\
&\quad +(k-1)\Big(S(\mathsf{C}_{n-1},k'-1)S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k)-S(\mathsf{C}_{n-1},k)S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k'-1)\Big) \\
&\quad +S(\mathsf{C}_{n-1},k'-1)S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k-1)-S(\mathsf{C}_{n-1},k-1)S(\mathsf{C}_{n-4}\cup\mathsf{C}_3,k'-1) \\
&\quad +(-1)^n\delta_{k'}S(\mathsf{C}_n,k)-(-1)^n\delta_k S(\mathsf{C}_n,k') \\
&= (k-1)(k'-1)f_{n-1}(k,k')+(k'-1)f_{n-1}(k-1,k') \\
&\quad +(k-1)f_{n-1}(k,k'-1)+f_{n-1}(k-1,k'-1) \\
&\quad +(-1)^n\delta_{k'}S(\mathsf{C}_n,k)-(-1)^n\delta_k S(\mathsf{C}_n,k').
\end{aligned}$$

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 $f_n(k, k') \geq 7S(\mathsf{C}_n, k)$ for $k' \in \{3, 4, 5\}$. Let $g_n(k, k') = (-1)^n\delta_{k'}S(\mathsf{C}_n, k) - (-1)^n\delta_k S(\mathsf{C}_n, k')$. There are 4 possible cases.

- *Case 1:* $k' \in \{4, 5\}$ *and* $k \geq k' + 2$.
  We have $g_n(k, k') = (-1)^n\delta_{k'}S(\mathsf{C}_n, k) \geq -6S(\mathsf{C}_n, k)$. Using the induction hypothesis and Lemma 7, Eq. (5) gives

$$\begin{aligned}
f_n(k,k') &\geq \Big(7(k-1)(k'-1)S(\mathsf{C}_{n-1},k)+7(k'-1)S(\mathsf{C}_{n-1},k-1)\Big) \\
&\qquad + \Big(7(k-1)S(\mathsf{C}_{n-1},k)+7S(\mathsf{C}_{n-1},k-1)\Big)-6S(\mathsf{C}_n,k) \\
&= 7(k'-1)S(\mathsf{C}_n,k)+7S(\mathsf{C}_n,k)-6S(\mathsf{C}_n,k) \\
&> 7S(\mathsf{C}_n,k).
\end{aligned}$$

- *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 $g_n(k, k') \geq -S(\mathsf{C}_n, 4)$, and we deduce from Lemma 10 (a) that $g_n(k, k') \geq -S(\mathsf{C}_n, 5)$;
  - if n is odd, then $g_n(k, k') \geq -\delta_{k'} S(\mathsf{C}_n, k) \geq -6S(\mathsf{C}_n, k)$.

  Hence, whatever n and (k, k'), $g_n(k, k') \geq -6S(\mathsf{C}_n, k)$. Since $f_{n-1}(k-1, k') = 0$, using again the induction hypothesis and Lemma 7, we deduce from Eq. (5) that

$$\begin{aligned} f_n(k, k') \geq& \Big(7(k-1)(k'-1)S(\mathsf{C}_{n-1}, k)\Big) + \Big(7(k-1)S(\mathsf{C}_{n-1}, k) + 7S(\mathsf{C}_{n-1}, k-1)\Big) - 6S(\mathsf{C}_n, k) \\ &= \Big(7(k'-1)S(\mathsf{C}_n, k) - 7(k'-1)S(\mathsf{C}_{n-1}, k-1)\Big) + \Big(7S(\mathsf{C}_n, k)\Big) - 6S(\mathsf{C}_n, k) \\ &= (7k'-6)S(\mathsf{C}_n, k) - 7(k'-1)S(\mathsf{C}_{n-1}, k-1). \end{aligned}$$

  Since $k \leq 6$, Lemma 10 (b) shows that $S(\mathsf{C}_{n-1}, k-1) \leq \frac{1}{3} S(\mathsf{C}_n, k)$ and we therefore have

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

- *Case 3:* $k' = 3$ *and* $k \geq 5$.
  As in the previous case, we have $g_n(k, k') \geq -6S(\mathsf{C}_n, k)$. The induction hypothesis gives $f_{n-1}(k, k') \geq 7S(\mathsf{C}_{n-1}, k)$, $f_{n-1}(k-1, k') \geq 7S(\mathsf{C}_{n-1}, k-1)$, $f_{n-1}(k, k'-1) \geq 0$, and $f_{n-1}(k-1, k'-1) \geq 0$. Hence, Eq. (5) becomes

$$\begin{aligned} f_n(k, k') \geq& 7(k-1)(k'-1)S(\mathsf{C}_{n-1}, k) + 7(k'-1)S(\mathsf{C}_{n-1}, k-1) - 6S(\mathsf{C}_n, k) \\ &= 7(k'-1)S(\mathsf{C}_n, k) - 6S(\mathsf{C}_n, k) \\ &> 7S(\mathsf{C}_n, k). \end{aligned}$$

- *Case 4:* $k' = 3$ *and* $k = 4$.
  We have $g_n(k, k') = (-1)^n 6S(\mathsf{C}_n, k) - (-1)^n 6S(\mathsf{C}_n, k')$ and we know from Lemma 10 (a) that $S(\mathsf{C}_n, 4) > S(\mathsf{C}_n, 3)$. Hence, $g_n(4, 3) \geq -6(S(\mathsf{C}_n, k) - S(\mathsf{C}_n, k'))$. Using the induction hypothesis, Eq. (5) gives

$$\begin{aligned} f_n(k, k') &\geq -7(k-1)(k'-1)S(\mathsf{C}_{n-1}, k) - 6\Big(S(\mathsf{C}_n, k) - S(\mathsf{C}_n, k')\Big) \\ &= 42S(\mathsf{C}_{n-1}, k) - 6\Big(S(\mathsf{C}_n, k) - S(\mathsf{C}_n, k')\Big). \end{aligned}$$

We therefore conclude from Lemmas 7 and 10 (c) that

$$\begin{aligned} f_n(4,3) &\geq \frac{42}{3}\Big(S(\mathsf{C}_n,4) - S(\mathsf{C}_n,3)\Big) - 6\Big(S(\mathsf{C}_n,4) - S(\mathsf{C}_n,3)\Big) \\ &= 8\Big(S(\mathsf{C}_n,4) - S(\mathsf{C}_n,3)\Big) \\ &> 8\Big(S(\mathsf{C}_n,4) - \frac{1}{8}S(\mathsf{C}_n,4)\Big) \\ &= 7S(\mathsf{C}_n,4). \end{aligned}$$

□

We now study the impact of the replacement of an induced $\mathsf{K}_3 \cup \mathsf{K}_1$ by C_4. It is easy to check that

- $\mathcal{A}(\mathrm{K}_3 \cup \mathrm{K}_1) = \frac{13}{4} > 3 = \mathcal{A}(\mathrm{C}_4)$, and
- $\mathcal{A}(2\mathrm{K}_3 \cup \mathrm{K}_1) = \frac{778}{175} > \frac{684}{154} = \mathcal{A}(\mathrm{K}_3 \cup \mathrm{C}_4)$.

Hence, $\mathcal{A}((p+1)\mathrm{K}_3 \cup \mathrm{K}_1) > \mathcal{A}(p\mathrm{K}_3 \cup \mathrm{C}_4)$ for $p = 0, 1$. We next prove that this inequality is reversed for larger values of p, that is $\mathcal{A}((p+1)\mathrm{K}_3 \cup \mathrm{K}_1) < \mathcal{A}(p\mathrm{K}_3 \cup \mathrm{C}_4)$ for $p \geq 2$. Proposition 5 is of no help for this proof since, whatever p, there are pairs (k, k') for which $S((p+1)\mathsf{K}_3 \cup \mathsf{K}_1, k)S(p\mathsf{K}_3 \cup \mathsf{C}_4, k') > S(p\mathsf{K}_3 \cup \mathsf{C}_4, k)S((p+1)\mathsf{K}_3 \cup \mathsf{K}_1, k')$, and other pairs for which the inequality is reversed. Also, it is not true that

$$\mathcal{A}((p+1)\mathsf{K}_3 \cup \mathsf{K}_1) - \mathcal{A}(p\mathsf{K}_3 \cup \mathsf{K}_1) > \mathcal{A}(p\mathsf{K}_3 \cup \mathsf{C}_4) - \mathcal{A}((p-1)\mathsf{K}_3 \cup \mathsf{C}_4)$$

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 $\mathcal{A}((p+1)\mathsf{K}_3 \cup \mathsf{K}_1)$ and $\mathcal{A}(p\mathsf{K}_3 \cup \mathsf{C}_4)$. This is what we do next, with the help of two lemmas.

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

$$\begin{aligned} \mathcal{B}(G \cup \mathrm{K}_2) &= \sum_{k=1}^{n}(k^2+k+1)S(G,k), \\ \mathcal{T}(G \cup \mathrm{K}_2) &= \sum_{k=1}^{n}(k^3+k^2+3k+2)S(G,k), \\ \mathcal{B}(G \cup \mathrm{K}_3) &= \sum_{k=1}^{n}(k^3+2k+1)S(G,k), \\ \mathcal{T}(G \cup \mathrm{K}_3) &= \sum_{k=1}^{n}(k^4+5k^2+4k+3)S(G,k). \end{aligned}$$

Proof As observed in [9],

$$S(G \cup \mathsf{K}_r, k) = \sum_{i=0}^{r} \binom{k-i}{r-i}\binom{r}{i}(r-i)!\, S(G, k-i). \tag{6}$$

Hence,

$$\begin{aligned}\mathcal{B}(G \cup \mathsf{K}_2) &= \sum_{k=1}^{n+2} S(G \cup \mathsf{K}_2, k) \\ &= \sum_{k=1}^{n+2} \Big(k(k-1)S(G,k) + 2(k-1)S(G,k-1) + S(G,k-2)\Big) \\ &= \sum_{k=1}^{n} (k^2+k+1)S(G,k)\end{aligned}$$

and

$$\begin{aligned}\mathcal{T}(G \cup \mathsf{K}_2) &= \sum_{k=1}^{n+2} kS(G \cup \mathsf{K}_2, k) \\ &= \sum_{k=1}^{n+2} \Big(k^2(k-1)S(G,k) + 2k(k-1)S(G,k-1) + kS(G,k-2)\Big) \\ &= \sum_{k=1}^{n} (k^3+k^2+3k+2)S(G,k).\end{aligned}$$

The values for $\mathcal{B}(G \cup \mathsf{K}_3)$ and $\mathcal{T}(G \cup \mathsf{K}_3)$ are computed in a similar way. □

Lemma 17 *If G is a graph of order n, then,*

$$\begin{aligned}\mathcal{B}(G \cup \mathrm{K}_3 \cup \mathrm{K}_1) &= \sum_{k=1}^{n} (k^4+k^3+5k^2+6k+4)S(G,k), \\ \mathcal{T}(G \cup \mathrm{K}_3 \cup \mathrm{K}_1) &= \sum_{k=1}^{n} (k^5+k^4+9k^3+15k^2+21k+13)S(G,k).\end{aligned}$$

Proof Let $G' = G \cup \mathsf{K}_3$. Equation (6) gives $S(G' \cup \mathsf{K}_1, k) = kS(G',k) + S(G',k-1)$. Hence, it follows from Lemma 16 that

$$\begin{aligned}\mathcal{B}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1) &= \sum_{k=1}^{n+4} \Big(kS(G',k) + S(G',k-1)\Big) \\ &= \sum_{k=1}^{n+3} kS(G',k) + \sum_{k=1}^{n+3} S(G',k) \\ &= \mathcal{T}(G') + \mathcal{B}(G') \\ &= \sum_{k=1}^{n} (k^4+k^3+5k^2+6k+4)S(G,k).\end{aligned}$$

Equation (6) gives

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

Hence, using again Lemma 16, we get

$$
\begin{aligned}
\mathcal{T}(G\cup \mathsf{K}_3\cup \mathsf{K}_1) &= \sum_{k=1}^{n+4}\Big(k^2S(G',k)+kS(G',k-1)\Big)\\
&= \sum_{k=1}^{n+3} k^2S(G',k) + \sum_{k=1}^{n+3}(k+1)S(G',k)\\
&= \sum_{k=1}^{n+3} k^2S(G',k) + \mathcal{T}(G') + \mathcal{B}(G')\\
&= \sum_{k=1}^{n}(k^5+k^4+9k^3+15k^2+21k+13)S(G,k).
\end{aligned}
$$

□

We are now ready to compare $\mathcal{A}(p\mathsf{K}_3\cup \mathsf{C}_4)$ with $\mathcal{A}((p+1)\mathsf{K}_3\cup \mathsf{K}_1)$.

Lemma 18 $\mathcal{A}(p\mathrm{K}_3\cup \mathrm{C}_4) < \mathcal{A}((p+1)\mathrm{K}_3\cup \mathrm{K}_1)$ *if* $p=0,1$ *and* $\mathcal{A}(p\mathrm{K}_3\cup \mathrm{C}_4) > \mathcal{A}((p+1)\mathrm{K}_3\cup \mathrm{K}_1)$.

Proof We have already mentioned that the lemma is valid for $p=0,1$. Hence, it remains to prove that $\mathcal{A}(p\mathsf{K}_3\cup \mathsf{C}_4) > \mathcal{A}((p+1)\mathsf{K}_3\cup \mathsf{K}_1)$ for $p\geq 2$. So assume $p\geq 2$ and let

$$
f(p) = \mathcal{T}(p\mathsf{K}_3\cup \mathsf{C}_4)\mathcal{B}((p+1)\mathsf{K}_3\cup \mathsf{K}_1) - \mathcal{B}(p\mathsf{K}_3\cup \mathsf{C}_4)\mathcal{T}((p+1)\mathsf{K}_3\cup \mathsf{K}_1).
$$

Since

$$\mathcal{A}(p\mathsf{K}_3 \cup \mathsf{C}_4) - \mathcal{A}((p+1)\mathsf{K}_3 \cup \mathsf{K}_1) = \frac{f(p)}{\mathcal{B}(p\mathsf{K}_3 \cup \mathsf{C}_4))\mathcal{B}((p+1)\mathsf{K}_3 \cup \mathsf{K}_1)},$$

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

$$\begin{aligned} S(G \cup \mathsf{C}_4, k) &= S(G \cup \mathsf{P}_4, k) - S(G \cup \mathsf{K}_3, k) \\ &= S(G \cup \mathsf{Q}_4, k) + S(G \cup \mathsf{P}_3, k) - S(G \cup \mathsf{K}_3, k) \\ &= \Big(S(G \cup \mathsf{K}_3 \cup \mathsf{K}_1, k) - S(G \cup \mathsf{K}_3, k)\Big) \\ &\quad + \Big(S(G \cup \mathsf{K}_3, k) + S(G \cup \mathsf{K}_2, k)\Big) - S(G \cup \mathsf{K}_3, k) \\ &= S(G \cup \mathsf{K}_3 \cup \mathsf{K}_1, k) - S(G \cup \mathsf{K}_3, k) + S(G \cup \mathsf{K}_2, k), \end{aligned}$$

which implies

$$\begin{aligned} \mathcal{B}(G \cup \mathsf{C}_4) &= \mathcal{B}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1) - \mathcal{B}(G \cup \mathsf{K}_3) + \mathcal{B}(G \cup \mathsf{K}_2), \text{ and} \\ \mathcal{T}(G \cup \mathsf{C}_4) &= \mathcal{T}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1) - \mathcal{T}(G \cup \mathsf{K}_3) + \mathcal{T}(G \cup \mathsf{K}_2). \end{aligned}$$

Hence, with $G = pK_3$, we get

$$\begin{aligned} f(p) &= \mathcal{T}(G \cup \mathsf{C}_4)\mathcal{B}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1) - \mathcal{T}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1)\mathcal{B}(G \cup \mathsf{C}_4) \\ &= \Big(\mathcal{T}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1) - \mathcal{T}(G \cup \mathsf{K}_3) + \mathcal{T}(G \cup \mathsf{K}_2)\Big)\mathcal{B}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1) \\ &\quad - \mathcal{T}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1)\Big(\mathcal{B}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1) - \mathcal{B}(G \cup \mathsf{K}_3) + \mathcal{B}(G \cup \mathsf{K}_2)\Big) \\ &= \mathcal{B}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1)\Big(\mathcal{T}(G \cup \mathsf{K}_2) - \mathcal{T}(G \cup \mathsf{K}_3)\Big) \\ &\quad - \mathcal{T}(G \cup \mathsf{K}_3 \cup \mathsf{K}_1)\Big(\mathcal{B}(G \cup \mathsf{K}_2) - \mathcal{B}(G \cup \mathsf{K}_3)\Big). \end{aligned}$$

Since $S(G, k) = 0$ for $k < 3$, we deduce from Lemmas 16 and 17 that

$$\begin{aligned} f(p) &= \sum_{k=1}^{n} a_k S(G,k) \sum_{k=1}^{n} b_k S(G,k) - \sum_{k=1}^{n} c_k S(G,k) \sum_{k=1}^{n} d_k S(G,k) \\ &= \sum_{k=3}^{n} \sum_{k'=3}^{n} (a_k b_{k'} - c_k d_{k'}) S(G,k) S(G,k') \\ &= \sum_{k=3}^{n} (a_k b_k - c_k d_k) S^2(G,k) && (7) \\ &\quad + \sum_{k'=3}^{n-1} \sum_{k=k'+1}^{n} (a_k b_{k'} - c_k d_{k'} + a_{k'} b_k - c_{k'} d_k) S(G,k) S(G,k') && (8) \end{aligned}$$

where

$a_k = k^4 + k^3 + 5k^2 + 6k + 4\,,$
$b_k = -k^4 + k^3 - 4k^2 - k - 1,$
$c_k = k^5 + k^4 + 9k^3 + 15k^2 + 21k + 13\,,$ and
$d_k = -k^3 + k^2 - k.$

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 Eq. (6) gives

$$\begin{aligned} S(G,3) = S(p\mathrm{K}_3,3) &= 6S((p-1)\mathrm{K}_3,3) \\ &< 18S(p-1)\mathrm{K}_3,3) + 24S((p-1)\mathrm{K}_3,4) \\ &= S((p\mathrm{K}_3,4) = S(G,4). \end{aligned}$$

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

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

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

$$\begin{aligned} h'(i,j) = & \Big(j^2 + 2j + 3\Big)i^6 + \Big(3j^3 + 25j^2 + 47j + 63\Big)i^5 \\ & + \Big(3j^4 + 52j^3 + 243j^2 + 437j + 533\Big)i^4 \\ & + \Big(j^5 + 37j^4 + 338j^3 + 1154j^2 + 2017j + 2267\Big)i^3 \end{aligned}$$

$$+\left(8j^5+161j^4+997j^3+2713j^2+4692j+4873\right)i^2$$
$$+\left(22j^5+290j^4+1258j^3+2729j^2+4784j+4443\right)i$$
$$+21j^5+172j^4+440j^3+575j^2+1112j+602.$$

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.

□

We are now ready to prove the main result of this section, where U_n $(n \geq 3)$ is the graph defined in Sect. 2.

Theorem 19 *If G is a graph of order $n \geq 3$ and maximum degree $\Delta(G) = 2$, then $\mathcal{A}(G) \leq \mathcal{A}(\mathrm{U}_n)$, with equality if and only if $G \simeq \mathrm{U}_n$.*

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 $G \simeq G' \cup \mathsf{P}_k \cup \mathsf{P}_{k'}$, then Eqs. (3) and (4) give $\mathcal{B}(G' \cup \mathsf{P}_k \cup \mathsf{P}_{k'}) = \mathcal{B}(G' \cup \mathsf{P}_{k+k'}) + \mathcal{B}(G' \cup \mathsf{P}_{k+k'-1})$ and $\mathcal{T}(G' \cup \mathsf{P}_k \cup \mathsf{P}_{k'}) = \mathcal{T}(G' \cup \mathsf{P}_{k+k'}) + \mathcal{T}(G' \cup \mathsf{P}_{k+k'-1})$. Moreover, we know from Proposition 2 that $\mathcal{A}(G' \cup \mathsf{P}_{k+k'-1}) < \mathcal{A}(G' \cup \mathsf{P}_{k+k'})$. Hence, Proposition 4 implies that $\mathcal{A}(G) = \mathcal{A}(G' \cup \mathsf{P}_k \cup \mathsf{P}_{k'}) < \mathcal{A}(G' \cup \mathsf{P}_{k+k'})$. Since $(G' \cup \mathsf{P}_{k+k'})$ is of order n and maximum degree 2, this contradicts the hypothesis that G maximizes $\mathcal{A}$.

We know from Lemma 3 that replacing a path P_k of order $k \geq 3$ by a cycle C_k strictly increases $\mathcal{A}(G)$. Moreover, Lemma 15 shows that replacing a cycle C_k of order $k \geq 6$ by $\mathsf{C}_{k-3} \cup \mathrm{K}_3$ 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 6, 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 $G \simeq \frac{n}{3}\mathrm{K}_3$ and if $n \bmod 3 = 2$ then $G \simeq \frac{n-5}{3}\mathrm{K}_3 \cup \mathrm{C}_5$. Finally, Lemma 18 shows that $G \simeq \frac{n-1}{3}\mathrm{K}_3 \cup \mathrm{K}_1$ if $n = 4$ or 7, and $G \simeq \frac{n-4}{3}\mathrm{K}_3 \cup \mathrm{C}_4$ if $n \bmod 3 = 1$ and $n \geq 10$. □

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 $\{3, \ldots, n-3\}$ 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 $\lfloor\frac{n}{\Delta(G)+1}\rfloor\mathrm{K}_{\Delta(G)+1} \cup$

$K_{n \bmod (\Delta(G)+1)}$ (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 12 vertices, using *PHOEG*[2]. We have thus determined that there is only one graph of order $n \leq 12$ and $\Delta(G) \neq 2$ (among more than 165 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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Availability of material and data https://phoeg.umons.ac.be/.

Declarations

Conflict of interest The authors have not disclosed any competing interests.

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